Interacting atoms in time-dependent potentials and artificial gauge fields

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For my family.
Summary

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This thesis considers novel phenomena arising in the few and many-body physics of ultracold atomic gases. The specific models considered are motivated by recent experimental developments. A main focus will be the theoretical description of systems used in the simulation of artificial gauge fields via time-modulated tuning of system parameters and via the coupling of internal atomic states by Raman lasers. A second aspect will be the study of systems with synthetic dimensions and the effects of the unconventional infinite range interactions that arise in this description. It explores time-dependent effects in the single and few particle setting and the collective many-body phases arising in these models.

Using the framework of Floquet theory it studies the interplay of time-dependence and particle-interactions both in continuum and lattice systems. In particular, it provides a general explanation for how heating effects can arise in interacting periodically time-dependent quantum systems, identifying an underlying mechanism for heating via two-particle collisions and the relevant scaling of the associated rates with system parameters. Furthermore, the general framework is applied to specific experimental set-ups. This yields heating rates and population dynamics in agreement with the experimental data. Finally, it also proposes improvements to the experiment that allow to limit the heating rates which is required to access the strongly interacting regime.
In the case of synthetic dimensions the focus lies on the intriguing interplay of artificial
gauge fields and strong particle interactions of atoms confined in optical lattices. In these
systems a suitable coupling of internal spin-states of the atoms allows to simulate an
additional finite dimension. In contrast to the typically encountered situation of short-
range interactions the particle interactions are infinite-range in this synthetic dimension.
In the strong coupling limit an effective description for this system is derived and its
ground state phase diagram is studied using numerical tools.
Preface

This thesis describes work undertaken in the Theory of Condensed Matter (TCM) group at the Cavendish Laboratories of the University of Cambridge under the supervision of Professor Nigel R. Cooper.

Chapters 1 and 2 give an introduction into the relevant background and provide the theoretical tools required in the main part of the thesis. Subsequent chapters are the result of original research, published in peer-reviewed journals.


This dissertation is the result of my own work and includes nothing which is the outcome of work done in collaboration except as declared in the Preface and specified in the text.

It is not substantially the same as any that I have submitted, or, is being concurrently submitted for a degree or diploma or other qualification at the University of Cambridge or any other University or similar institution except as declared in the Preface and specified in the text. I further state that no substantial part of my dissertation has already been
submitted, or, is being concurrently submitted for any such degree, diploma or other qualification at the University of Cambridge or any other University of similar institution except as declared in the Preface and specified in the text

This thesis does not exceed 60,000 words.
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1. Introduction

1.1. Ultracold Atomic Gases

Ultracold quantum gases are dilute clouds of charge-neutral atoms trapped in vacuum cells and cooled down to quantum degeneracy by laser and evaporative cooling [5–8].

They allow very precise control over the microscopic system parameters, such as the strength and type of the interactions, the kinetic energy of the particles, the realisation of essentially perfect, defect free lattices with a variety of geometries, and confinement to different dimensionalities. A sketch of ultracold atoms in a two dimensional optical lattice is shown in Fig. 1.1. Experimentally these systems can be coherently manipulated on the quantum level and most of their properties tuned (in space and time) via adjustment of external fields, such as laser beams or magnetic fields. They are very well isolated from their environment and can in most cases be treated as closed and

\[ \bar{a} \sim n^{-1/3}, \quad \lambda_T \sim \frac{\hbar^2}{(MK_bT)} \]

[\text{For an ideal gas of identical particles with mass } M \text{ in three dimensions with number density } n \text{ in equilibrium at temperature } T, \text{ the mean characteristic separation scales as } \bar{a} \sim n^{-1/3}, \text{ whereas the thermal de Broglie wavelength behaves like } \lambda_T \sim \frac{\hbar^2}{(MK_bT)}. \text{ For } \lambda_T \gtrsim \bar{a} \text{ quantum effects become relevant [4].}]

Figure (1.1) Artistic interpretation of an ultracold atomic gas in a two-dimensional optical lattice
1. Introduction

Bosonic atomic gases [4] at sufficiently low temperatures are known to condense into a Bose-Einstein condensate (BEC), schematically shown in Fig. 1.2. One of the first experimental achievements was the creation of Bose-Einstein condensates with Rubidium [10] and Sodium atoms [11] in the laboratory in 1995, quantum degeneracy in Fermionic gases was demonstrated in 1999 [12–14]. Fermionic ultracold atoms [4, 15] undergo a crossover from Bardeen-Cooper-Schrieffer pairing of fermionic atoms [16] to Bose-Einstein condensation of tightly bound bosonic molecules (for a recent review of the BEC-BCS crossover see [17]) as a function of their interaction strength. The condensation of bound bosonic molecules of fermionic atoms on the BEC side was first experimentally observed in 2003 [18–20], and the full BEC-BCS crossover was experimentally studied soon after [21]. Since then, ultracold atomic systems have been used to study a wide variety of quantum phenomena, such as matter-wave-interference [22], long-range phase-coherence [23], superfluidity, vortices and vortex lattices [24, 25], the superfluid-Mott insulator transition [26, 27], the realisation of the Tonks-Girardeau Gas in 1D [28] and the Berezinskii–Kosterlitz–Thouless transition in 2D [29].
1.1. Ultracold Atomic Gases

Figure (1.3) Illustration of the quantum gas microscope [30]. A high aperture optical system is used to simultaneously image the atoms with a resolution $\sim 600$ nm as well as to create an optical lattice potential. Taken from [31].

An exciting recent development are new experimental techniques that allow to image and control ultracold atomic gases in situ with resolution on the single atom scale [7]. Quantum gas microscopes have been realised for bosonic [30, 32] and fermionic [33, 34] gases and been applied to study the superfluid-Mott transition on the single site level [35, 36]. They also enable the measurement of site-resolved correlations [37] and entanglement entropies in quantum many-body systems [38]. The experimental setup used in [30] is illustrated in Fig. 1.3. It uses a trap close to a dielectric surface created by evanescent waves, an optical potential and a magnetic trap. Trapping the atoms very close to the surface allows to exploit a solid-immersion effect and increase the geometric aperture of the imaging system. This enables to probe and image atoms with a resolution of the order of 600 nm. In addition, the imaging system can also be used to directly project an optical potential onto the trapped atoms.

For a comprehensive review of the field of ultracold atomic systems we refer to the excellent available literature [4–8, 15].
1. Introduction

1.1.1. Trapping and Dimensionality

For most experiments, the resulting trapping potential can be approximated as a simple harmonic potential

\[ V(x, y, z) = \frac{1}{2} M \left( \omega_x^2 x^2 + \omega_y^2 y^2 + \omega_z^2 z^2 \right) \]  

(1.1)

where \( M \) is the atomic mass and \( \omega_i \) is the trapping frequency in direction \( x_i \). Associated with the harmonic confinement is the characteristic trapping energy scale \( \hbar \omega_i \) and the characteristic length scale \( l_i = \sqrt{\hbar/(M \omega_i)} \). These correspond to the energy \( E_n = \hbar \omega_i (n + 1/2) \) of the \( n \)-th eigenstate and the characteristic size of the eigenstates via \( \langle x_i^2 \rangle - \langle x_i \rangle^2 = l_i^2 (n + 1/2) \) where the expectation value is defined in the \( n \)-th eigenstate \( \psi_n \) of the oscillator in direction \( x_i \), i.e. \( \langle O \rangle = \langle \psi_n | O | \psi_n \rangle \). Importantly, for the ground-state the oscillator length \( l_i \) also gives the distance over which the probability density falls off to \( |\psi_0(l_i)/\psi_0(0)|^2 = 1/e \), thus, the spatial extent on which it is exponentially localised.

In an equilibrium situation, when all other energy scales in the system are small compared to the trapping energy, in particular for temperatures \( k_b T \ll \hbar \omega_i \), motion along that direction is frozen out, and the effective dimensionality of the system is consequently reduced. Thus, by changing the frequencies \( \omega_i \) it is possible to create effective three-, two- and one-dimensional systems. This tuneability of the effective dimension of ultracold atomic systems is one of the reasons why they provide such a versatile tool for quantum simulation, and justifies to study them in all dimensions. It will be important to keep this in mind when we consider situations of strong confinement, e.g. quasi-one-dimensional systems, and extensions to weakly confined, higher dimensional settings and discuss the resulting differences in physical behaviour.

\[ ^2 \text{More recently, it has become experimentally feasible to optically trap atoms in a uniform "box"-like trap [39].} \]
1.1. Interactions

At low temperatures and in the dilute limit the interactions between the atoms can be effectively described via two-body contact interactions of the form

\[ V(r) = g_{\text{eff}} \delta(r), \]  

(1.2)

where \( \delta(r) \) is the Dirac delta function at the particle separation \( r \) and \( g_{\text{eff}} \) an effective interaction parameter that depends on the dimensionality and the trapping potentials. In 3D for untrapped particles it is given by

\[ g_{\text{eff}} = \frac{4\pi \hbar^2 a_s}{2m_r} \]

with \( m_r = M/2 \) the reduced mass of particles of mass \( M \) and \( a_s \) the s-wave scattering length [5]. This approximation is valid for a wide range of systems, provided longer range forces, such as dipol-dipol interactions in the case of dipolar gases, are not present.

The success of this approximation lies in reproducing the correct low-energy scattering behaviour of the underlying microscopic interaction potential as outlined below [5]. Considering scattering of a generic two-body potential \( V(r) \) we seek solutions to the Schrödinger equation for the relative motion

\[ \left( \frac{\hat{p}^2}{2m_r} + V(r) \right) \psi_k(r) = E_k \psi_k(r), \]  

(1.3)

with energy \( E_k = \frac{\hbar^2 k^2}{2m_r} \). Due to the centrifugal barrier for higher angular momentum channels, scattering of atoms at sufficiently low temperatures is dominated by the lowest allowed angular momentum collisions, i.e. s-wave for bosons and p-wave for fermions. The scattering amplitude \( f(k) \) in the case of s-wave scattering describes the asymptotic form of the scattered states via

\[ \psi_k \sim e^{ikr} + f(k) \frac{e^{ikr}}{r}. \]

It is completely determined by the corresponding phase-shift \( \delta_0(k) \) via \( f(k) = \frac{1}{k \cot \delta_0(k) - ik} \). At low energies \( f(k) \rightarrow \frac{1}{-1/a_s + r_e k^2 - ik} \) which defines the scattering length \( a_s \) and the effective range \( r_e \) of the underlying potential \( V(r) \). In the regime of ultracold collisions \( ka_s \ll 1 \) and the two-body collisions are

\[ ^3 \text{More precisely, the pseudo-potential } V(r) (\cdots) = g_{\text{eff}} \delta(r) \delta_r (r \cdots) \text{ should be used. If the wavefunctions are regular at the origin this reduces to } V(r) = g_{\text{eff}} \delta(r). \]
1. Introduction

Figure (1.4) Adapted from [40]. Two channel model of a Feshbach resonance. Shown are two molecular potential curves of a closed $V_c(R)$ channel and the background or open channel $V_{bg}(R)$ as a function of inter-atomic separation $R$. If the energy of an incoming scattering state $E$ of two particles is close to the energy of a molecular bound state $E_c$ in the closed channel, the mixing between the channels becomes strong, and the scattering length shows resonant behaviour. For ultracold atomic gases collisions mainly take place near $E = 0$, and resonance corresponds to tuning the energy of the bound state $E_c$ close to threshold.

completely determined by the scattering length $a_s$ via

$$f(k) = \frac{-a_s}{1 + ik a_s} \quad (1.4)$$

The use of Eq. (1.2) as an approximation for low-energy scattering is now explained by the fact that the low-energy limit of the scattering length in Eq. (1.4) is in fact the exact result at all values of $k$ for the delta pseudo-potential. Thus, the delta pseudo-potential reproduces the scattering amplitude and the corresponding phase-shifts which ensures that the asymptotic form of the scattering states is the same as for the true microscopic potential.

By using different atomic species the scattering length and the strength of the interactions can be changed while keeping other system parameters the same. The scattering length can also be tuned in experiment via Feshbach resonances. A Feshbach resonance refers to
an energetic resonance condition in a two-particle scattering process in different channels as depicted in Fig. 1.4. Channels correspond to different molecular states of the two atoms in the scattering event: the open channel connects to the state of two unbound particles at large separations, in contrast a channel is closed if it has a higher molecular energy at large separations than two free particles. A Feshbach resonance occurs if the energy $E$ of two incoming particles in an open channel is close to the energy of a bound molecular state $E_c$ in a closed channel [40]. By changing the energy difference of the bound-molecular state and the atomic scattering state, the mixing between the channels and, thus, the resulting scattering length can be tuned. Dependent on the magnetic moments of the molecular states this can be achieved via magnetic fields, leading to magnetic Feshbach resonances, or via optical means leading to optical Feshbach resonances.

The control over the scattering length and consequently the effective interactions makes Feshbach resonances one of the essential tools of ultracold gas experiments. They enable the realisation of large tunable attractive and repulsive interactions for ultracold atomic gases.

1.1.3. Optical Lattices

**Figure (1.5)** Illustration of optical lattices. (a) Up to three pairs of counter-propagating lasers illuminate a cloud of ultracold atoms. (b) One pair of lasers splits the system into a 1D array of quasi-two dimensional “pancakes” (c) Two orthogonal pairs of lasers split the system into a 2D lattice of quasi-1D tubes (d) Three orthogonal pairs of lasers create a 3D lattice of harmonically confined atoms at each lattice site.

Another important tool for controlling ultracold atoms are optical lattices [5–8]. Since neutral atoms experience a light-shift potential proportional to the laser intensity, a standing light wave creates an almost perfect defect-free lattice potential. The origin of this potential is the interaction of atoms with laser light described by the dipole Hamiltonian
1. Introduction

[41, 42]. The laser light is far detuned from an atomic transition between a stable and an electronically excited state of the atoms. Importantly, the ratio of spontaneous emission from the excited state to the induced optical potential for the atoms in the groundstate can be systematically suppressed by working at sufficiently large detuning as it scales as \( 1/\Delta_e \) where \( \Delta_e \) is the detuning from atomic resonance. We provide the details of the derivation in Appendix A. The resulting conservative potential can be expressed as \( V(x) = \alpha |E|^2 \), where \( \alpha \) is the scalar polarizability of the atoms which generically depends on the laser frequency, and \( E(x) \) is the electric field at position \( x \).

For two counter-propagating lasers with wave-vectors \( k_L \) and \( -k_L \) the resulting potential is given by

\[
V_L(r) = V_0 \sin^2(k_L \cdot r)
\]

where \( r \) is the position and \( V_0 \) controls the lattice depth and is proportional to the laser intensity. For \( k_L = |k_L|e_x \) the resulting lattice has well defined minima at \( x_j = jd \) with lattice constant \( d = \pi/|k_L| \). The natural energy scale in optical lattices is given by the recoil energy \( E_R = \hbar^2 k_L^2/(2M) \), it corresponds to the kinetic energy an atom of mass \( M \) would have after absorbing or emitting a photon with wavevector \( k_L \) when initially at rest. For a sufficiently deep lattice the dynamics of the atoms at low temperatures is well captured by the Hubbard Hamiltonian [5, 8]

\[
\hat{H} = -t \sum_{\langle i,j \rangle} \hat{a}_i^\dagger \hat{a}_j + \hat{U}_{\text{int}}
\]

where \( \hat{a}_i^\dagger \) creates an atom at lattice site \( i \) and \( t \) denotes the tunnelling matrix element between nearest neighbour sites \( \langle i,j \rangle \). The interaction \( \hat{U}_{\text{int}} \) arises from contact interactions which leads to on-site density-density interactions of the form \( \hat{U}_{\text{int}} = U_0 \sum_j \hat{n}_j(\hat{n}_j - 1) \) for spinless bosons where \( U_0 \) gives the strength of the interactions and \( \hat{n}_j = \hat{a}_j^\dagger \hat{a}_j \) is the density at site \( j \). More generally, for spinful particles one obtains \( \hat{U}_{\text{int}} = \sum_{j,\sigma,\sigma'} U_{\sigma\sigma'} \hat{a}_j^\dagger \sigma \hat{a}_j^\dagger \sigma' \hat{a}_j \sigma \hat{a}_j \sigma' \) where \( U_{\sigma\sigma'} \) is the potentially species-dependent interaction strength.

Optical lattices provide a very adaptable and highly controllable experimental tool. By combining standing waves in different directions, or using more complex interference patterns of multiple lasers with possibly different wavelengths, a variety of one-, two- or three-dimensional lattices with different geometries can be created, such
1.1. Ultracold Atomic Gases

as superlattices [43], triangular [44], honeycomb [45] and Kagomè lattices [46]. The simplest case of a 1D lattice, a square 2D lattice and a cubic 3D lattice are shown in Fig. 1.5.

In experiments, the lattice depth, lattice constant and geometry can be tuned directly by adjusting the intensity, frequency and phase of the laser beams. In stark contrast to solid-state systems where the crystal lattice structure is mostly predetermined by the constituent atoms and fixed after growing the material, the optical lattice potential can be changed in time during the experiment by adjusting the laser beams, for example the lasers, and thus the lattice potential, can be switched off to observe the free expansion of the gas cloud, or the amplitude of the lasers can be changed over time. This will allow us to study and exploit the consequences of time-modulated or shaken optical lattices which will be covered in more detail in Section 1.2.4.

The simulation and detailed study of the Hubbard model as one of the paradigmatic models of solid-state physics with ultracold atoms [5, 7, 47–49] was one of the first experimental successes of cold atoms in optical lattices. For bosonic atoms and repulsive interactions at integer filling the system undergoes a phase transition from a superfluid to a Mott insulator as the ratio of interaction to kinetic energy \( U/t \) is tuned above a (dimension-dependent) critical value [26, 50, 51], at any incommensurate filling there remains a finite superfluid density for \( t \neq 0 \). The phases can be understood from the extreme limits of \( t = 0 \) in which the groundstate of the system has integer filling at every lattice site, and the limit of \( U = 0 \) in which particles are non-interacting and form a phase-coherent superfluid state spanning the whole lattice. This transition can be experimentally accessed both by changing the interactions as described above or increasing the potential depth, thereby reducing \( t \). Spin 1/2 fermionic atoms evolve from a metallic state over a strongly interacting fermi-liquid to a fermionic Mott insulator as the interaction strength is increased [27, 52]. In the strongly interacting regime the anti-ferromagnetic coupling between spins emerging from super-exchange processes [53] allows the simulation of quantum magnetism [54]. Further, it would allow to understand high-temperature superconductivity in the fermionic Hubbard model [55] via quantum simulation. Even though some progress has recently been made in observing (short)-range anti-ferromagnetic correlations [56, 57], accessing this low-temperature physics is experimentally extremely challenging. Thus, one of the main challenges remaining is to
develop methods to prepare low-entropy states and to better control technical heating due to spontaneous emission [7, 58].

Using atoms with larger number $N$ of internal states, such as alkaline atoms with SU($N$)-invariant interactions [59–62] opens up a whole range of additional phenomena. The SU($N$) Hubbard-model is predicted to show a variety of magnetically ordered phases and chiral spin-liquids [60, 63, 64], but is theoretically very challenging to study, and experiments might provide additional insight into the exotic physics of high-spin magnetism. We discuss one of the possible uses of these additional internal states in the framework of “synthetic” dimensions in Section 1.2.5 and discuss some of the consequences in these models on the many-body physics in Chapter 5.

1.2. Artificial Gauge Fields

![Artistic interpretation of a shaken optical lattice, yielding a peierl’s substitution $p \rightarrow p - A$ corresponding to an artificial gauge field.]

The aim of this section is to provide a brief introduction to artificial magnetic fields for ultracold atomic gases. It will provide the necessary background and the models studied in later chapters. In Section 1.2.3 and Section 1.2.4 we will discuss respectively the creation of artificial gauge fields via dressing of states in the continuum and via time-periodic modulation of optical lattices. The role of interactions and scattering in such schemes will be the topic of Chapter 3 and Chapter 4. In Section 1.2.5 we introduce the concept of synthetic gauge fields in “synthetic dimensions”, a system which we will study in the many-body context in Chapter 5.
1.2. Artificial Gauge Fields

1.2.1. Introduction

As described above ultracold atomic gases are charge-neutral, thus, they do not couple to magnetic fields via the Lorentz-force. The basic idea of artificial magnetic or gauge fields for ultracold atoms is to engineer a Hamiltonian in which the momentum operator $p$ of the atoms is shifted to $p - A$ corresponding to the canonical momentum of a charged particle in a magnetic field.

In the continuum we require a kinetic contribution to the Hamiltonian of the form

$$\hat{H}_{\text{kin}} = \frac{\left(\hat{p} - \hat{A}_{\text{art}}\right)^2}{2M}. \quad (1.7)$$

In the case of a periodic (one-dimensional) lattice quantum particles with a charge $q$ under the influence of a magnetic field described by the potential $A$ acquire a phase

$$\phi_j = \frac{q}{\hbar} \int_{x_j}^{x_{j+1}} A \cdot dx$$

when moving from site $x_j = jd$ to site $x_{j+1}$. For sufficiently deep lattices, the effect of the vector-potential can be captured in the tight-binding Hamiltonian via the introduction of complex hopping phases

$$\hat{H}_{\text{kin}} = -t \sum_j e^{i\phi_j} \hat{a}_{j+1} \hat{a}_j + \text{h.c.} \quad (1.8)$$

which is known as the Peierls substitution [65, 66]. This concept is illustrated for the case of a shaken optical lattice in Fig. 1.6.

There have been long-standing research efforts to find ways to cause neutral atoms to behave as if under the influence of a gauge field [5, 67–71], and there have now been several successful experimental implementations of artificial gauge fields using schemes inspired by these proposals [25, 72–81]. This extends the capabilities of ultracold gases as simulators of quantum many-body systems to phenomena usually associated with electrons in magnetic fields. Such gauge fields can mimic the orbital effects of magnetic fields on a charged particle, e.g. Landau level and Quantum Hall physics, and allow the realisation of topological energy bands with non-zero Chern numbers, and is expected to lead to novel many-body phases of degenerate fermionic or bosonic atoms. In ultracold atomic systems one can even realise more exotic situations, such as non-abelian
1. Introduction

gauge fields. In the case of the Quantum Hall effect of a homogeneous two-dimensional electron gas, the energy bands are flat Landau levels with topological character. More generally, flat bands show particularly interesting behaviour as the kinetic energy of particles is small compared to the interaction energies. When interactions dominate strongly correlated many-body states can arise with exotic properties. Interesting physics that is expected in these situations includes the fractional quantum Hall effect with the associated fractionalised excitations and more generally quantum spin liquids. Ultracold atomic systems also offer the opportunity to synthesise band structures not found in solid state materials, e.g. bands with Chern numbers \( C > 1 \), and study the resulting FQH states and Chern insulators [82–87]. Interactions, therefore, play a special role for ultracold atomic gases in artificial gauge fields.

In the continuum two main proposals have been put forwards to generate artificial magnetic fields, working via rotating the system [68] which we introduce in Section 1.2.2, and the coherent coupling of internal states in dressed states schemes in Section 1.2.3. For atoms confined in deep optical lattices, the very first proposals used spin-dependent optical lattices combined with Raman lasers, a scheme called laser-assisted tunnelling [88–90]. We will not discuss this in detail, as it is not directly relevant to the models we study in this thesis. The basic idea is to trap different internal states on different sublattices and restore tunnelling through coupling them with a resonant laser field. It can be used to realise both artificial gauge fields [88–90] and synthetic spin-orbit coupling [91–94]. More recently, the concept of Floquet-engineering [76, 84, 95–100] has emerged as a promising route towards realising artificial gauge fields and more generally Hamiltonians with novel properties. We discuss the specific applications to shaken or modulated optical lattices in Section 1.2.4. Finally, we discuss the concept of “synthetic” dimensions [101, 102] in Section 1.2.5.

1.2.2. Rotating Gases

The first proposals to generate an artificial magnetic field relied on rotating atomic gases [5, 67, 68]. Considering a (non-interacting) atomic gas in an axisymmetric harmonic trap in a frame rotating about the symmetry axis \( \hat{z} \) with angular frequency \( \Omega \), the single
particle Hamiltonian is [68]

\[
\hat{H} = \frac{\hat{p}^2}{2M} + 1/2M\omega^2_\perp (x^2 + y^2) + 1/2M\omega^2_\parallel z^2 - \Omega \cdot \mathbf{r} \times \hat{\mathbf{p}}
\]

\[
= \frac{\hat{p} - M\Omega \times \mathbf{r}}{2M} + 1/2M(\omega^2_\perp - |\Omega|^2)(x^2 + y^2) + 1/2M\omega^2_\parallel z^2
\]

(1.9)

This can be identified with the Hamiltonian of a charged particle with charge \( q \) moving under the influence of a magnetic field \( \mathbf{B} \) with \( qB = 2M\Omega \) in a modified harmonic trap with new trap frequency \( \tilde{\omega}^2_\perp = \omega^2_\perp - |\Omega|^2 \). Thus, in a rotating frame the Coriolis force is seen to be equivalent to the Lorentz force. At \( |\Omega| = \omega_\perp \) the system reduces to particles in a uniform magnetic field in a quasi-two-dimensional setting, and the familiar physics of the Quantum Hall effect emerge. Experimentally, rotation of the atomic gas can be induced via stirring with a rotating optical [25] or magnetic potentials [103]. This has been used to nucleate single vortices and the formation of regular vortex lattices has been observed [25]. However, approaching the fast-rotating limit is problematic as the system becomes unstable [5]. This can be prevented by adding an additional quartic confinement [104]. Alternatively, a fast rotating BEC can be created by evaporatively cooling a slowly rotating cloud along the rotation axis [105], thus achieving \( \Omega > 0.99\omega_\perp \).

The strongly correlated physics of the FQHE is expected to emerge in the regime of low filling factors \( \nu = n_{2D} \frac{\hbar}{qB} \), where \( n_{2D} \) is the two dimensional density. For experiments with rotating gases the filling factor is limited by the maximally allowed rotation frequency and the comparably large particle densities. Experimental filling factors are in the region of \( \nu \sim 500 \) [106], deep in the vortex lattice regime [68]. Thus, the realisation of the strongly correlated phases is currently out of reach of experiments. A second limitation is given by the fact that the magnetic field emerges in the rotating frame. Consequently, any static non-axisymmetric potentials in the lab-frame will lead to collective excitations and heating of the desired quantum-state at rest in the rotating frame [68]. The methods we discuss in the following do not suffer from this specific problem and allow the realisation of large flux densities.

\(^{4}\)Stability of the system requires the gas to remain trapped, i.e. \( |\Omega| \leq \omega_\perp \). Note that this also limits the maximal achievable magnetic field to \( qB \leq 2M\omega_\perp \).
1. Introduction

1.2.3. Dressed State Schemes in the Continuum

The method to create artificial magnetic fields described in this section works in the continuum. It is based on coupling a number of internal states in a spatially dependent way, and treating the spatial motion of the atoms separately from this parametrical dependence, leading to an adiabatic phase that is acquired during spatial motion of the atoms which resembles the phase of a magnetic field [69, 70, 107, 108]. That atom-light interactions can be used to create scalar and vector gauge potentials for neutral atoms has first been put forward in [107], where the focus was on the resulting scalar potential. Consequently, specific laser configurations were discussed focusing on creating the vector gauge field via space-dependent couplings [109, 110] or position dependent detunings [108].

This scheme relies on two main ingredients. Firstly, the system needs to have at least two internal states that allow a suitable coupling and whose energies and/or coupling can be tuned spatially. Secondly, there needs to be one state in the basis of “dressed” states with regards to which the spatial motion can be treated as adiabatic. The artificial gauge field coupling to the spatial motion of this state arises from the adiabatic elimination of all other “dressed” states. The simplest realisation is provided by a two-level system. We consider the coupling of a ground state \( |g\rangle \) to an excited state \( |e\rangle \) of an atom with mass \( M \) via a laser described by a Hamiltonian of the form [69]

\[
\hat{H} = \frac{\hat{p}^2}{2M} + \frac{\hbar \Omega}{2} \begin{pmatrix}
-\cos \theta & e^{-i\phi} \sin \theta \\
\sin \theta & \cos \theta
\end{pmatrix}
\]  

(1.10)

where the time-dependence has been dropped in the rotating wave-approximation and \( \Omega \) is the (generalised) Rabi frequency. The Rabi frequency \( \Omega_R = \Omega \sin \theta \) characterises the strength of the atom-light coupling between the relevant states, and is connected to the atom and laser properties via \( \Omega_R = \frac{q}{\hbar} \langle e \mid \vec{E} \cdot \vec{r} \mid g \rangle \). It is given by the expectation value of the dipole operator \( \vec{q} \vec{r} \), where \( q \) is the charge of the electron, between the coupled states, and the amplitude of the electric field \( \vec{E} \). The diagonal terms \( \hbar \Omega \cos \theta \) are set by the detuning of the transition from the atomic resonance, i.e. \( \hbar \Omega \cos \theta = E_e - E_g - \hbar \omega_L \) with the energy of the uncoupled states \( E_{e/g} \) and the laser frequency \( \omega_L \). We obtain two dressed states \( \chi^{(\pm)} \) with energies \( E^{(\pm)} = \pm \hbar \Omega / 2 \) and adiabatic elimination of the excited...
1.2. Artificial Gauge Fields

Figure (1.7) Level scheme of $[111]$. Magnetic sublevels of $^{87}\text{Rb}$ atoms in the $F = 1$ manifold are split in energy by an applied magnetic field and then coupled by two Raman lasers with wave-vectors $k_1$ and $k_2$ through a near-resonant two-photon process via an intermediate excited state. $\delta$ is the two-photon detuning which is spatially varied to create the artificial gauge field. The single-photon transition is detuned from resonance by $\Delta \gg \delta$. Taken from [69].

state $\chi^{(+)}$ leads to the Hamiltonian for $\chi^{(-)}$

$$\hat{H}^{(-)}_{\text{ad}} = \frac{\left(\hat{p} - A^{(-)}\right)^2}{2M} + W^{(-)} + E^{(-)}$$

(1.11)

where $W^{(-)}$ is an additional scalar potential which does not matter for the present discussion. Importantly, we obtained the term $A^{(-)} = i\hbar \langle \chi^{(-)} | \nabla | \chi^{(-)} \rangle = -\hbar \sin^2(\theta/2)\nabla \phi$ which couples linearly to the momentum as in the case of an ordinary magnetic field.

There are different possible experimental realisations of such effective two-level systems. If one works with only two states and couples directly to an excited state, the life-time of the dressed states is limited by the spontaneous emission from the excited state $|e\rangle$, and one has to select the relevant states carefully to limit heating on the experimental time scales. Alternatively, one may couple two or more states selected from a ground-state manifold via 2-photon transitions through an intermediate excited state [108]. Choosing the single photon detuning $\Delta$ between the excited state and the groundstate manifold large compared to the Rabi frequencies of the transitions ensures that the spontaneous
emission due to the contribution of the excited state remains small. However, as detailed
in Appendix D, if the detuning is large compared to the excited state fine structure
splitting, the two-photon Raman coupling for $\Delta m_F = \pm 1$ transitions scales with $\Delta^2$ as
well and large detuning does not improve the ratio of off-resonant scattering to $\Omega$. This
can be avoided by working with $\Delta m_F = 0$ transitions [108].

Experimentally, synthetic gauge fields have been realised using the three magnetic
hyperfine states in the $F = 1$ manifold of $^{87}$Rb [74, 111, 112] with a level-scheme as
depicted in Fig. 1.7. In their setup the artificial gauge field is created by spatially varying
the two-photon transition detuning $\delta$ leading to a non-vanishing artificial magnetic
field.

A related concept is that of optical flux lattices [82, 113–116]. These rely on coupling a set
of internal atomic states in a similar way as described for the dressed state schemes, but
they apply outside of the adiabatic limit. Their main advantage is that they can realise consi-
iderably higher flux densities and are thus better suited to access the strongly-correlated
regime [82]. In addition, they only require a small number of lasers, which makes them
simpler to implement experimentally, and they do not require deep-optical lattices redu-
cing potential heating due to light-scattering and are valid beyond the tight-binding limit
[113] which the schemes in the following sections work in.

One of the limitations of these scheme is that it relies on having a suitable set of internal
states which makes it species dependent.\textsuperscript{5} As part of our general treatment of scattering
theory in the Floquet setting in Chapter 3 we consider the role of interactions and time-
dependence in dressed-state schemes as an application to experimentally relevant settings
in Section 3.4.1.

\subsection*{1.2.4. Time-periodic Modulation of Optical Lattices}

The scheme described in this section works by time-periodic modulation or “shaking” of an
optical lattice [76, 84, 95–100, 117]. As quantum systems with periodic time-dependence
\textsuperscript{5}This is true if the internal states are assumed to be spin-states. Principally, they could also be chosen as
states of a suppressed additional spatial direction in which case the scheme applies to arbitrary atomic
species.
they can be described within Floquet-Theory. We will consider an intuitive example below and leave the general theoretical description until after our introduction to Floquet theory in Chapter 2. The artificial magnetic field emerges in the high-frequency approximation, which we introduce in Section 2.4. The basic idea is that for a modulation at a frequency $\omega$ large compared to all system energies, the effective dynamics can be well captured within a time-independent effective Hamiltonian which if the time-dependence is properly designed turns out to contain the artificial gauge field.

Such dynamic optical lattices have recently been used to realise Bloch-bands with non-zero Chern numbers [79, 81] and Bose-Einstein condensation in the resulting topological band structure has been achieved [118]. The experiments in [78, 79, 81, 118] rely on resonant modulation of the optical potential. Starting from a static optical lattice with an energy off-set between neighbouring sites of size $\Delta$, either via a superlattice or in a Wannier-Stark-ladder configuration, which inhibits tunnelling for $t \ll \Delta$, they restore tunnelling with a time-periodically modulated potential of frequency $\omega = \Delta/\hbar$. The tunnelling matrix elements pick up a phase $\phi$ related to the differential phase of the lattice modulation on neighbouring sites, in analogy to the phase given by the Peierl’s substitution. These schemes allow the realisation of large synthetic fluxes, specifically, the experiments [79, 81] achieve a flux $\Phi = \pi/2$ per plaquette of the two-dimensional optical lattice. By measuring the transverse Hall response of the system to an applied linear force [119] this allowed the first measurement of a Chern number in an ultracold atomic system [81]. The experiments [81] also revealed significant heating and population transfer into higher bands which have been attributed to the periodic driving. Such heating is problematic if strongly correlated phases, e.g. fractional Quantum Hall states, are to be realised in Floquet-engineered settings. We provide an explanation of the heating and population dynamics in the experimental setting due to the interplay of the time-dependence and particle interactions in Chapter 4.

Intuitively, the lattice schemes can be understood in a two-site picture. Imagining two sites whose energy is modulated in time differentially, a particle sees at time $\tau$ a phase of $\phi \sim \Delta E(\tau)$. The complex hopping phase corresponds to the time average over one period $T$ of this phase, i.e. $e^{i\phi} \sim \langle e^{i\Delta E(\tau)} \rangle_T$. To make this precise consider bosons on two sites ($a$
where $\Delta$ is the energy offset between $a$ and $b$ sites and is assumed to be large compared to $t$ inhibiting tunnelling. Particles on site $a$ ($b$) are created by the operator $\hat{a}^\dagger$ ($\hat{b}^\dagger$) with corresponding densities $\hat{n} = \hat{a}^\dagger \hat{a}$ ($\hat{b}^\dagger \hat{b}$). The last line describes the differential time-periodic modulation $\hat{V}(\tau)$ of different sites with dimensionless strength $\kappa$ and phase factors $\nu_a(b)$. To restore tunnelling we assume $\Delta = \hbar \omega$ and consider the high-frequency limit. To this end we transform into a rotating frame via

\[
\hat{R}(\tau) = \exp \left[ -\frac{i}{\hbar} \left( \hat{\Delta} + \int_0^\tau \hat{\nu}(\tau') d\tau' \right) \right] = \exp \left[ -i \omega \hat{n}_b - \nu_a \right] + \kappa \left( (-e^{i\omega \tau} (\nu_a \hat{n}_a + \nu_b \hat{n}_b) + e^{-i\omega \tau} (\nu_a^* \hat{n}_a + \nu_b^* \hat{n}_b)) \right]
\]

The transformed Hamiltonian $\hat{H}_R = \hat{R}^\dagger(\tau) \hat{H}(\tau) \hat{R}(\tau) - i \hbar \hat{R}^\dagger(\tau) \partial_\tau \hat{R}(\tau)$ takes the form

\[
\hat{H}_R(\tau) = -t \sum_{k=-\infty}^{\infty} e^{ik\omega} e^{i(k\omega + \phi)} J_k(2\kappa |\Delta|) \hat{b}^\dagger \hat{a} + h.c.
\]

with $\delta_\nu = \nu_b - \nu_a$ and $\phi = \arg(\nu_b - \nu_a)$ and $J_k$ denotes the $k$-th Bessel function of the first kind [120]. We can now take the limit $\omega \to \infty$ and only keep the first order term in the high-frequency expansion, Eq. (2.14), which is just the time-average, i.e.

\[
\hat{H}\left(\tau\right)^{(1)} = \hat{H}_{av} = -te^{i\phi} J_1(2\kappa |\Delta|) \hat{b}^\dagger \hat{a} + h.c.
\]

This result shows that the tunnelling between sites was restored with a renormalised amplitude $tJ_1(2\kappa |\Delta|)$ proportional to the first Bessel function $J_1$. We obtain the first Bessel function here as the offset was chosen as $\Delta = 1 \times \hbar \omega$. Moreover, for vanishing differential modulation $\delta_\nu = 0$, and tunnelling remains suppressed to zero. Finally, we induced a complex hopping phase $\phi = \arg(\nu_b - \nu_a)$ which depends on the differential

\[\text{Note that the limit } \omega \to \infty \text{ also implies } t/\Delta = t/(\hbar \omega) \to 0\]
1.2. Artificial Gauge Fields

phase between the $a$ and $b$ sites of the modulation pattern.

This simple example illustrates a general method to create complex hopping phases in arbitrary lattice geometries via time-periodic modulation of site-energies. Considering for example a square two-dimensional lattice with sites at positions $(m, n)$ and nearest neighbour tunnelling, the gauge invariant flux would be given by summing the hopping phases $\phi_{(m,n)\rightarrow(m',n')}$ for hopping from site $(m, n)$ to site $(m', n')$ over a plaquette. This gives

$$
\Phi^{(m,n)} = \sum \phi_{(m,n)\rightarrow(m',n')}
= \phi_{(m,n)\rightarrow(m+1,n)} + \phi_{(m+1,n)\rightarrow(m+1,n+1)} + \phi_{(m+1,n+1)\rightarrow(m,n+1)} + \phi_{(m,n+1)\rightarrow(m,n)}
= 2\pi n^{(m,n)}_{\phi}
$$

which defines the flux $n^{(m,n)}_{\phi}$ per plaquette. Each of these phases can in turn be controlled by controlling the phases $\nu_{(m,n)}$ of the modulation pattern. In the limit of low flux density $n_{\phi} \ll 1$ the system can be described via the continuum theory [84, 85] and we recover the physics of the FQHE effect. Furthermore, low filling fractions $n/n_{\phi}$ can experimentally be realised in optical lattice systems. For large flux densities genuinely new physics can emerge that has no counterpart in the continuum [86–88, 121].

We will consider scattering and heating in a modulated lattice as one of the applications of our Floquet scattering Theory in Section 3.4.2 and the band population dynamics following from Floquet scattering in a modulated superlattice potential in Chapter 4.

1.2.5. Synthetic Dimensions

The final method we describe is based on the idea of “synthetic” dimensions [101, 102]. It relies on coupling internal states of the atoms in such a way as to simulate the physics of motion along a real lattice direction.\(^7\)

\(^7\)We will be focussing on a finite number of internal spin states here, but recent proposals also use harmonic oscillator states in a similar manner [122]
1. Introduction

**Figure (1.8)** Illustration of the method of “synthetic” dimensions. Shown is a one-dimensional system with 3 internal states \( m = -1, 0, 1 \). Particles hop along the real lattice with amplitude \( t \) and along the spin-direction with amplitude \( \Omega e^{i\phi} \). The groundstate shows chiral edge states indicated by the red and blue arrows.

Experimentally, these methods have so far been implemented in one-dimensional optical lattices, both for fermionic and bosonic species, and the corresponding two-dimensional physics, such as (chiral) edge-states, reminiscent of the edge physics of the Quantum Hall effect [123] have been observed [124, 125]. Experimentally, these chiral edge modes can be imaged directly via state-resolved imaging of the atomic cloud [124, 125]. It offers the additional prospect of realising higher than three-dimensional systems, e.g. a recent proposal suggests to simulate 4-dimensional Quantum Hall physics in cold atom setups [126].

The basic idea is similar to schemes described above in that it relies on coupling internal states of the atoms via Raman lasers which is interpreted as a synthetic tunnelling element \( t_{syn} \sim \Omega e^{2ik_R \cdot x} \) where \( \Omega \) denotes the strength of the coupling and \( k_R \cdot x \) the running phase of the Raman lasers. The different internal states are interpreted as sites of a “synthetic” lattice dimension. The spatial dependence of this running phase is now exploited to engineer a topologically non-trivial lattice Hamiltonian, see Fig. 1.8 for an illustration of a “synthetic” three-leg ladder system. Ideally, one would have a large number of internal states, \( N = 2I + 1 \) for an atomic spin \( I \), at one’s disposal, both to have a sufficiently large “bulk” region in the synthetic dimension and to reduce finite size effects such as the scattering of the chiral edge states as they are generically not topologically protected. A first distinction to a “real” dimension is the strong non-homogeneity of the tunnel couplings along the spin direction which stems from the Clebsch-Gordon coefficients associated with the specific atomic transitions. Secondly, interactions are particularly interesting in this setting, as due to their \( SU(2I + 1) \)-invariance they are infinite range along the synthetic dimension. While the resulting model shows a rich variety of phases [127, 128], it is unclear if it can host fractional quantum Hall states [129]. We study
1.2. Artificial Gauge Fields

Figure (1.9) Dispersion of atoms with internal spin states \( m_z = -1, 0, 1 \) in a one-dimensional lattice coupled via Raman-beams with running phase \( \phi = 2kRd = 1 \) and \( \Omega_R/t = 0.2 \), see Eq. (1.17). Arrows indicate the spin-composition of the groundstate band in the two minima. Colorcoded is the expectation value \( \langle S_z \rangle \) with \( S_z = \text{diag}(-1, 0, 1) \).

these types of systems in the limit of strong interactions and strong Raman coupling in Chapter 5.

To understand this scheme in some more detail, we consider the simplest model that can show proper (chiral) edge modes, i.e. we require at least 3 internal states which implies \( I = 1 \), which also corresponds to the experiments [124, 125]. The Hamiltonian for atoms with a spin \( I = 1 \) and 3 degenerate magnetic sublevels loaded into a one-dimensional optical lattice reads as

\[
\hat{H} = \sum_{j=1}^{1} \sum_{m_z=-1}^{1} -t \hat{a}_{j+1,m_z}^\dagger \hat{a}_{j,m_z} + \Omega_{m_z} + \frac{\Omega_R}{t} e^{i\phi j} \hat{a}_{j+1,m_z}^\dagger \hat{a}_{j,m_z}^\dagger + \text{h.c.} \tag{1.17}
\]

where \( \hat{a}_{j,m_z}^\dagger \) creates an atom in internal state \( m_z \) at site \( x_j = jd \), with the lattice spacing \( d \), the phase \( \phi = 2kRd \) is the running phase of the Raman beams, and \( \Omega_{m_z} \) is the atom-light coupling strength of the different hyperfine-levels [102, 130, 131]. We remark that generically the synthetic dimension naturally is of finite extent and has open-boundaries at spin-states \( m_z = \pm I \) unless one specifically engineers an additional coupling between these states.\(^8\) Note, that in the

\(^8\) There are proposals to generate such couplings via the use of additional lasers [102], they generically require either many-photon transitions, additional rf fields or to address each transition via spin-dependent light-shifts. Thus, they are experimentally harder to realise, in particular for large spins \( I \).
present case of $I = 1$ the couplings are actually homogeneous, $g_{m_z} = g = \sqrt{2}$, and periodic boundary conditions in the synthetic dimension can also be experimentally realised. The non-interacting Hamiltonian Eq. (1.17) can for closed boundary conditions in the real direction be diagonalised in each momentum sector separately. We display the resulting band structure as a function of $q$ for $\Omega_R/t = 0.2$ and $\phi = 1$ in Fig. 1.9. Of particular note is the resulting ground-state band which has minima at opposite momenta with opposite spin-composition. These are the chiral edge modes of the system mentioned above, each propagating along one of the edges of the synthetic dimension, which here correspond to $m_z = +1$ and $m_z = -1$, in opposite directions along the real dimension.

1.3. Outline of Thesis

In this chapter we have introduced the toolbox of ultracold atomic gases in Section 1.1. In particular, we have discussed how they can be confined in different geometries and dimensions and the type of interactions most prevalent in these systems. Then, we discussed different schemes to extend the capabilities of ultracold atoms by engineering artificial magnetic fields for charge-neutral atoms in Section 1.2. This served a two-fold purpose, it provided the relevant background on the theoretical proposals and experimental realisations and introduced the basic models which we will study in more detail later on. The attentive reader will have noticed that after introducing the most common type of interactions encountered in ultracold atomic gases, we have mostly discussed the non-interacting single-particle physics of the models in the following. On the other hand, we have emphasised that one of the advantages of cold-atomic gas systems is their wide tunability, and in particular the ability to engineer the (many-body) interactions. In fact, the effects of interactions, their interplay with time-dependence and gauge fields will be the main focus and combining theme in all the work that will be presented in this thesis.

In Chapter 2 we begin by introducing the treatment of periodically time-dependent quantum systems within Floquet-Theory. This chapter will provide us with a framework but also offer additional freedom in engineering the topology of the synthetic dimension [132].
1.3. Outline of Thesis

in which to understand the concept of Floquet-engineering and Floquet scattering. We will discuss the high-frequency approximations mentioned above and the theoretical tools which we will employ in the following chapters.

Being equipped with these tools, we discuss the general scattering properties of time-dependent Hamiltonians under perturbation via (weak) two-body contact interactions in Chapter 3. We phrase the question in terms of scattering theory in a rotating frame of the time-dependent non-interacting Hamiltonian, and sufficiently weak interactions such that a treatment within perturbation theory is sufficient. We show how time-dependent potentials in presence of interactions generically lead to “inelastic” scattering and illustrate this in a simple toy model. After these preparatory explorations, we discuss the role of interactions in two specific applications relevant to the dressed state and modulated lattice schemes described in Section 1.2.3 and Section 1.2.4.

Using the insights we have gained, we tackle the experimental setup used to realise the Harper-Hofstadter Hamiltonian [78, 81] in Chapter 4. Specifically, we are concerned with the experimentally observed heating rates and band population dynamics whose control as described above are of crucial importance in the quest for strongly-correlated physics. Using scattering rates computed via the Floquet-Fermi-Golden rule from the full non-interacting time-dependent Floquet-states we obtain population dynamics in agreement with the experimental observations. Having established these Floquet scattering processes as a viable explanation of the heating and population dynamics in this experiment, we consider how they can be suppressed in the experiment via additional confining potentials.

Finally, in Chapter 5 we study the many-body physics of bosonic atoms emerging in “synthetic” dimensions in the limits of strong interactions and strong Raman coupling between the internal states. The physics is governed by the interplay of the exotic infinite range interactions, and frustration of the hopping due to the artificial gauge field. We derive an effective model of spinless hardcore bosons. Using Density-Matrix-Renormalisation-Group calculations we obtain the phase-diagram at flux $\Phi = \pi$, including supersolid and pair-superfluid phases.

The thesis can thus be broadly divided into two parts. Chapter 3 and Chapter 4 will study the interplay of the explicit time-dependence of Floquet states and interactions in systems
used to simulate artificial gauge fields. As described above in these systems we find Floquet scattering to be a relevant process. However, it will also turn out that in specific cases the interactions commute with the time-dependence. Specifically, this is the case for Raman coupled spin-states used to create the synthetic dimensions studied in Chapter 5 and we will therefore not focus on the Floquet aspect for this system. Even though this approach does not suffer from Floquet scattering it has a number of different limitations. Firstly, the required Raman transitions lead to off-resonant light scattering which as we discussed cannot be reduced by working with far-detuned light fields. Secondly, the approach is species-dependent as it relies on coupling different internal states of the atoms, while the modulated optical lattices can be used for any atomic species. Thirdly, the length of the synthetic dimension is fundamentally of finite, small extent. In particular, it is unclear whether these systems can host fractional quantum hall states which are expected to occur in true two dimensional systems. Thus, the approaches working with Floquet engineering in two dimensional optical lattices, though potentially suffering from Floquet scattering, are still relevant to explore all the physics. In particular, as we argue, the Floquet scattering may be reduced by appropriate design of the experiment, whereas the limitation of the finite extent of synthetic dimensions cannot be removed. Finally, we emphasise again that in both cases it is the inclusion of interactions in the description which leads to the phenomena we discuss.
2. Introduction to Floquet Theory

The work described in Chapter 3 and 4 relies on Floquet theory [133–135], in its application to quantum mechanical systems with periodic time-dependence. Coherent control of quantum many-body systems via time-periodic driving has become recognised as a highly useful and flexible tool in recent years, for reviews see [95–97, 117, 136, 137]. It not only allows the realisation of artificial gauge fields as described in the last chapter, but also opens the opportunity to study genuinely new physics not accessible in an equilibrium setting. While it enters into the regime of non-equilibrium physics we will see that many of the usual notions from static quantum mechanics carry over to the Floquet case which makes it simpler to study theoretically than the generic fully time-dependent case.

Notable achievements include dynamic localisation in BECs [138, 139], coherent AC-induced tunnelling in lattices [140, 141], the coherent control of dressed matter waves and the dynamic phase-transition between the Mott and superfluid state [142, 143], coherent band coupling [144, 145], coherent control of interaction blockade with applications to cooling [146], the realisation of a tunable Ising model [147], the realisation of systems with topologically non-trivial properties, such as Floquet-topological insulators [148–152], the Haldane-model [80], anyonic Hubbard models [153, 154] and density-dependent-tunnelling and dynamic gauge-fields [154–156].

In this chapter we provide an introduction to the general concepts required for the following discussion and introduce the notational conventions used in the remainder of the thesis. In Section 2.1 and Section 2.2 we discuss the notions directly required for the discussion in Chapter 3 and Chapter 4. We will start with reviewing Floquet’s theorem and the form of the solutions it provides for time-periodically dependent Hamiltonians, briefly discuss the notion of quasi-energy and the freedom of choice in defining them, and conclude
2. Introduction to Floquet Theory

with the notion of an extended Hilbert space and the corresponding inner product defined therein. In Section 2.3 and Section 2.4 we describe a different approach to Floquet systems based on an effective description via a time-independent Floquet Hamiltonian. This description underlies Floquet engineering, the idea of simulating a desired time-independent Hamiltonian via proper design of a periodically driven quantum system. Finally, we introduce the high-frequency approximations frequently used to obtain the Floquet Hamiltonian from the full time-dependent Hamiltonian.

We would like to emphasise that these two approaches work in different regimes, the second approach breaks down in the presence of resonances which is precisely the case which we will be considering. Some of the main results will in fact be concerned with the case when an effective description is not valid and when the description only via the Floquet Hamiltonian and its spectrum is not sufficient.

2.1. Floquet Theorem and Quasi Energies

Consider a time-varying Hamiltonian $\hat{H}(\tau)$ that is periodic in time, $\hat{H}(\tau+T) = \hat{H}(\tau)$, where $T = 2\pi/\omega$ is the oscillation period and $\omega$ the associated frequency. The corresponding time-dependent Schrödinger equation

$$\left[\hat{H}(\tau) - i\hbar \frac{\partial}{\partial \tau}\right] |\Psi(\tau)\rangle = 0$$

allows solutions of a specific form called Floquet states. These may be written as

$$|\Psi_\alpha(\tau)\rangle = \exp[-i\epsilon_\alpha \tau / \hbar]|\Phi_\alpha(\tau)\rangle,$$

(2.2)

where $|\Phi_\alpha(\tau)\rangle$ is called the Floquet mode which has the same time-periodicity as the Hamiltonian, i.e. it satisfies $|\Phi_\alpha(\tau+T)\rangle = |\Phi_\alpha(\tau)\rangle$, and $\epsilon_\alpha$ is called the quasi-energy which is only defined up to multiples of $\hbar \omega$. Due to the time-periodicity of the Floquet modes one may expand them as

$$|\Phi_\alpha(\tau)\rangle = \sum_m e^{i m \omega \tau} |\phi_m^{\alpha}\rangle.$$

(2.3)
2.1. Floquet Theorem and Quasi Energies

where \( |\phi_m^\alpha\rangle = \frac{1}{T} \int_0^T d\tau e^{-im\omega \tau} |\Phi_\alpha(\tau)\rangle \) are the Fourier-components of the Floquet mode \( |\Phi_\alpha(\tau)\rangle \), e.g. they are generic elements of the Hilbert space. Clearly, the same physical state is obtained from

\[
|\Psi_\alpha(\tau)\rangle = \exp[-i(\epsilon_\alpha + m\hbar \omega)\tau/\hbar] \exp[im\omega \tau] |\Phi_\alpha(\tau)\rangle = \exp[-i\epsilon_m^\alpha \tau/\hbar] |\Phi_m^\alpha(\tau)\rangle,
\]

where the shifted states are defined as \( |\Phi_m^\alpha(\tau)\rangle = \exp[im\omega \tau] |\Phi_\alpha(\tau)\rangle \) with quasi-energy \( \epsilon_m^\alpha = \epsilon_\alpha + m\hbar \omega \) for any integer number \( m \).

The formal analogy to Bloch’s theorem is now evident: just as the (discrete) spatial translational invariance of a lattice Hamiltonian leads to Bloch functions formed from a plane wave part and a periodic part labelled by the crystal or quasi-momentum \( k \), so too does the invariance of the Hamiltonian under discrete time translation \( \tau \to \tau + T \) cause the Floquet states to consist of a simple phase part and a time-periodic part labelled by the quasi-energy \( \epsilon_\alpha \). Just as the Bloch quasi-momentum \( k \) is only defined up to reciprocal lattice vectors and conventionally taken to lie in the first Brillouin zone (BZ), so is the Floquet quasi-energy only defined up to addition of \( \hbar \omega \). One may then define \( \epsilon_0^\alpha \) to lie in the range \( -\hbar \omega/2 < \epsilon_0^\alpha \leq \hbar \omega/2 \). However, as we discuss below, other conventions for the Floquet energies may be more suitable and physically transparent: for example one might choose \( \epsilon_\alpha^0 \) in such a way as to most closely correspond to the eigenenergies of a static Hamiltonian, or to correspond to the choice which maximises the norm of \( |\phi_\alpha^0\rangle \).

At this point it is worth noting that in the most generic case the concept of an energy is not well-defined for a Floquet system anymore. The energy \( E \) is strictly speaking only well defined for a static Hamiltonian, or more generally in the presence of a continuous time-translation symmetry, in which case the full time dependence of the eigenstates \( |\psi\rangle \) reduces to a simple phase evolution via \( |\psi\rangle(\tau) = e^{-iEt/\hbar} |\psi\rangle(\tau = 0) \), up to some time-dependent gauge choice. Importantly, even for a static Hamiltonian the energy of a single state is not well defined, it only gains meaning when compared to a different state and when a coupling between these states is present as otherwise any energy can be gauged arbitrarily by state dependent unitary transformations. However, one may easily envisage cases in which talking about an energy becomes meaningful. For example, one...
might prepare a system in some eigenstate of a static Hamiltonian, then switch on a
time-dependent perturbation, and after switching off the perturbation measure the energy
of the evolved system with respect to the eigenstates of the static Hamiltonian. In this
scenario the energies before switching on and after switching off the perturbation are well
defined and the difference is meaningful. Finally, there is usually a very obvious choice for
a static reference Hamiltonian \( \hat{H}_{\text{ref}} \) to compare states against. In that case preparing states
with respect to \( \hat{H}_{\text{ref}} \), then switching on the time-dependent Hamiltonian \( \hat{H}(\tau) \), and after
some time measuring the overlaps of the evolved state with respect to the eigenstates
of well defined energy of \( \hat{H}_{\text{ref}} \) also defines an energy. A most simple example of such a
reference Hamiltonian would be to consider free particles.

### 2.2. Extended Hilbert Space

We define the Hermitian operator
\[
\mathbf{h} = \hat{H}(\tau) - i\hbar \partial_{\tau}
\]
in an extended Hilbert space \( \mathcal{H} \otimes \mathcal{T} \) given by the direct product of the Hilbert space \( \mathcal{H} \) on which \( \hat{H} \) acts and the space of
\( T \)-periodic functions \( \mathcal{T} \). States in this extended space will be denoted as \(|\phi\rangle\rangle\), and as
the functions \( e^{im\omega \tau} \) form a basis of \( \mathcal{T} \) may be expanded as
\[
|\phi\rangle\rangle = \int_{-\infty}^{\infty} e^{im\omega \tau} |\phi_m\rangle
\]
as sums
over states \(|\phi_m\rangle\) in \( \mathcal{H} \). One sees that the Floquet modes themselves satisfy an eigenvalue
equation
\[
\mathbf{h}|\Phi_\alpha\rangle\rangle = \epsilon_\alpha |\Phi_\alpha\rangle\rangle, \tag{2.5}
\]
Moreover, clearly the shifted Floquet modes \(|\Phi_m^\alpha\rangle\rangle\) satisfy the same equation, but with
their shifted eigenvalues \( \epsilon_m^\alpha \). As eigenfunctions of a Hermitian operator they form a
complete and orthogonal basis set with respect to a suitably extended inner product. This
is achieved via \[134, 157\]
\[
\langle\langle \Phi_\alpha | \Phi_m^\beta \rangle\rangle = \frac{1}{T} \int_0^T d\tau \langle\Phi_\alpha^\alpha(\tau) | \Phi_m^\beta(\tau) \rangle = \delta_{\alpha,\beta} \delta_{n,m}, \tag{2.6}
\]
which is seen to be the time-average over a period \( T \) of the usual inner product
\[
\langle\Phi_\alpha^\alpha(\tau) | \Phi_m^\beta(\tau) \rangle
\]
in \( \mathcal{H} \). Moreover, at equal times the Floquet modes form a complete set for the Hilbert
2.3. Effective Hamiltonian and Floquet Engineering

This section presents an alternative approach to Floquet-systems that is better suited to Floquet-engineering and describing many-body physics, but which will not be required for the main results of this work. It also provides the connection between the approach taken in this thesis and much of the other work on Floquet-systems in the literature [95–97, 117, 136, 137].

At the heart of Floquet engineering is the effective or Floquet Hamiltonian, a time-independent Hamiltonian governing the time-evolution of the system at stroboscopic times \( t_n = \tau_0 + nT \), see Eq. (2.11). Here, we take a rather unconventional route to obtain it, based on the previous discussion, which, however, makes the connection to Floquet’s theorem and the form of the solutions it provides for the time-periodic Schrödinger equation very explicit.

Using a full-set of solutions given by the Floquet modes in Eq. (2.3) one may define a unitary-time-dependent transformation via

\[
\hat{U}_F(\tau, \tau_0) = \sum_\alpha |\Phi_\alpha(\tau)\rangle \langle \Phi_\alpha(\tau_0)|.
\]  

(2.8)

We note that for this choice, by the periodicity of the Floquet modes and their completeness, we have \( \hat{U}_F(\tau_0 + T, \tau_0) = \hat{U}_F(\tau_0, \tau_0) = \hat{1}_H \). The transformed Hamiltonian turns out to be time-independent, i.e.

\[
\hat{H}_F^{\tau_0} = \hat{U}_F^{\dagger}(\tau, \tau_0)\hat{H}(\tau)\hat{U}_F(\tau, \tau_0) - i\hbar \hat{U}_F^{\dagger}(\tau, \tau_0)\partial_\tau \hat{U}_F(\tau, \tau_0)
\]

\[
= \sum_\alpha \epsilon_\alpha |\Phi_\alpha(\tau_0)\rangle \langle \Phi_\alpha(\tau_0)|
\]  

(2.9)
With the full time-evolution given by

\[
\hat{U}(\tau, \tau_0) = \hat{U}_F(\tau, \tau_0) \exp \left[ -\frac{i}{\hbar} \hat{H}_F^\tau (\tau - \tau_0) \right].
\] (2.10)

This equation now allows a simple interpretation of the time-evolution of Floquet systems. The periodic time-dependence of the Floquet modes encapsulated in \(\hat{U}_F(\tau, \tau_0)\) represents what is typically called “micromotion” in the literature. The linear phase evolution given by the time-independent effective Hamiltonian \(\hat{H}_F^\tau\), which is often called Floquet Hamiltonian, and the quasi-energies \(\varepsilon_\alpha\) is similar to the evolution of a truly time-independent quantum system. We note that the Floquet Hamiltonian \(\hat{H}_F^\tau\) depends parametrically on the time \(\tau_0\), however the explicit spectral representation in Eq. (2.9) shows that the spectrum is in fact independent of \(\tau_0\).

This choice to obtain the Floquet Hamiltonian is clearly not unique, any unitary time-independent transformation of \(\hat{H}_F^\tau\) yields an equally valid choice, but has the advantage that it directly generates the stroboscopic evolution via

\[
\hat{U}(\tau_0 + T, \tau_0) = \exp \left[ -\frac{i}{\hbar} T \hat{H}_F^\tau \right].
\] (2.11)

This equation is central to the Floquet engineering approach. The idea is to tailor the time-dependent Hamiltonian \(\hat{H}(\tau)\) in such a way as to realise a Floquet Hamiltonian \(\hat{H}_F^\tau\) of the desired form. Then the behaviour of the time-dependent system at the stroboscopic times \(\tau_n = \tau_0 + nT\) exactly matches the dynamics as generated by the time-independent Hamiltonian \(\hat{H}_F^\tau\).

### 2.4. High-Frequency Approximations

In terms of understanding the effects of coherent time-periodic driving of quantum systems an efficient method to obtain the Floquet Hamiltonian \(\hat{H}_F^\tau\) for a given time-dependent Hamiltonian \(\hat{H}(\tau)\) is required. Strictly speaking, for the Floquet engineering aspect, one would, in fact, like to obtain a suitable Hamiltonian \(\hat{H}(\tau)\) given a desired static Hamiltonian \(\hat{H}_{\text{target}}\). Clearly, the formal approach taken above, in making use of...
2.4. High-Frequency Approximations

the full eigenstates of a time-dependent generically interacting many-body Hamiltonian is not feasible in practice in almost all cases. Thus, one requires an approximate scheme that still provides a valid description at least on the time-scales and energy-scales one is interested in. Such an approach is provided by high-frequency approximations [96, 97, 117, 137, 158–161].

To understand these, it is useful to first expand the time-periodic Hamiltonian in its frequency modes as

\[ \hat{H}(\tau) = \sum_m e^{im\omega \tau} \hat{H}_m, \]  

(2.12)

where \( \hat{H}_m = \frac{1}{T} \int_0^T d\tau e^{-im\omega \tau} \hat{H}(\tau) \). If the driving frequency \( \hbar \omega \) is large compared to the terms \( \hat{H}_m \neq 0 \), one can hope that an expansion in the inverse frequency might yield a suitable description of the dynamics. The expansion takes the form

\[ \hat{H}_F \approx \sum_{n=1}^{n_{\text{max}}} \hat{H}_F^{(n)}, \quad \hat{U}_F(\tau) \approx \exp \left[ \sum_{n=1}^{n_{\text{max}}} \hat{G}^{(n)}(\tau) \right]. \]  

(2.13)

For our purposes only the explicit forms of \( \hat{H}_F^{(n)} \) with \( n = 0, 1 \) are required,

\[ \hat{H}_F^{(1)} = \hat{H}_0, \]  

(2.14)

\[ \hat{H}_F^{(2)} = \sum_{m \neq 0} \frac{[\hat{H}_m, \hat{H}_{-m}]}{m\hbar \omega}. \]  

(2.15)

Expressions for \( \hat{G}^{(n)}(\tau) \) and higher orders can be found in the references given above. From a practical point of view, and in the cases which we will be considering, one often engineers the time-dependent Hamiltonian in such a way that the approximate Floquet Hamiltonian \( \hat{H}_F \approx \sum_{n=1}^{0(1)} \hat{H}_F^{(n)} \) corresponds to the desired target Hamiltonian \( \hat{H}_{\text{target}} \).

The validity of the high-frequency approximation for interacting many-body systems is far from obvious [158]. The breakdown of these expansions is directly related to resonances in the full quasi-energy spectrum and to heating-up under the full dynamics [162–166]. For systems with a locally unbounded spectrum, these resonances must always exist even in the high-frequency limit. It is precisely these types of situations we will be
2. Introduction to Floquet Theory

considering in Chapter 3 and Chapter 4. Thus, our approach is complementary in that it provides explicit time-scales for the heating of the system and allows to obtain stability regions in parameter space in which the high-frequency approximation on which Floquet engineering is often based remains valid.

2.5. Summary

We have briefly introduced the results of Floquet’s theorem as relevant to the following work. Solutions take the form of products of plane wave factors and Floquet modes given in Eq. (2.2), with the expansion of Floquet modes in Eq. (2.3). We discussed the gauge freedom in defining the quasi-energy and mentioned motivations for different choices which will be further discussed in detail and for specific examples in Chapter 3. The formulation presented above allows one to carry over many of the techniques known from time-independent quantum mechanical systems and extend them to the time-periodic case by use of the scalar product Eq. (2.6). Specifically, this will form the basis of the extension of the Fermi golden rule to the Floquet setting called the Floquet Fermi golden rule (FFGR) discussed in Section 3.2.1 and used to discuss two-particle scattering for time-periodic Hamiltonians.

In a second part, we introduced the notion of Floquet engineering based on the effective description via a time-independent Floquet Hamiltonian and its approximation in the high-frequency limit. These are important to connect to developments in the wider context of coherent control of quantum many-body systems via periodic driving and provide the underlying theoretical framework to motivate some of the models we are going to study. We discussed some aspects of why this description might break down and argued that in the cases we will be considering this is naturally the case.
3. Scattering Theory for Floquet-Bloch States

Figure (3.1) Sketch of a scattering event with incoming energy $E_0$ by a time-dependent potential with frequency $\omega$ in which the incoming particles (red) gain energy during the collision and end up in a higher energy state (blue).

In this chapter we study the scattering properties of particles that are subjected to time-periodic Hamiltonians. Our study is motivated by recent experimental implementations of artificial gauge fields for gases of ultracold atoms. Making use of Floquet theory, we focus on translationally invariant situations in which the single-particle dynamics can be described in terms of spatially extended Floquet-Bloch waves. We develop a general formalism for the scattering of these Floquet-Bloch waves. We show how static interactions can be seen to become time-dependent in a Floquet frame of reference, and thus, how the scattering of Floquet-Bloch states be understood to be equivalent to scattering of time-independent states via a time-periodic potential. A two-particle scattering process in this interpretation is illustrated in Fig. 3.1. An important role is played by the conservation of Floquet quasi-energy, which is defined only up to the addition of integer multiples of $\hbar \omega$ for a Hamiltonian with period $T = 2\pi/\omega$. We discuss the consequences of this for the interpretation of “elastic” and “inelastic” scattering in cases of physical interest. We illustrate our general results with applications to: the scattering of a single particle in a Floquet-Bloch state from a static potential; and, the
scattering of two bosonic particles in Floquet-Bloch states through their interparticle interaction. We analyse examples of these scattering processes in models that are closely related to the schemes used to generate artificial gauge fields in cold-atom experiments, through optical dressing of internal states, or through time-periodic modulations of tight-binding lattices. We show that the effects of scattering cannot, in general, be understood by an effective time-independent Hamiltonian, even in the limit $\omega \to \infty$ of rapid modulation. We discuss the relative sizes of the elastic scattering (required to stabilize many-body phases) and of the inelastic scattering (leading to deleterious heating effects). In particular, we describe how inelastic processes that can cause significant heating in current experimental set-up can be switched off by additional confinement of transverse motion.

### 3.1. Introduction

The methods to generate artificial gauge fields discussed in Section 1.2 generically exploit time-dependent driving or light-fields.\(^1\) As we discussed in Chapter 2 quantum mechanical systems with a periodic time-dependence allow a treatment within Floquet theory [133, 134]. We focus on two of the methods to create artificial gauge fields, the dressed state schemes in the continuum Section 1.2.3 and the time-periodic modulation of (deep) optical lattices Section 1.2.4 to make contact with recent experiments [75, 78, 79, 81, 167]

With the experimental achievement of artificial gauge fields using these techniques, or at least the resulting single-particle phenomena, it is of great interest to consider the consequences for systems of many interacting quantum particles. Much work has been done in exploring the effective interactions between particles in the dressed-state bands [112, 168–174]. However, this work has largely ignored the aspects relating to the periodic

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\(^1\)The case of rotation is special in settings where any potentials that are static in the laboratory frame have perfect cylindrical symmetry. Then, in the frame of reference co-rotating with any stirring potential the Hamiltonian is time-independent, so energy is absolutely conserved. In general, without cylindrical symmetry of the static potentials, rotation at angular frequency $\omega$ also leads to a time-periodic Hamiltonian and only conservation of quasi-energy.
time-dependence giving conservation only of the Floquet quasi-energy, though note the complementary work in Refs. [175, 176].

Generally, time-periodic driving with characteristic angular frequency $\omega$ allows the absorption of energy quanta $\hbar \omega$ from the field. At the single particle level, there is periodic energy transfer, as typical of a Rabi oscillation in a dressed state, which does not lead to entropy generation or other heating processes. However, in the presence of inter-particle interactions, one can anticipate that this energy absorption can cause forms of “inelastic” scattering that can have a heating effect. Possible processes include the excitation of particles into higher bands or even particle loss, or absorption of energy into transverse directions also resulting in heating and loss of particles from the experimental region. These processes necessitate investigation.

Scattering through time-periodically modulated potentials has been studied previously in other contexts [177–180]. In particular, the transport properties of time-driven mesoscopic systems have been investigated [181, 182] and formulations been given within the Keldysh formalism [183] as well as in the Floquet framework [184]. A general formulation for oscillating scatterers in terms of a Floquet scattering matrix was developed in [185]. The study of the transport in periodically driven systems and the associated scattering properties is still an active field of research [186–190]. The novelty of the systems considered here is that the non-interacting Hamiltonian will be periodically driven and the scattering will be caused by static two-body interactions, not by an external oscillating one-body scattering potential. Due to the Floquet structure of the single-particle states the interactions will effectively become time-dependent. Importantly, this also means that for the systems we consider the asymptotic states will be time-dependent, in contrast to the situation usually assumed in transport measurements in which the time-dependence is restricted to the scattering region. Thus, while the underlying theory describing the scattering processes and the resulting phenomena (like the absorption of quanta $\hbar \omega$ from the photon field during scattering) is similar, the physical origin of those processes is very different. Such systems have been studied in the context of atom-atom and atom-electron collisions in intense laser fields and a perturbation theory in the particle-interactions has been established [191–194].

We shall study the scattering processes that arise in these time-driven systems. The
focus will be on elucidating the role of two-body elastic scattering processes, required for the realisation of strongly-correlated many-body phases, as compared to inelastic two-body processes which will limit experimental lifetimes or the temperatures achievable in experiments. We will begin with a discussion of scattering theory in the Floquet framework in Section 3.2. Therein, we will show how to phrase scattering in a “Floquet” frame of reference, derive the FFGR to calculate the corresponding scattering rates, discuss “elastic” and “inelastic” processes and generic properties of Floquet scattering. These will be illustrated in a simple toy model in Section 3.3. We will then apply this general framework to two model systems for artificial gauge fields in Section 3.4: Firstly, Section 3.4.1 will present a two-level system coupled by laser fields which will serve to illustrate effects of time-periodic driving on the scattering properties in the continuum case. Secondly, in Section 3.4.2 we will consider a lattice with time-modulated on-site energies to highlight similarities and differences to the continuum. Therefore, our results on two-particle scattering are directly relevant to current and future cold gas experiments realising artificial gauge fields.

3.2. Scattering Theory in the Floquet Framework

The theory of scattering within the Floquet framework [191] is most conveniently described in the interaction picture of quantum mechanics. The conceptional difference in the scattering of Floquet states arises from the fact that the interaction picture will be defined with respect to a time-periodic non-interacting Hamiltonian \( \hat{H}_0(\tau) \) in contrast to the more conventional case of a static non-interacting Hamiltonian. The special properties of the associated propagator, encoding the fact that energy is only conserved modulo \( \hbar \omega \), will ultimately lead to inelastic scattering processes.

We consider a Hamiltonian of the form \( \hat{H}(\tau) = \hat{H}_0(\tau) + \hat{V} \), which is split into a non-interacting part \( \hat{H}_0 \) that describes free particle motion, and an interaction \( \hat{V} \) that will describe the particle scattering. The non-interacting Hamiltonian \( \hat{H}_0(\tau) \) consists of a static part and a time-periodic single particle coupling term that is strong and thus must be treated in a non-perturbative way, whereas the interaction \( \hat{V} \) will be treated in the framework of perturbative scattering theory. We assume that \( \hat{V} \) is time-independent, as
3.2. Scattering Theory in the Floquet Framework

this will be relevant in the physical situations discussed later, but the analysis can be readily extended to general time-dependent $\hat{V}(\tau)$.

We define the unitary time-evolution operator $\hat{U}_0(\tau, \tau')$ associated with $\hat{H}_0(\tau)$ by

$$|\Psi_0(\tau')\rangle = \hat{U}_0(\tau, \tau')|\Psi_0(\tau)\rangle.$$  \hspace{1cm} (3.1)

Due to the time-dependence of $\hat{H}_0(\tau)$ this operator generically depends on both start and end times. Due to the time-periodicity of $\hat{H}_0(\tau)$, it has the spectral representation

$$\hat{U}_0(\tau, \tau') = \sum_\alpha e^{-i\epsilon_\alpha(\tau' - \tau)/\hbar}|\Phi_{0,\alpha}(\tau')\rangle\langle\Phi_{0,\alpha}(\tau)|$$  \hspace{1cm} (3.2)

$$= \sum_{a,n,m} e^{-i\epsilon_a(\tau' - \tau)/\hbar} e^{-i(n\omega_\tau - m\omega_\tau')}|\phi_{0,\alpha}^a\rangle\langle\phi_{0,\alpha}^n|$$  \hspace{1cm} (3.3)

We define the states in the interaction picture in the usual way via

$$|\Psi^I(\tau)\rangle = \hat{U}_0(\tau, \tau_0)|\Psi(\tau)\rangle$$  \hspace{1cm} (3.4)

which then satisfy the Schrödinger equation

$$i\hbar\partial_\tau |\Psi^I(\tau)\rangle = \hat{V}^I(\tau)|\Psi^I(\tau)\rangle$$  \hspace{1cm} (3.5)

with

$$\hat{V}^I(\tau) = \hat{U}_0(\tau, \tau_0)\hat{V}\hat{U}_0(\tau, \tau_0).$$  \hspace{1cm} (3.6)

The corresponding time-evolution operator $\hat{U}^I(\tau, \tau_0)$ then satisfies the differential equation

$$i\hbar\partial_\tau \hat{U}^I(\tau, \tau_0) = \hat{V}^I(\tau)\hat{U}^I(\tau, \tau_0)$$  \hspace{1cm} (3.7)

with the initial condition $\hat{U}^I(\tau, \tau_0) = \hat{1}$. Rewritten as an integral equation

$$\hat{U}^I(\tau, \tau_0) = \hat{1} - \frac{i}{\hbar} \int_{\tau_0}^\tau d\tau' \hat{V}^I(\tau')\hat{U}^I(\tau_0, \tau')$$  \hspace{1cm} (3.8)
it allows the usual iterative solution in the Dyson series

\[
\hat{U}^1(\tau, \tau_0) = \hat{I} - \frac{i}{\hbar} \int_{\tau_0}^{\tau} d\tau' \, \hat{V}^1(\tau') + O(\hat{V}^2).
\] (3.9)

The full unitary evolution operator is then given by

\[
\hat{U}(\tau, \tau_0) = \hat{U}_0(\tau, \tau_0) \hat{U}^1(\tau, \tau_0).
\] (3.10)

This treatment clarifies in what way the usual scattering theory can be applied to Floquet states. The only difference arises via the use of the propagator \(\hat{U}_0(\tau, \tau_0)\), Eq. (3.2), whose structure therefore determines the differences to the standard case of a time-independent Hamiltonian.

Special attention should be given to the form of \(\hat{V}^1(\tau)\) in Eq. (3.6). Since every Floquet state generically contains components that evolve with phases \(e^{-i(\epsilon_1 + m\hbar\omega)\tau/\hbar}\) for all integer \(m\), \(\hat{V}^1(\tau)\) will most generally contain time-dependent terms oscillating with \(e^{-i(\Delta\epsilon + m\hbar\omega)\tau/\hbar}\) where \(\Delta\epsilon = \epsilon_1 - \epsilon_2\) is the quasi-energy difference of any two Floquet states. Therefore, it is immediately apparent that generically a transition between an initial state with quasi-energy \(\epsilon_1\) and a final state with quasi-energy \(\epsilon_f = \epsilon_1 + m\hbar\omega\) for any integer \(m\) can be induced by a static interaction \(\hat{V}\) due to the structure of the Floquet states. Specifically, we obtain

\[
\hat{V}^1(\tau) = \sum_{\alpha, \beta} e^{-i(\epsilon_\alpha - \epsilon_\beta)\tau/\hbar} \left( \sum_{m, n} e^{-i(m-n)\omega\tau} \langle \phi^m_{0,\alpha} | \hat{V} | \phi^n_{0,\beta} \rangle \right) |\Psi_{0,\alpha}(\tau_0)\rangle \langle \Psi_{0,\beta}(\tau_0)|
\] (3.11)

where the bracketed part describes a time-periodic interaction operator in the Floquet frame of reference. This allows the following intuitive interpretation of scattering processes of Floquet states by static interactions: Transforming to the Floquet frame of reference makes the non-interacting Floquet states time-independent, but now they see a periodically varying interaction potential. If the structure of the Floquet modes and the interaction is such that different frequency components are coupled, i.e. \(\langle \phi^m_{0,\alpha} | \hat{V} | \phi^n_{0,\beta} \rangle \neq 0\) for \(m \neq n\), the interaction in the Floquet frame of reference becomes periodically time-dependent and thus allows the emission or absorption of energy quanta \(\hbar\omega\). Thus, the scattering of Floquet states is closely related to the scattering of time-independent states.
by time-dependent potentials. It is in this interpretation that Fig. 3.1 is seen to generically apply to the two-particle scattering of Floquet states. It may also be interpreted as the micromotion induced by \( \hat{H}_0(\tau) \) not commuting with the interaction \( \hat{V} \). If on the other hand, the interaction operator remains time-independent due to the specific structure of the interactions or the Floquet modes, possibly due to symmetries of the problem, energy changing scattering will not be allowed and energy will be strictly conserved. We will see an illustration of this phenomenon in the scattering properties of the toy model in Section 3.3. However, we emphasise that this statement is true in a non-perturbative sense and for generic many-body systems.

Keeping only the term that is first order in \( \hat{V} \) in the Dyson series, Eq. (3.9), leads to the Born approximation. This reduces to the application of the FFGR for transition rates.

Considering the representation Eq. (3.11) for the scattering potential in the Floquet frame of reference, the effect of higher orders can be understood as follows: Firstly, it will renormalise the quasi-energy of the states via terms of form \( V^{n,m}_\alpha \beta \cdots V^{m',n'}_{\beta',\alpha'} \) with \( V^{n,m}_\alpha \beta = \langle \phi^m_{0,\alpha} | \hat{V} | \phi^n_{0,\beta}\rangle \), i.e. transitions that return via a number of intermediate states back to the original state. Secondly, there will be couplings of the form \( V^{n,m}_\alpha \beta \cdots V^{m',n'}_{\beta',\gamma} \) that couple two different states \( \alpha \) and \( \gamma \) via a number of intermediate states. In the most generic case, the direct matrix element \( V^{n,m}_{\alpha,\gamma} \) does not vanish for any combination of \( \alpha, \gamma, n \) and \( m \), i.e. transitions between all states with an arbitrary photon transfer \( n - m \) is already allowed in first order. If this is the case, the first order terms are expected to be dominant for weak interactions. If the direct transition were forbidden the second order term would become relevant and give the leading behaviour.

### 3.2.1. Floquet Fermi Golden Rule

The extension of Fermi’s golden rule to the Floquet framework was presented in [195]. Since it will be central to the applications described below, we present a simple derivation of the FFGR following from the Floquet propagator in Eq. (3.10).
We consider a case in which $\hat{V}$ is switched on at $\tau = 0$ and compute transition rates from an initial state $|\Psi_i\rangle$ to a final state $|\Psi_f\rangle$. We take the initial state at $\tau = 0$ and the final state at all times to be Floquet eigenstates of the unperturbed Hamiltonian $\hat{H}_0(\tau)$, i.e. $|\Psi_i(\tau = 0)\rangle = |\Phi_{0,i}\rangle(\tau = 0)$ and $|\Psi_f(\tau)\rangle = e^{-iH_0\tau}|\Phi_{0,f}\rangle(\tau)$. For notational simplicity we drop this subscript indicating the states to be eigenstates of the unperturbed Hamiltonian in the following.

Thus, the amplitude of interest is

$$A(i \rightarrow f, \tau) = \langle \Psi_f(\tau) | U(0, \tau) | \Psi_i(\tau = 0) \rangle$$

$$= \langle \Psi_f(\tau) | \hat{U}_0(0, \tau)\hat{U}^\dagger(0, \tau) | \Psi_i(\tau = 0) \rangle$$

$$= \langle \Psi_f(\tau = 0) | \hat{U}^\dagger(0, \tau) | \Psi_i(\tau = 0) \rangle.$$  

Using the expansion up to first order of the time-evolution operator $\hat{U}^\dagger(0, \tau)$ we obtain for the transition amplitude in the case of $i \neq f$

$$A(i \rightarrow f, \tau) = \frac{-i}{\hbar} \int_0^\tau d\tau' \langle \Psi_f(0) | \hat{\Phi}(\tau') | \Psi_i(0) \rangle$$

$$= \frac{-i}{\hbar} \int_0^\tau d\tau' \langle \Psi_f(0) | \hat{U}_0(\tau', 0)\hat{U}^\dagger(0, \tau') | \Psi_i(0) \rangle$$

$$= \frac{-i}{\hbar} \int_0^\tau d\tau' e^{-i(\epsilon_i - \epsilon_f)\tau'/\hbar} \langle \Phi_i(\tau') | \hat{\Phi}(\tau') \rangle$$

$$= \sum_{n,m} \frac{-i}{\hbar} \int_0^\tau d\tau' e^{-i(\epsilon_i - \epsilon_f - (n-m)\omega)\tau'/\hbar} \langle \phi_{im}^m | \hat{\Phi}(\tau') \rangle$$

$$= \sum_{n,m} \frac{e^{-i(\epsilon_i - \epsilon_f - (n-m)\omega)\tau'/\hbar}}{(\epsilon_i - \epsilon_f - m\omega)} V^m_{ni}$$

$$= \sum_{l,m} \frac{e^{-i(\epsilon_i - \epsilon_f - m\omega)\tau'/\hbar}}{(\epsilon_i - \epsilon_f - m\omega)} V^{m+l}_{ni}$$

where to get from Eq. (3.16) to Eq. (3.17) we used the spectral representation of the propagator Eq. (3.2) and the orthogonality of the Floquet modes at equal times. In Eq. (3.19) we have defined the matrix-element $V^m_{ni} = \langle \phi_{im}^m | \hat{\Phi}(\tau') \rangle$ of the perturbation $\hat{V}$ between the $n$-th Fourier component $|\phi_{in}^n\rangle$ of the initial Floquet mode $|\Phi_i(\tau)\rangle = \sum_n e^{i\omega_n \tau} |\phi_{in}^n\rangle$ and the $m$-th Fourier component $|\phi_{im}^m\rangle$ of the final Floquet mode $|\Phi_f(\tau)\rangle = \sum_m e^{i\omega_m \tau} |\phi_{im}^m\rangle$. 

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\[ \sum_m e^{im\omega \tau} |\psi_m^f\rangle. \]

From the transition probability, \( P(i \rightarrow f, \tau) = |A(i \rightarrow f, \tau)|^2 \), one derives the FFGR by computing the rate \( \gamma_{i \rightarrow f} = \lim_{\tau \rightarrow \infty} P(i \rightarrow f, \tau)/\tau \). In contrast to the derivation of the usual Fermi golden rule, the amplitude contains two sums over the Fourier components of the Floquet modes. The sum over \( m \) allows the emission/absorption of energy quanta \( m\hbar\omega \) during the scattering process. In computing the transition rates, \( m \) is fixed by the resonance condition \( \epsilon_i - \epsilon_f = m\hbar\omega \). With this in mind the standard steps lead to

\[ \gamma_{i \rightarrow f} = \sum_{m,l,n} \frac{2\pi}{\hbar} \delta(\epsilon_i - \epsilon_f - m\hbar\omega) V_{if}^{nn+m} V_{fi}^{l+m}. \]  

(3.21)

As a final step we may rewrite this in a more convenient form as

\[ \gamma_{i \rightarrow f} = \sum_m \frac{2\pi}{\hbar} \delta(\epsilon_i^0 - \epsilon_f^0 - m\hbar\omega) |\langle \Phi_m^f | \hat{V} | \Phi_0^i \rangle|^2 \]  

(3.22)

where \( |\Phi_m^f(\tau)\rangle = e^{im\omega \tau} |\Phi_0^f(\tau)\rangle \) are the shifted Floquet modes. Written in this way the rate has the same form as the conventional Fermi's golden rule apart from the additional summation over \( m \) and the use of the extended scalar product. The explicit sum over \( m \) justifies the remarks that only quasi-energy is conserved or equivalently that energy is only conserved up to quanta of \( \hbar\omega \). Transitions with the absorption/emission of \( m\hbar\omega \) will occur within the FFGR if \( V_{if}^{nn+m} = \langle \delta_f^n | \hat{V} | \delta_i^{n+m} \rangle \neq 0 \) for some \( n \), i.e. if the interaction couples different Fourier components of the Floquet modes.

3.2.2. Inelastic Scattering

In light of the fact that for a time-periodic Hamiltonian only the quasi-energy is conserved, it is important to consider the definition of “inelastic scattering” in these circumstances. One obvious choice for the quasi-energies is to reduce them to a BZ, i.e. to choose \( -\hbar\omega/2 < \epsilon_i^0 \leq \hbar\omega/2 \). However, this choice may be inconvenient and even hide some of the relevant physics. We illustrate this by describing two simple examples.
3. Scattering Theory for Floquet-Bloch States

Single-particle Floquet scattering in an unbounded dispersion

As a first example consider a single particle for which the Floquet energy spectrum of $\hat{H}_0(\tau)$ consists of Floquet-Bloch waves with a parabolic energy dispersion as a function of the dimensionless wavevector $k$, with $e_k^0 = \hbar\omega(k^2 - 1/2)$, which we display in Fig. 3.2\(^2\). The single-particle states of this unperturbed time-periodic Hamiltonian can be fully described by an energy dispersion that is a continuous function of wavevector $k$. Within the Floquet framework, one can equally well choose to reduce the quasi-energies to a BZ, shown as the set of bold curves in Fig. 3.2. In terms of the reduced quasi-energies the dispersion is discontinuous and there is a discrete infinite set of quasi-energetically degenerate momenta. When a potential $\tilde{V}$ that breaks translational symmetry is introduced, it can cause one-body scattering from an initial state (e.g. the red dot) to the final states of the same quasi-energy (e.g. the green or blue dots). Given the simple nature of the parabolic energy dispersion for the unperturbed single particle, it is natural to call the transition to a different branch “inelastic” (red to blue) and the transition staying within the same branch “elastic” (red to green). This may be conveniently achieved by defining $e_k^0 = \hbar\omega(k^2 - 1/2)$ to depend continuously on the dimensionless wavevector $k$ (i.e. not to be restricted to $-\hbar/\omega < e_k^0 \leq \hbar\omega/2$), and by considering the whole family of periodically repeated dispersions (the dashed lines in Fig. 3.2): “inelastic” scattering (i.e. between different branches) then corresponds to a change in the Floquet index $m$.

Two-particle Floquet scattering in a bounded dispersion

The relevance of these considerations becomes even more apparent for two-particle scattering. As a second example, we consider scattering of two particles occupying an energy band (on a lattice) that has a bounded dispersion, e.g. each particle experiences the band structure of the form $e_k^0/(\hbar\omega) = -0.4 \cos(k)$ depending on the dimensionless quasimomentum $k$, shown in Fig. 3.3 with its periodic repetitions\(^3\). From a naive interpretation

\(^2\)The dimensions and energy offset are chosen for presentational convenience. We shall present a model leading to a similar case in Section 3.3 below.

\(^3\)We discuss a model in a 1D lattice leading to a similar dispersion in Section 3.4.2. The explicit value of 0.4 is chosen for presentational convenience, any value such that twice the bandwidth is larger than...
3.2. Scattering Theory in the Floquet Framework

Figure (3.2) Unbounded single-particle dispersion $\frac{\epsilon_k^0}{(\hbar \omega)} \propto k^2$ as a function of dimensionless wavevector $k$ reduced to the first BZ (bold) and continuous dispersion with periodically repeated images (dashed). Scattering an initial state (red/middle) to final state (green/left) would be considered elastic and scattering from initial state (red/middle) to a different branch (blue/right) would be considered inelastic. When regarding these processes with respect to the continuously defined dispersions, elastic scattering corresponds to no change in the Floquet index $m$ whereas inelastic scattering changes $m$.

of the single-particle spectrum, in which one ignores the periodically repeated spectra, one would say that two particles at the bottom of the band $k = 0$ with quasi-energy $\epsilon = -0.4\hbar \omega$ would be forbidden from scattering by energy conservation. However, the total two-particle energy is $\epsilon_2 = -0.8\hbar \omega$ which would have to be mapped to a quasi-energy $0.2\hbar \omega$ to lie in the range $(-\hbar \omega/2, \hbar \omega/2)$. Thus, scattering is in fact allowed to a number of states for which $\epsilon^0(k_1) + \epsilon^0(k_2) = 0.2\hbar \omega$. One such possible scattering event is depicted in the figure where the two initial particles in the band minimum (red) scatter to a final state (blue). One might also consider the reduced two-particle dispersion, which is shown with contours in Fig. 3.3. Clearly, scattering from the centre to arcs around the corners of the BZ now becomes possible, so two particles in the band minimum are not stable anymore. Those are processes that become allowed only within the Floquet description and will be called inelastic. If the (two-particle) quasi-energies are defined to be continuous with respect to the variable $k$ those correspond to a term $m \neq 0$. For example, using the viewpoint of the repeated zone for the quasienergy, the above scattering process

$h\omega$ would do.
3. Scattering Theory for Floquet-Bloch States

![Figure (3.3)](image)

**Figure (3.3)** (a) Bounded single-particle dispersion $\epsilon(k)/(\hbar\omega) = -0.4 \cos(k)$ as a function of dimensionless quasimomentum $k$ in the energy BZ with periodically repeated images (b) contours of the reduced two-particle quasi-energy $\epsilon(k_1) + \epsilon(k_2)$. Depicted is a two-particle scattering process during which two particles initially in the band-minimum (red balls) scatter into higher quasi-energy states (blue balls). This process conserves the reduced two-particle quasi-energy or equivalently can be viewed as one particle scattering into the lower shifted dispersion (grey ball).

involves the transition of one particle (depicted grey in Fig. 3.3) to a copy of the Floquet band shifted down by $\hbar\omega$ (i.e. a transition with $m = 1$).

**Conclusions for generic Floquet scattering**

Based on these examples, and the applications below, we provide a general definition of “inelastic scattering” of Floquet-Bloch waves. We consider the Floquet-Bloch spectrum for a single particle, and define the quasi-energy for $m = 0$, $\epsilon_{k,\sigma}^0$, to be a continuous function of the wavevector $k$ (which will be a vector in dimensions $d > 1$). The index $\sigma$ accounts for any other discrete quantum numbers – e.g. band, or spin indices – which characterize the Floquet-Bloch state. The full set of Floquet modes is obtained via $\epsilon_{k,\sigma}^m = \epsilon_{k,\sigma}^0 + m\hbar\omega$. In any scattering event, the particle (or particles) must start and finish in states labelled by these indices $(k,\sigma,m)$ (at long times before and after the collision). We define all those scattering events which involve a change of either the discrete label $\sigma$ or of the Floquet index $m$ (or both) to be “inelastic”. This definition of inelastic scattering accounts both for collisions in which the band index (of one or both) particles changes, and for collisions
that would not have occurred under a naive interpretation of the energy bands where
the repeated copies spaced by $\hbar\omega$ are ignored.

At this point it is again useful to recall the discussion of energy and quasi energy in
Section 2.1. In the cases we will be considering below the quasi energies contains a
contribution corresponding to the energy of free particle motion. In that case it is sensible
to consider the Hamiltonian of free particles as a reference with respect to which it is
meaningful to say the kinetic energy of a state changed during a Floquet scattering event
and this occurs exactly if the momentum of the particle changed during the scattering
process. Equivalently, one may consider particles prepared in some bandstructure $E_\sigma$
with discrete indices $\sigma$ of a static Hamiltonian, add a time-dependent perturbation, and
ask after scattering in which bands of the static Hamiltonian the particles end up. This
assumes that the time-dependent perturbation is either localised in time or in space, such
that the description via the static Hamiltonian makes sense at either long times after the
collision or after particles have left the interaction region.

3.3. Toy Model

To illustrate the preceding discussion of the scattering properties of Floquet states, we
consider a toy model for scattering in the presence of Raman dressing of internal states.
We consider a single particle (or relative particle co-ordinate) with two internal states,
and the Hamiltonian $\hat{H}(\tau) = \hat{H}_0(\tau) + \hat{V}$ with

$$\hat{H}_0(\tau) = \frac{\hat{p}^2}{2M} \mathbb{1} + \begin{pmatrix} 0 & \Omega e^{i\omega \tau} \\ \Omega e^{-i\omega \tau} & \hbar \omega \end{pmatrix}. \quad (3.23)$$

A physical implementation would be provided by shining a laser beam on an atom with
mass $M$. We restrict the atomic dynamics to only two states $|g\rangle$ and $|e\rangle$, which are
coupled with strength $\Omega$ by a laser with frequency $\omega$. We assume the laser frequency
to be resonant with the transition frequency between the groundstate $|g\rangle$ and the elec-
tronically excited state $|e\rangle$. Further assuming that the lifetime of the excited state $|e\rangle$
is long compared to the timescales we are considering, we may neglect spontaneous
emission.
As the simplest interaction we may consider an immobile scatterer at the origin

\[ \hat{V} = \delta(x) \begin{pmatrix} g_0 + g_1 & g_c \\ g_c & g_0 - g_1 \end{pmatrix}, \] (3.24)

where we assume that the different atomic levels \(|g\rangle\) and \(|e\rangle\) interact with a state dependent strength \(g_0 + g_1\) and \(g_0 - g_1\) respectively, and that the scatterer couples the different states with a strength \(g_c\). In the interpretation of a relative particle coordinate the internal states \(|\psi\rangle\) and \(|\bar{e}\rangle\) would correspond to internal states for the two-atom system, the laser coupling would have to be between these molecular states, and the interaction \(\hat{V}\) could arise from contact interactions between the atoms.

The Floquet modes of the non-interaction system are given as

\[ \Phi^m_{k,\sigma} = \frac{1}{\sqrt{2L}} e^{i\omega\tau} e^{ikx} \begin{pmatrix} 1 \\ \sigma e^{-i\omega\tau} \end{pmatrix} \] (3.25)

with quasi-energies \(\epsilon^m_{k,\sigma} = \frac{\hbar^2 k^2}{2M} + \sigma \Omega + m\hbar\omega\), where \(L\) is the system size and labels are the momentum \(k\), the band index \(\sigma = \pm 1\) and the Floquet mode number \(m\). Note that this actually corresponds to two shifted copies of a single parabolic dispersion which is shown in Fig. 3.2 and for which the implications within the Floquet framework have been outlined above.

We begin the discussion of scattering by a treatment within the FFGR. The rate of scattering from an initial state \(\Psi_i\) to a final state \(\Psi_f\) is given by Eq. (3.22) as described in Section 2.1. The argument of the quasi-energy conserving \(\delta\)-function reads

\[ \frac{\hbar^2 k^2}{2M} = \frac{\hbar^2 k^2}{2M} + (\sigma_i - \sigma_f)\Omega - m\hbar\omega \] (3.26)

which shows that a transition to a final state with \(m < 0\) (\(m > 0\)) corresponds to an absorption (emission) of energy \(m\hbar\omega\) from the driving field. This may be converted into kinetic energy or into a change of the bands, or both. Transitions with \(m = 0\) can still convert the difference between the band energies into kinetic and vice-versa, but the total energy of the states remains the same.
3.3. Toy Model

We take the initial and final state to be \( \Phi_i = \Phi_{k_i, \sigma_i}^0 \) and \( \Phi_f = \Phi_{k_f, \sigma_f}^m \) and the matrix element is computed as

\[
\langle \langle \Phi_f^m | \hat{V} | \Phi_i^0 \rangle \rangle = \frac{1}{(2L)^2} \delta_{m,0} \left[ (g_0 + g_1) + (g_0 - g_1) \sigma_i \sigma_f \right]
\]  

(3.27)

As the Floquet modes (Eq. (3.25)) contain two frequency components at \( m \) and \( (m + 1) \), single-particle scattering within the FFGR allows at most the absorption of a single quantum \( \hbar \omega \). Moreover, clearly for \( g_c = 0 \) no processes with absorption of energy from the laser field take place, i.e. there is no change in the Floquet index \( \Delta m = 0 \), and particles can only scatter between the two bands. However, for \( g_c \neq 0 \) particles can absorb energy during scattering \( \Delta m \neq 0 \).

The elastic scattering rate is given by

\[
\gamma_{k_i, \sigma_i \rightarrow k_f, \sigma_f} = \frac{1}{L} \frac{2\pi}{\hbar} |g_0|^2 \rho_{\sigma}(e_i).
\]  

(3.28)

with the density of states \( \rho_{\sigma}(e) \) defined for the single particle dispersion \( e_{k, \sigma}^0 \) per unit length, i.e. \( \rho_{\sigma}(e) = 1/L \sum_k \delta(e - e_{k, \sigma}^0) \). For the inelastic rates we distinguish between those processes which only convert kinetic energy into band energy and vice versa which for our basis choice correspond to no change in \( m \) and those that change \( m \).

The inelastic rate for band changing collisions with no change in the Floquet index \( m \) is

\[
\gamma_{k_i, \sigma_i \rightarrow k_i, \sigma_i} = \frac{1}{L} \frac{2\pi}{\hbar} |g_1|^2 \rho_{\sigma}(e_i),
\]  

(3.29)

assuming that a band-changing transition is energetically allowed by Eq. (3.26) with \( m = 0 \). The inelastic scattering rate with a change in Floquet index \( m \) by 1 is given by

\[
\gamma_{k_i, \sigma_i \rightarrow k_f, \sigma_f} = \frac{1}{2L} \frac{\pi}{2\hbar} |g_c|^2 \rho_{\sigma}(e_i \pm \hbar \omega).
\]  

(3.30)

In 1D the corresponding cross sections read \( \sigma_{el} = \frac{2M^2 \hbar^4}{\pi^2 k^2} \) for elastic collisions for which \( k = k_i = \pm k_f \). For band changing collisions with no change in Floquet index we obtain \( \sigma_{inel}^{m=0} = \frac{2M^2 \hbar^4}{\pi^2 k_i k_f} \) where \( k_i \) and \( k_f \) satisfy Eq. (3.26) with \( m = 0 \). The inelastic scattering cross section for absorption/emission of \( \hbar \omega \) is \( \sigma_{inel}^{m \neq 0} = \frac{2M^2 \hbar^4}{4\pi^2 k_i k_f} \) where \( k_i \) and \( k_f \) satisfy
3. Scattering Theory for Floquet-Bloch States

Eq. (3.26) with \( m = \pm 1 \). The divergences in the cross sections at low energies (small \( k_i \)) stem from two factors. Firstly from the division by the incoming flux which accounts for the \( 1/k_i \) factor present in all cross sections, and secondly from the final density of states which is proportional to \( 1/k_f \) in 1D.

We assume a regime in which changes of the bands are not allowed in collisions without absorption of energy, i.e. initial particles in the lower band with \( \epsilon_i < 2\Omega \). Further we restrict to \( \epsilon_i < \hbar \omega \) and \( \hbar \omega > 2\Omega \), such that emission of a photon during scattering is not possible and scattering between bands becomes allowed with the absorption of a photon. In that case the ratio of the total cross sections is given by

\[
\frac{\sigma_{1D}^{inel}}{\sigma_{1D}^{el}} = \frac{g_c^2}{4g_0^2} \left[ \frac{1}{\sqrt{1 + \hbar \omega / \epsilon_i^{\text{kin}}} + \frac{1}{\sqrt{1 + (\hbar \omega - 2\Omega) / \epsilon_i^{\text{kin}}}}} \right]
\]

(3.31)

with \( \epsilon_i^{\text{kin}} = \hbar^2 k_i^2 / (2M) \). These expressions suggest that to achieve strong elastic scattering as compared to inelastic scattering it is advantageous to work at small \( \epsilon_i^{\text{kin}} \). However, at very low energies the Born-Approximation becomes invalid, certainly breaking down when \( \sigma_{el} \gtrsim 1 \), thus for \( \epsilon_i^{\text{kin}} \lesssim \frac{M g_c^2}{2e} \). Using this value in Eq. (3.31) we obtain a natural lower limit for the ratio of inelastic to elastic cross sections. We remark that in 1D the Born approximation for the \( \delta \) potential becomes exact only in the limit of large momenta. Therefore, the divergence observed above for low energies is expected, and we cannot access the regime of collisions at low initial momenta.

The corresponding expression in 2D is

\[
\frac{\sigma_{2D}^{inel}}{\sigma_{2D}^{el}} = \frac{g_c^2}{4g_0^2} \times 2,
\]

(3.32)

where the factor of 2 is due to the fact that the inelastic scattering cross section has two contributions from the band-changing and the band-conserving scattering processes. Thus, in 2D there is no energy dependence, and the relative size of inelastic and elastic scattering is simply controlled by the ratio of the relevant interaction parameters. In 3D
3.3. Toy Model

one finds

$$\frac{\sigma_{\text{inel}}^{3D}}{\sigma_{\text{el}}^{3D}} = \frac{g_c^2}{4g_0^2} \left[ \sqrt{1 + \hbar \omega / \epsilon_i^{\text{kin}}} + \sqrt{1 + (\hbar \omega - 2\Omega) / \epsilon_i^{\text{kin}}} \right] \tag{3.33}$$

which shows that inelastic scattering becomes increasingly important compared to elastic scattering at low kinetic energies. Unless $g_c/g_0$ is very small, this could lead to experimental difficulties in achieving stable strongly correlated phases of dressed-state particles at low energies in 3D settings. This model provides a simple example of how the suppression of inelastic compared to elastic scattering for low-energy particles may be favoured by the confinement of free motion to low dimensions. In 3D, the strength of the $\delta$-potential is related to the physical scattering length via $g \sim a_s$. Moreover, the exact scattering amplitude in the limit of $k a_s \ll 1$ is given by $a_s$ which coincides with the result given by the Born approximation. Therefore, the Born approximation becomes exact for $gk \ll 1$ which is the limit we are considering.

We emphasize that the inelastic scattering rate and cross sections only depend on $\omega$ via the final density of states. In particular, in the limit $\omega \to \infty$, the rate vanishes in 1D, but is constant in 2D and divergent in 3D. We note that taking the limit $\omega \to \infty$ also implies that the final momenta increase as $k_f \sim \sqrt{\omega}$. In 1D this actually implies that the Born-approximation becomes exact, but in 3D we leave the regime of validity of the Born approximation. However, a more careful limit scaling the amplitude of the interaction potential as $g \sim 1/\sqrt{\omega}$ ensures that $k_f g \ll 1$ and the Born approximation remains valid. This scaling does not affect the considered ratio of elastic to inelastic scattering, thus, our conclusions remain unchanged. Thus, the dynamics in higher than 2 dimensions cannot possibly be described by an average Hamiltonian even for $\omega \to \infty$, but rather inelastic scattering with an infinitely high energy transfer occurs in this case. In view of the contact interaction, the matrix element remains nonzero for arbitrarily high momentum transfer, hence arbitrarily large final state energy. We emphasise that in the case of the real physical potential this would be cut-off at some maximal energy scale corresponding to a microscopic length scale of interaction potential. In addition, higher angular momentum channels will become relevant at higher energies and using the approximation via a $\delta$-potential ceases to be valid.

We now consider the effects of higher orders of the scattering potential. From the Dyson series, Eq. (3.9), one can see that to order $\hat{V}^n$ transitions with an energy absorp-
tion/emission of $n\hbar\omega$ are allowed for this specific model if $g_c \neq 0$. However, in this case it is more transparent to perform a unitary transformation to the eigenstates of the non-interacting Hamiltonian.

$$\tilde{H} = \hat{U}^\dagger \hat{H} \hat{U} - i\hbar \hat{U}^\dagger \partial_\tau \hat{U}$$

$$= \frac{\hat{p}^2}{2M} \mathbb{1} + \begin{pmatrix} \Omega & 0 \\ 0 & -\Omega \end{pmatrix} + \tilde{V}(\tau)$$

(3.34)

with

$$\tilde{V}(\tau) = \begin{pmatrix} g_0 & g_1 \\ g_1 & g_0 \end{pmatrix} + g_c \begin{pmatrix} \cos \omega \tau & i \sin \omega \tau \\ -i \sin \omega \tau & \cos \omega \tau \end{pmatrix}.$$  

(3.35)

In this representation $\tilde{V}(\tau)$ contains two frequency components at $\pm \omega$ and at order $\tilde{V}(\tau)^n$ allows the absorption of $n\hbar\omega$ of energy. This derivation has the additional advantage that it provides a natural explanation for the inelastic scattering in this model. Whenever the unitary transformation that diagonalises the time-periodic non-interacting Hamiltonian $\hat{H}_0(\tau)$ commutes with the interaction $\hat{U}^\dagger \hat{V} \hat{U} = \hat{V}$ (or, more generally, leaves it time-independent) no inelastic scattering can occur. This exactly corresponds to the case in which $\hat{V}(\tau)$, Eq. (3.6), only picks up the trivial phase dependence due to the difference in quasi-energies. We also note that in this frame the model corresponds to the scenario shown in Fig. 3.1, of time-independent states with fixed energy scattering through a time-periodic potential.

This toy model is special in two aspects. Each Floquet mode contains only two frequency components, because the Hamiltonian contains only rotating-wave terms. Moreover, in the internal state basis each internal state component has a single oscillation frequency. As a consequence, inelastic scattering only occurs if these internal states are coupled by the interaction, i.e. if $g_c \neq 0$. If one adds counter-rotating terms to the Hamiltonian, the Floquet modes do in fact contain all frequency components and inelastic scattering is possible even for $g_c = 0$.

From the discussion of this toy model we draw the following conclusions. Firstly, the scattering properties of a time-periodic Hamiltonian are not encapsulated by some effective time-independent Hamiltonian: of the infinite set of momentum states that have the same quasi-energy, and therefore could be coupled by scattering, we have found
that the rate of coupling depends both on the detailed time-dependence of the Floquet modes and on the structure of the interaction. In particular, the scattering properties of a time-periodic Hamiltonian with frequency $\omega$ cannot be described by an effective “time-averaged” Hamiltonian even in the limit $\omega \to \infty$. Secondly, we have shown how the FFGR may be used to compute transition rates to lowest order in the interaction potential, and that higher order corrections captured by the full Dyson Series can modify the picture emerging from FFGR but do not change the qualitative scattering properties.

3.4. Applications

Following these preliminary considerations, and the development of the formalism of scattering theory for particles in time periodic Hamiltonians, we now turn to discuss applications to situations of physical interest. We shall consider the two-particle scattering processes in cases where the one-particle states are Bloch waves arising from some “dressed” states. We consider two cases that are representative of physical implementations that have recently been studied in experiments: the use of Raman coupling of internal states to generate gauge fields in the continuum; and the use of periodic modulation of site energies to form vector potentials on optical lattices. Our interest will be in the sizes of “inelastic” two-body scattering processes (which have deleterious effects of heating) as compared to the remaining elastic processes (which are required for the formation of strongly correlated phases). Although our approach may be applied to fermions or bosons, or to two distinguishable particles, and may be extended to any general interaction potentials, for simplicity we focus on the case of bosons with contact interactions.

3.4.1. Dressed State Model

We consider a model for the creation of artificial vector potentials in the continuum by dressing of two internal states, $\sigma = \pm$, similar to the experimental implementations [74, 108, 111, 112, 144, 145, 196–198]. However, the states may be either internal (spin)
3. Scattering Theory for Floquet-Bloch States

states of the atomic species coupled by optical transitions or subbands of an additional spatial dimension coupled by a suitable time-periodic potential perturbation \([144, 145]\) \(^4\). In the second case we will not explicitly model the optical potentials used to create these subbands and select them from other bands. Rather, in our model below we will completely suppress this dimension and consider scattering of particles moving along a different dimension. Similar considerations also apply in the case of coupling harmonic oscillator eigenstates as in \([122]\), where now we would have to consider an infinite set of states. For simplicity we will mainly treat the system in one dimension assuming tight confinement in the other two directions. We will briefly comment on the extension to a 2D model by adding free motion in a second dimension.

The system is described by the Hamiltonian \( \hat{H}(\tau) = \hat{H}_0(\tau) + \hat{H}_{\text{int}} \). The non-interacting time-dependent part \( \hat{H}_0(\tau) \) is

\[
\hat{H}_0(\tau) = \int \text{d}x \sum_{\sigma, \sigma'} \hat{\Psi}_{\sigma'}^\dagger(x) \left[ \frac{\hat{p}^2}{2M} \delta_{\sigma', \sigma} + \hat{V}_{\sigma', \sigma}(x, \tau) \right] \hat{\Psi}_\sigma(x),
\]

(3.36)

where \( \hat{\Psi}_\sigma(x) \) is a creation operator for bosons with mass \( M \) in internal state \( \sigma \). The coupling matrix \( \hat{V} \) describes the internal dynamics of the atoms interacting with the laser field. It is given by

\[
\hat{V}(x, \tau) = \hbar/2 \begin{pmatrix} -\Delta & \Omega e^{i\omega \tau + 2ik_r x} \\ \Omega e^{-i\omega \tau - 2ik_r x} & \Delta \end{pmatrix},
\]

(3.37)

with an energy splitting \( \hbar \Delta \) between internal states and the coupling of strength \( \hbar \Omega \) between internal states due to the laser fields taken to be of the rotating wave form. As described in \([108]\) such a system may arise as the effective two-level description of Raman-coupled spin-states in which case the splitting and coupling strength are also to be understood as effective quantities for the two-photon transitions involved. In this case \( \omega \) corresponds to the frequency difference of two Raman lasers and \( k_r \) is the wavelength of the counter propagating Raman lasers. We derive \( \hat{V} \) from the underlying experimental setup in Appendix B.1 discussing the use of the rotating wave approximation and the

\(^4\)Selecting only two bands in an optical lattice requires the bandstructure to be sufficiently anharmonic to not be subject to resonant couplings to higher bands. This has been explicitly checked to be the case in \([144]\).
3.4. Applications

adiabatic elimination of excited states. Importantly, the rotating wave approximation is performed with respect to a frequency corresponding to a groundstate-excited state manifold splitting which is large compared to all remaining quantities in the Hamiltonian and the kinetic energies of the particles.

We consider interactions described by the following Hamiltonian

\[ \hat{H}_{\text{int}} = \frac{1}{2} \int dx \sum_{\sigma} g_\sigma \hat{\Psi}_\sigma^\dagger(x) \hat{\Psi}_\sigma^\dagger(x) \hat{\Psi}_\sigma(x) \hat{\Psi}_\sigma(x) + g_2 \sum_{\sigma} \hat{\Psi}_{1\sigma}^\dagger(x) \hat{\Psi}_{2\sigma}^\dagger(x) \hat{\Psi}_{1\sigma}(x) \hat{\Psi}_{2\sigma}(x) \\
+ g_c \sum_{\sigma} \hat{\Psi}_{1\sigma}^\dagger(x) \hat{\Psi}_{2\sigma}^\dagger(x) \hat{\Psi}_{1\sigma}(x) \hat{\Psi}_{2\sigma}(x) \]

(3.38)

which contains general contact interactions with species-dependent strength \( g_\sigma \), interspecies coupling with strength \( g_2 \) and species-changing coupling with strength \( g_c \). The relative sizes of these couplings depend on the physical origin of the two internal states. For two (hyperfine) spin states, the \( g_c \) term does not conserve the spin projection and is therefore not present if spin-rotation symmetry is preserved\(^5\). However, if the two internal states are two states of position motion – for example two vibrational sub-bands [144, 145] – then \( g_c \) is proportional to the usual contact interaction modified by a geometric factor describing the wave function overlap between bands. In the specific case of Refs. [144, 145] the two internal states are the \( s \)- and \( p \)-bands of an optical lattice, and the couplings are \( g_\sigma \propto g \int dx |w_\sigma(x)|^4 \), \( g_2 \propto g \int dx |w_\sigma(x)|^2 |w_p(x)|^2 \) and \( g_c \propto g \int dx w_s^*(x) w_s^*(x) w_p(x) w_p(x) \) where \( g \) is the appropriate one-dimensional contact interaction strength and \( w_\sigma \) the Wannier orbital of the band \( \sigma = s(p) \). Thus, the couplings \( (g_\sigma, g_2 \text{ and } g_c) \) are all non-zero and of comparable magnitude. In the case of coupling harmonic oscillator eigenstates [122], all internal states would be coupled by contact interactions. We note that keeping the term \( g_c \) that couples states that are split by \( \hbar \Delta \), but not the counter-rotating terms for the Raman lasers is consistent as the rotating wave approximation is performed on a larger frequency scale \( \omega_L \gg \Delta \) as detailed in Appendix B.1.

\(^5\)We note that for strong dipolar interactions, such processes are allowed for spin states, with the internal angular momentum taken up by relative orbital angular momentum of the two particles.
Single-Particle States

Our discussion of the single particle states follows the one given in [70] with the main exception that the explicit time-dependence of the states is kept within the Floquet theory description.

The non-interacting Hamiltonian \( \hat{H}_0 \) couples only two components and can be expressed with respect to the operators \( \hat{\phi}^\dagger_1(k) = \hat{\phi}^\dagger_{1,k+k_r} \) and \( \hat{\phi}^\dagger_2(k) = \hat{\phi}^\dagger_{2,k-k_r} e^{-i\omega t} \), where \( \hat{\phi}^\dagger_{\sigma,k} \) creates an internal state \( \sigma \) particle in a plane-wave state. \( \hat{H}_0 \) reduces to a sum over independent \( 2 \times 2 \) blocks of the form

\[
\hat{H}_0(k) = \begin{pmatrix}
\frac{\hbar^2(k+k_r)^2}{2M} - \hbar \delta / 2 & \hbar \Omega / 2 \\
\hbar \Omega / 2 & \frac{\hbar^2(k-k_r)^2}{2M} + \hbar \delta / 2
\end{pmatrix}
\]

(3.39)

where \( \hbar \delta / 2 = \hbar \Delta / 2 - \hbar \omega / 2 \) and an overall constant energy shift \( \hbar \omega / 2 \) was dropped. Note that this implies that the eigenstates will be mixtures of different (internal) states at different momenta where the composition will depend on the quasi-momentum \( k \).

We choose the recoil energy \( E_r = \hbar^2 k_r^2 / 2M \) as the unit of energy and \( k_r \) as the unit of momentum defining dimensionless parameters \( \tilde{\Omega} = \hbar \Omega / E_r, \tilde{\delta} = \hbar \delta / E_r \) and \( \tilde{k} = k / k_r \). The Hamiltonian becomes

\[
\hat{H}_0(k) = E_r \begin{pmatrix}
(\tilde{k} + 1)^2 - \tilde{\delta} / 2 & \tilde{\Omega} / 2 \\
\tilde{\Omega} / 2 & (\tilde{k} - 1)^2 + \tilde{\delta} / 2
\end{pmatrix}
\]

(3.40)

and the Floquet modes are

\[
\Phi^m_{k,\sigma} = N_{k,\sigma} \begin{pmatrix}
\tilde{\delta} + 4\tilde{k} + \sigma \sqrt{\tilde{\Omega}^2 + \left(4\tilde{k} - \tilde{\delta}\right)^2} \\
\tilde{\Omega}
\end{pmatrix} e^{in\omega t}
\]

(3.41)

with the normalisation factor

\[
N_{k,\sigma} = 1 / \sqrt{L} \left[ \left(\tilde{\delta} + 4\tilde{k} + \sigma \sqrt{\tilde{\Omega}^2 + \left(4\tilde{k} - \tilde{\delta}\right)^2} \right)^2 + \tilde{\Omega}^2 \right]^{-1/2}
\]

(3.42)

for a system of size \( L \). Defining the components of the \( \sigma = \pm \) eigenvector with respect
Figure (3.4) Dispersion $E/E_r$ as a function of $k/k_r$, see Eq. (3.44), including an energy offset to have zero minimum. The top row shows the dispersion for $\hbar \delta/E_r = 0$ and $\hbar \Omega/E_r = 1$ in (a) and $\hbar \Omega/E_r = 4$ in (b), the bottom row (c) and (d) for the same parameters in the case of $\hbar \delta/E_r = 1$. Colourcoded is the expectation value $\langle S_z \rangle$ with $S_z = \text{diag}(-1, 1)$ in the $\sigma = \pm$ basis.

Note at this point that the coupling in the rotating wave approximation leads to a wave function in which each component in the internal state basis has a single oscillation frequency, i.e. $m \omega$ and $(m+1) \omega$ for the components of $\Phi^m_{k,\sigma}$. As a consequence, inelastic scattering processes can only occur if these internal states are coupled by the interaction as we have seen in the discussion of the toy model in Section 3.3.
The corresponding quasi-energies are

\[
\epsilon_{k,\sigma}^m = E_r \left[ \tilde{k}^2 + \sigma \sqrt{\tilde{\Omega}^2 + \left( 4\tilde{k} - \delta \right)^2} \right] + m\hbar\omega. \tag{3.44}
\]

The dispersion for different characteristic values of the parameters is shown in Fig. 3.4. Firstly, for no detuning \(\hbar\delta/E_r = 0\) both bands are symmetric around \(k/k_r = 0\). The character of the lower band changes as a function of \(\hbar\Omega/E_r\) as we discuss in the following. For \(\hbar\Omega/E_r < 4\) (left column of the Fig. 3.4) it has three distinct extrema of which the one at \(k/k_r = 0\) is a maximum and two global degenerate minima at \(k/k_r = \pm |k_0|\). For \(\hbar\Omega/E_r \geq 4\) (right column of Fig. 3.4) it only has a single global minimum at \(k/k_r = 0\). The gap between upper and lower band is in both cases given by \(\hbar\Omega\). For non-zero detuning, both bands become skewed lifting the symmetry under \(k \to -k\) and the degeneracy between the minima of the lower band present for \(\hbar\Omega/E_r < 4\). The shift of the minimum of the dispersion to non-zero \(k\) can be interpreted as due to the induced artificial magnetic field [69]. In particular, for small momenta the dispersion is quadratic around this minimum and thus directly corresponds to the dispersion of a charged particle in a magnetic field.

Note that the non-interacting Hamiltonian \(\hat{H}_0\) is invariant under two continuous symmetry operations: modified spatial translations generated by \(O_\hat{p} = \hat{1}\hat{p} + k_r\hat{\sigma}_z\), and modified temporal translations generated by \(O_\hat{E} = \hat{1}i\hbar\partial_\tau - \hbar\omega\hat{\sigma}_z/2\) where \(\hat{\sigma}_z = \text{diag}(1, -1)\) denotes the third Pauli matrix. The corresponding finite symmetry operations are translations multiplied by a state dependent phase factor, \(\text{diag}(e^{ik_r a}, e^{-ik_r a})\hat{T}_{x \to x+a}\) and \(\text{diag}(e^{-i\omega a/2}, e^{i\omega a/2})\hat{T}_{\tau \to \tau+a}\). These symmetries imply the conservation of both the momentum \(k\) and the energy \(E\). The single-particle states can thus be characterised by their momentum \(k\) and energy \(E\), both of which can take unbounded values: there is no BZ for momentum or energy, owing to the existence of these continuous symmetries. It is for this reason that no BZ structure (in energy or momentum) appears in Fig. 3.4.
Figure (3.5) Sketch of the generic scattering processes we are considering for the states defined in Eq. (3.43) with quasi-energies given in Eq. (3.44). The initial state consists of two particles in the lower band (red) and depending on the frequency $\omega$ and model parameters three different scattering processes may be allowed, with both particles remaining in the lowest band (light blue), one particle being scattered into the second band (blue) and both particles ending up in the higher band (deep blue). Black arrows indicate the spin-composition of the single-particle states. Colourcoded is the expectation value $\langle S_z \rangle$ with $S_z = \text{diag}(-1, 1)$ in the $\sigma = \pm$ basis.

Two-body scattering

We now study whether, through their mutual interaction, two particles that both start in plane-waves states in the lower band can undergo scattering into the higher band or scattering into higher quasi-momentum states in the same band via the absorption of energy quanta $h\omega$ from the time-dependent fields. The generic situation we are considering is shown in Fig. 3.5. The initial state is given by two particles in the lower band (red) and depending on the frequency $\omega$ and model parameters three different scattering processes may be allowed, with both particles remaining in the lowest band (light blue), one particle being scattered into the second band (blue) and both particles ending up in the higher band (deep blue).
In discussing the two-body scattering, it is interesting to consider the interplay of the interparticle interaction \( \hat{H}_{\text{int}} \) and the above finite symmetry operations. One finds that these symmetries commute with the \( g_\alpha \) and \( g_2 \) terms, but that both symmetries are broken by the \( g_c \) coupling term. However, there remains a discrete symmetry, namely, when including the \( g_c \) interaction term the full Hamiltonian is still invariant under discrete spatial and temporal translations by \( x \to x + \pi/k_r \) and \( \tau \to \tau + 2\pi/\omega \). Thus, while in the non-interacting model both momentum \( k \) and energy \( E \) are strictly conserved, in the presence of the \( g_c \) interaction term scattering processes that change the momentum by integer multiples of \( 2k_r \) and the energy by multiples of \( \hbar\omega \) are allowed; or, put differently, for \( g_c \neq 0 \) only quasi-momentum and quasi-energy remain conserved quantities.

We compute the two-body scattering rate using the FFGR (Eq. (3.22)). We take two particles in the lower band \( \Phi_{m,k,-} \) with their momentum centred at the minimum \( k_0 \) of the single-particle dispersion, i.e. \( k_1 = k_0 + k \) and \( k_2 = k_0 - k \) respectively, as the initial state, i.e.

\[
|\psi_i\rangle = \hat{\Psi}_{k_1,-}^\dagger \hat{\Psi}_{k_2,-}^\dagger |\text{vac}\rangle,
\]

with quasi-energy \( \epsilon_i = \epsilon_{k_1,-}^0 + \epsilon_{k_2,-}^0 \) defined via the single-particle energies given in Eq. (3.44). The final state is taken to consist of two particles in any of the bands with momentum \( q_1 \) and \( q_2 \)

\[
|\psi_f\rangle = |\psi_{q_1,\sigma_1;q_2,\sigma_2}\rangle = \hat{\Psi}_{q_1,\sigma_1}^\dagger \hat{\Psi}_{q_2,\sigma_2}^\dagger |\text{vac}\rangle.
\]

with corresponding quasi-energy \( \epsilon_f = \epsilon_{q_1,\sigma_1}^0 + \epsilon_{q_2,\sigma_2}^0 \). The general two-particle Floquet mode can be written as a four-component spinor in the basis of (internal) states \( |1\rangle |1\rangle, |1\rangle |2\rangle, |2\rangle |1\rangle \) and \( |2\rangle |2\rangle \) as

\[
\Phi_{m,\sigma_1,\sigma_1;\sigma_2,\sigma_2}^m = \hat{P} \begin{pmatrix}
a_{\sigma_1}(k_1)a_{\sigma_2}(k_2)e^{ik_r(x+y)} \\
a_{\sigma_1}(k_1)b_{\sigma_2}(k_2)e^{-ik_r(y-x)}e^{-i\omega \tau} \\
b_{\sigma_1}(k_1)a_{\sigma_2}(k_2)e^{-ik_r(x-y)}e^{-i\omega \tau} \\
b_{\sigma_1}(k_1)b_{\sigma_2}(k_2)e^{-2ik_r(y-x)}e^{-2i\omega \tau}
\end{pmatrix} \times e^{ik_1x + ik_2y} e^{im\omega \tau}
\]

where \( \hat{P} \) denotes symmetrisation of the wave function under exchange of single-particle
quantum numbers as we consider bosonic particles.

As we are interested in inelastic processes with the absorption of a non-zero number of photons, the relevant matrix element is \( \langle \Phi^m | \hat{H}_{\text{int}} | \Phi^0 \rangle \) for non-zero \( m \). Therefore, the usual scalar product \( \langle \Phi^m | \hat{H}_{\text{int}} | \Phi^0 \rangle \) contains an overall oscillating factor of \( \exp[-im\omega \tau] \) stemming from the last factor in Eq. (3.47). This factor can only be cancelled to yield a non-zero time-average if different components of the spinors are coupled by \( \hat{H}_{\text{int}} \). Thus, the only relevant coupling for inelastic scattering is the one given by \( g_c \) coupling the states \( |1\rangle |1\rangle \) to \( |2\rangle |2\rangle \). For this process the energy of exactly two two-photon transitions, i.e. \( m = 2 \) in Eq. (3.22), is absorbed; simultaneously, the centre of mass momentum changes by \( 4k_r \), owing to the fact that the running Raman beams impart a momentum kick of \( 2k_r \) during the two-photon transition.

In the following we focus on the results for the case of two low-energy particles, \( k \to 0 \), i.e. the initial state has both particles in the same minimum of the lower band of the quasi-energy dispersion. We obtain stability regions in the parameter space of \((\Omega, \omega)\) in which inelastic processes are kinematically forbidden, shown in Fig. 3.6. These regions are derived from the quasi-energy conservation in the FFGR and the constraints on the final centre of mass momentum. Generally, as \( \Omega \) increases the gap to the higher band increases as well, making transitions from the initial state in \((-,-)\) to those with at least one excited particle in a higher band \([(+, -), (-, +) \text{ or } (+, +)]\) forbidden as only an energy of \( 2\hbar\omega \) is available. Conversely, as \( \omega \) is increased there is a threshold above which particles can be excited into higher bands. For no detuning \( \hbar\delta / E_r = 0 \) the dispersion is symmetric and has two degenerate minima for \( \hbar\Omega / E_r < 4 \) at \( k = \pm |k_{\text{min}}| \neq 0 \). Therefore, there are two distinct initial states with \( k_0 = \pm |k_{\text{min}}| \) and stability regions for both cases are shown. The thin dashed lines that split off and go up for \( \hbar\Omega / E_r < 4 \) corresponds to \( k_0 = +|k_{\text{min}}| \) and the bold that go down to \( k_0 = -|k_{\text{min}}| \), i.e. with both particles starting in the right or the left minimum of the lower band respectively. This is readily explained by the fact that for \( k_0 = -|k_0| \) particles starting in the left minimum of the dispersion get scattered close to the right minimum when increasing their quasimomentum by \( 2k_r \) and therefore have a lower energy and threshold \( \omega \). This breaking of the symmetry \( k \to -k \) that is apparent in the dispersion is due to the fact the the coupling matrix in Eq. (3.37) contains a running wave term \( \exp[i\omega \tau + 2ik_r x] \) which explicitly sets a direction in space.
Figure (3.6) Stability diagram for (a) $\hbar \delta / E_r = 0$ and (b) $\hbar \delta / E_r = 16$ with initial state of two particles with quasi-momentum $k_1 = k_2 = k_0$ in the minimum of the lower band. For no detuning and $\hbar \Omega / E_r < 4$ the both cases of $k_1 = k_2 = +|k_0|$ (dashed lines) and $k_1 = k_2 = -|k_0|$ (full lines) are shown, with detuning the minimum of the single particle dispersion is unique, see Fig. 3.4. Shaded regions correspond to parameter regimes in which inelastic scattering is allowed. The bottom region (A) in light blue corresponds to inelastic scattering where both particles remain in the lower bands, i.e. the $(-, -)$-final state, in the middle region (B) particles can scatter either into the $(-, -)$ or the $(+, -)$-final state and in the top region (C) scattering into all states $(-, -), (+, -)$ and $(+, +)$ is allowed. The thick dashed gray lines of constant $\omega \hbar / E_r$ and of constant $\Omega \hbar / E_r$ correspond to the cuts along which the scattering rate is shown in Fig. 3.7 and Fig. 3.8.
3.4. Applications

With detuning the degeneracy is lifted and the minimum is unique for all parameter values.

We now turn to the computation of the scattering rates, the allowed final states can be parametrised as \( \Phi_m(q) = \Phi_m^{\sigma_1, k_0, q, \sigma_2, k_0 + 2k_r - q} \). To compute the total scattering rate one integrates over these final states

\[
\frac{\mathrm{d}n}{\mathrm{d}r} = \frac{2\pi}{\hbar} \sum_{\sigma_1, \sigma_2, m \neq 0} \frac{L}{2\pi} \int dq \left| \langle \langle \Phi_m(q) | \hat{H}_{\text{int}} | \Phi_0^\sigma \rangle \rangle \right|^2 \delta(\epsilon_i - \epsilon_f(q) - m\hbar\omega)
\]

\[
= \frac{1}{\hbar L E_r} \sum_{\sigma_1, \sigma_2, m \neq 0} L^2 \int d\epsilon_i \frac{d(q/k_r)}{d(\epsilon_f/E_r)} \left| \langle \langle \Phi_m(q) | \hat{H}_{\text{int}} | \Phi_0^\sigma \rangle \rangle \right|^2 \delta(\epsilon_i - \epsilon_f - m\hbar\omega)
\]

\[
= \frac{g_c^2 k_r}{\hbar L E_r} \Gamma^{1D}
\]

which defines the intensive dimensionless scattering rate \( \Gamma^{1D} \) for inelastic processes. Due to the dependence on the 1D-density of states \( \Gamma^{1D} \) will diverge at the borders of the stability regions in Fig. 3.6 whenever a scattering channel opens or closes and the density of states of the final state diverges. A plot of \( \Gamma^{1D} \) for characteristic parameter values is shown in Fig. 3.7 with these divergences clearly visible. Away from those points the dimensionless rate is \( \Gamma^{1D} \approx 0.2 - 0.4 \). We remark again that for coupled spin-states \( g_c = 0 \) and no inelastic scattering occurs, whereas for subbands \( g_c \neq 0 \) generally.

The elastic scattering rates are comparatively easier to compute. For simplicity we focus on the case of spin-independent coupling strengths \( g_\sigma = g_2 = g \), no detuning \( \tilde{\delta} = 0 \) and consider the limit of \( k \to 0 \) for which the leading behaviour can be given explicitly. A more detailed discussion of the elastic scattering properties can be found in [74].

As mentioned before the non-species-changing interaction terms (\( g_\sigma \) and \( g_2 \)) conserve the total momentum and only the relative momentum can be changed during scattering. Moreover, in first order \( g_c \) does not contribute to the elastic scattering rate as it always changes both the energy and the total momentum of the colliding particles. Neglecting higher order effects of \( g_c \) and in the limit of \( k \to 0 \) the particles behave like spinless bosons with a modified dispersion relation interacting via a contact interaction and
Figure (3.7) Dimensionless scattering rate $\Gamma^{1D}$ defined in Eq. (3.48), for an initial state with particles in the lower band with momentum $k = \pm |k_0|$ getting inelastically scattered. In the top row for no detuning $\hbar \delta / E_r = 0$ as a function of $\hbar \omega / E_r$ for fixed $\hbar \Omega / E_r = 4$ in (a) and as a function of $\hbar \Omega / E_r$ for fixed $\hbar \omega / E_r = 7$ in (b) (dashed $k = +|k_0|$, full $k = -|k_0|$) and at the bottom for $\hbar \delta / E_r = 16$ as a function of $\hbar \omega / E_r$ for fixed $\hbar \Omega / E_r = 16$ in (c) and as a function of $\hbar \Omega / E_r$ for fixed $\hbar \omega / E_r = 20$ in (d) as indicated by the dashed lines in Fig. 3.6. The rate shows divergences at the opening/closing of scattering channels corresponding to the borders in Fig. 3.6 at which the density of states of the final states diverges.
all differences that occur in their elastic scattering is entirely due to density of states effects.

The elastic scattering rates within FGR are given by

\[
\Gamma_{el} = \begin{cases} 
\frac{1}{(\tilde{\Omega}/4)^2 - 1} \frac{1}{k/k_r} & \text{for } \tilde{\Omega} < 4 \\
2\frac{(k/k_r)^3}{(k/k_r)^3} & \text{for } \tilde{\Omega} = 4 \\
\frac{1}{1 - 4/\tilde{\Omega} k/k_r} & \text{for } \tilde{\Omega} > 4
\end{cases}
\tag{3.49}
\]

where in the case of \(\tilde{\Omega} = 4\) the dispersion is quartic \(\epsilon(k) \propto k^4\) and consequently the divergence is \(1/k^3\) instead of the usual \(1/k\) for a parabolic dispersion. We emphasize again that these rates are the same as for undressed particles with the modified dispersion interacting via a contact interaction. In the limit of \(k \to 0\) the dressing of particles only changes the dispersion and the density of states, not the interactions themselves.

To relate both the inelastic and elastic scattering rates to the corresponding cross sections, the rates have to be divided by the incident flux. For simplicity we again focus on the case of \(\tilde{\delta} = 0\) and the limit of \(k \to 0\) for which the incoming flux for our initial state is

\[
J_{in} = \frac{2\hbar k}{ML} \left[ 1 - \left( \frac{\tilde{\Omega}}{4} \right)^2 \right] \text{ for } \tilde{\Omega} < 4 \\
J_{in} = \frac{2\hbar k}{ML} \left( \frac{k}{2k_r} \right)^2 \text{ for } \tilde{\Omega} = 4 \tag{3.50} \\
J_{in} = \frac{2\hbar k}{ML} \left[ 1 - \frac{4}{\tilde{\Omega}} \right] \text{ for } \tilde{\Omega} > 4
\]

For \(\tilde{\Omega} \neq 4\) these factors together with Eq. (3.49) and Eq. (3.48) give a divergence of \(1/k^2\) and \(1/k\) for the elastic and inelastic scattering cross section respectively in the same way as discussed in the toy model above. The case of \(\tilde{\Omega} = 4\) is special as the dispersion then becomes quartic \(\epsilon(k) \propto k^4\). The corresponding \(1/k^6\) and \(1/k^3\) behaviour of the elastic and inelastic scattering cross sections is entirely due to the dispersion and density of states effects and is not related to the dressing of the states. In both cases the divergence at low
3. Scattering Theory for Floquet-Bloch States

$k$ signals a failure of the Born-Approximation.

Following the discussion of the toy model, in 1D the elastic rate should dominate over the inelastic rate at low $k$ and at lower overall interaction strengths when the ratio of $g_c/g$ is kept fixed.

Extension to two dimensions

The above model has motion only along one dimension, as relevant for the motion along tubes with transverse confinement frequencies large compared to $\omega$. In systems with weak confinement in the transverse directions there are additional inelastic scattering channels. Here we consider the case of a two-dimensional system as is required to generate a non-vanishing effective magnetic field. For now, we ignore any spatial dependence of the laser fields along the second direction, which we denote $y$. The setting is then a two-dimensional system tightly confined in the $z$-direction, with the Raman-lasers running along the $x$-direction and free motion in $y$.

The discussion straightforwardly generalises to this case. We define

$$\epsilon_f(q, k_y) = \epsilon_f(q, k_y = 0) + E_y = \epsilon_q + E_y$$

where the additional energy is given by $E_y = 2E_r(k_y/k_r)^2$ and $k_y$ is the relative momentum in the $y$-direction of a two-particle state. Note that inelastic scattering processes remain gapped in this case even for particles remaining in the same band as the absorption of photons is always coupled to a change in the centre of mass momentum in this model which changes the energy.

Taking an initial state with no relative momentum $k_y^i = 0$ and a final state with relative momentum $k_y^f = q_y$ we define the matrix element of the interaction Hamiltonian as

$$I_{q,q_y}^m = \langle \Phi_f^m(q, q_y) | \hat{H}_{\text{int}} | \Phi_i^0 \rangle$$

(3.52)
and get for the inelastic scattering rate

\[
\frac{dn}{d\tau} = \frac{2\pi}{\hbar} \sum_{\sigma_1 \sigma_2; m \neq 0} \left( \frac{L}{2\pi} \right)^2 \int dq_y \int dq \left| f_{q,qy}^m \right|^2 \delta(\epsilon_i - \epsilon_f(q, q_y) - m\hbar\omega)
\]

\[
= \frac{1}{2\pi \hbar L^2 E_r^2} \sum_{\sigma_1 \sigma_2; m \neq 0} L^4 \int dE_y \frac{d(q_y/k_r)}{d(E_y/E_r)} \int d\epsilon_q \frac{d(q/k_r)}{d(\epsilon_q/E_r)} \left| f_{q,qy}^m \right|^2 \delta(\epsilon_i - \epsilon_q - E_y - m\hbar\omega)
\]

\[
= \frac{g^2_c}{2\pi \hbar L^2 E_r} \Gamma^{2D}
\]

(3.53)

where as before \(\Gamma^{2D}\) is a dimensionless intensive rate constant for inelastic scattering processes. Note that \(g_c\) is now defined differently, while it was an effective quantity for a 1-dimensional system before it is now the corresponding quantity for a 2D confined system. The two-dimensional rate \(\Gamma^{2D}\) is not expected to diverge at the opening or closing of scattering channels anymore, but rather to exhibit jumps which is confirmed in Fig. 3.8. Note that the scattering rate does not vanish in the limit \(\omega \to \infty\). The situation is the same as in the toy model discussed in Section 3.3, where the rate vanishes in 1D simply due to the decreasing density of states, whereas in 2D with a constant density of states the rate does not vanish in the large \(\omega\) limit. In the 3D case (not shown), the density of states increases as \(\sqrt{\omega}\) for large drive frequency, again leading to large scattering for \(\omega \to \infty\). In terms of the relation of inelastic to elastic scattering, the expectation is that in 2D elastic and inelastic scattering should scale in the same way as functions of \(k\) for low momenta as the density of states is \(k\) independent, whereas in 3D the inelastic rate should dominate at low \(k\) because of the suppression of elastic scattering due to the vanishing density of states.
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**Figure (3.8)** Dimensionless scattering rate $\Gamma^{2D}$ defined in Eq. (3.53), for an initial state with particles in the lower band with momentum $k = \pm |k_0|$ and relative momentum $k_y = 0$ getting inelastically scattered for the extension to a 2D setting with free motion in a transverse direction. In the top row for no detuning $\hbar \delta / E_r = 0$ as a function of $\omega \hbar / E_r$ for fixed $\hbar \Omega / E_r = 4$ in (a) and as a function of $\hbar \Omega / E_r$ for fixed $\omega \hbar / E_r = 7$ in (b) (dashed $k = +|k_0|$, full $k = -|k_0|$) and at the bottom for $\hbar \delta / E_r = 16$ as a function of $\omega \hbar / E_r$ for fixed $\hbar \Omega / E_r = 16$ in (c) and as a function of $\hbar \Omega / E_r$ for fixed $\omega \hbar / E_r = 20$ in (d) as indicated by the dashed lines in Fig. 3.6. The rate shows jumps at the opening/closing of scattering channels corresponding to the borders in Fig. 3.6.
3.4.2. Modulated lattice

We now turn to a model of a lattice with modulated on-site energies. This is a simplified version of the modulation protocols used in [75, 78, 167] used to create artificial magnetic fields in optical lattices. Despite its simplifications it should still capture the novel scattering properties which become important due to the periodic driving. Our discussion describes generic features of two-particle scattering in models using modulated optical lattices as described in Section 1.2.4. Our work is complementary to that of Ref.[175, 176] which considered many-particle systems in shaken optical lattices.

Our model consists of a one-dimensional superlattice with time-periodic modulation of on-site energies sketched in Fig. 3.9. The superlattice causes a staggered energy offset between sites, and the site-modulation resonantly restores the suppressed tunnelling along the lattice. We shall assume that the resulting bandwidth $\Delta_w$ is small compared to the modulation frequency, $\Delta_w \ll \hbar \omega$. However, we shall allow for the possibility that $\hbar \omega$ is close to the interband transition energy $\Delta_g$, allowing inelastic scattering into this higher band. We therefore retain two bands of the original one-dimensional lattice (i.e. there are two Wannier states per local minimum of the potential). After a discussion of the one-dimensional model we comment on the inclusion of an additional free direction of motion. We consider bosons described by a field-operator $\hat{\Psi}(x)$ loaded into such an optical superlattice of length $L$. The Hamiltonian for this system is given by $\hat{H} = \hat{H}_0(\tau) + \hat{H}_{\text{int}}$,

$$\hat{H}_0(\tau) = \int \! dx \, \hat{\Psi}^{\dagger}(x) \left[ -\frac{\hbar^2}{2M} \frac{d^2}{dx^2} + V_1 \sin^2(kx) + V_2 \cos^2(kx/2) \right] \hat{\Psi}(x) + \int \! dx \, \hat{\Psi}^{\dagger}(x) \left[ V_\omega \cos^2(kx/2 + \omega \tau/2) \right] \hat{\Psi}(x),$$

$$\hat{H}_{\text{int}} = \frac{g}{2} \int \! dx \, \hat{\Psi}^{\dagger}(x) \hat{\Psi}^{\dagger}(x) \hat{\Psi}(x) \hat{\Psi}(x),$$

where the first line of Eq. (3.54) describes the kinetic energy and superlattice potential with strength $V_1$ and $V_2$ created by standing light-waves with wavevectors $k$ and $k/2$, and the second line gives the modulation of on-site energies with strength $V_\omega$ and modulation frequency $\omega$ which can be created by two running-wave beams as described in [167].
3. Scattering Theory for Floquet-Bloch States

**Figure (3.9)** Sketch of the one-dimensional time-periodically driven lattice potential defined in Eq. (3.54), different time-slices are colour-coded. The lattice is staggered with an energy offset $V_2$ between neighbouring sites which suppresses tunnelling along the lattice. Tunnelling is then restored by resonantly modulating the site-energies with a modulation strength $V_\omega$ at frequency $\hbar \omega = V_2$. Note that the neighbouring wells are modulated with a phase-shift of $\pi$ resulting in maximal differential modulation. For illustrational purposes the staggering $V_2$ and the modulation $V_\omega$ are exaggerated in the figure.

Energies and lattice depth will be measured in terms of the recoil energy $E_r = \frac{\hbar^2 k^2}{2M}$ which we define with respect to the unstaggered lattice, i.e. $k_r = k$, and we assume the lattice to be deep $V_1 > E_r$ in order to obtain well separated bands.

The last part, Eq. (3.55), gives the usual 1D contact interaction between atoms of strength $g$. Assuming a tight-confinement by a harmonic potential in the transverse radial direction, it is given by $g = \frac{4 \hbar^2 a_s}{a_s^3 M}$, where $a_s$ is the 3D s-wave-scattering length of the true interaction potential and $a_\perp = \sqrt{2 \hbar/(M \omega_\perp)}$ the radial confinement length of the harmonic trap with frequency $\omega_\perp$ [199].

We begin by mapping the Hamiltonian $\hat{H}_0(\tau)$ onto a tight-binding Hamiltonian with two orbitals per lattice site at positions $x_j = jd$ with $d = \pi/k$. To this end the bosonic field-operator $\hat{\Psi}(x)$ is expanded in terms of the Wannier functions of the two lowest bands of the Hamiltonian with $V_2 = V_\omega = 0$, i.e. in the Wannier functions of the simple optical lattice without the superlattice potential. Writing

$$\hat{\Psi}(x) = \sum_j w_1(x - x_j) \hat{a}_j + w_2(x - x_j) \hat{b}_j,$$  \hspace{1cm} (3.56)
where \( \hat{a} (\hat{b}) \) are field operators for Wannier states in the first (second) band, one obtains the tight-binding model as

\[
\hat{H}_0(\tau) = \sum_{ij} \left( -t_{ij}^{(1)} \hat{a}_i^\dagger \hat{a}_j - t_{ij}^{(2)} \hat{b}_i^\dagger \hat{b}_j + \text{h.c.} \right) \\
+ \sum_1 \frac{1}{2} \left[ 1 + (-1)^j \right] \left[ V_2 + V_\omega \cos(\omega \tau) \right] \hat{a}_j^\dagger \hat{a}_j \\
+ \sum_1 \frac{1}{2} \left[ 1 + (-1)^j \right] \left[ V_2 + V_\omega \cos(\omega \tau) + \Delta_g \right] \hat{b}_j^\dagger \hat{b}_j,
\]

(3.57)

where,

\[
t_{ij}^{(n)} = \int dx \, w_n^2(x-x_i) \left[ \frac{-\hbar^2}{2M} \frac{d^2}{dx^2} + V_1 \sin^2(kx) \right] w_n(x-x_j)
\]

(3.58)

and \( \Delta_g \) is the energy gap between the first (a) and second (b) band. We note that we did not include an interband tunnelling term of the form \( (\hat{a}_i^\dagger \hat{b}_j + \text{h.c.}) \) in Eq. (3.57) as this term is forbidden by parity conservation in the case of \( s \) and \( p \) bands. We remark that we do not require the wannier functions \( w_n(x) \) explicitly. We will reformulate the problem in terms of the Bloch functions below, which define the \( t_{ij}^{(n)} \) uniquely via their dispersion.

The superlattice potential \( V_2 \cos^2(kx/2) \) is seen to lead to a staggering in the tight-binding model which suppresses tunnelling along the lattice due to the energy difference \( V_2 \) between neighbouring sites. Tunnelling can then be restored by modulating the lattice on resonance \( \hbar \omega = V_2 \) whereby the necessary energy is provided by absorption and emission of photons. The parameters need to satisfy \( V_2 > t_{ij}^{(n)} \) such that in the staggered lattice tunnelling is suppressed. Moreover, to obtain clearly separated bands the gap \( \Delta_g \) should be bigger than the band-width of the Bloch bands. Finally, to avoid resonant excitation from the lowest to the highest band \( \hbar \omega \) should be smaller than the gap. Additionally, the time-dependent modulation \( V_\omega \) should not be too strong, as will become apparent in the derivation below. In the high frequency regime the relevant quantity to measure the effect of the modulation is \( \kappa = V_\omega / (\hbar \omega) \) which should be of order 1, whereas in the low frequency regime \( V_\omega \) should be comparable to \( V_2 \) and smaller than \( V_1 \). This leads to a hierarchy of energy-scales \( \Delta_g, V_1 > V_2 = \hbar \omega \approx V_\omega > t_{ij}^{(n)} \).
Single-Particle States

We proceed to obtain the single-particle spectrum of the non-interacting Hamiltonian $\hat{H}_0$. As it is only translationally invariant with respect to translations by 2 lattice sites $l \rightarrow l + 2$, i.e. the translational symmetry is reduced compared to the unstaggered lattice, it is convenient to introduce an enlarged unit cell and distinguish even ($l = 2n$) and odd ($l = 2n + 1$) sites. As seen from Eq. (3.57) the odd sites do not experience the time-modulation, whereas the even sites are offset by $V_2$ and modulated in time by $V_ω$.

As we doubled the unit cell, the Brillouin zone will be reduced. We define the operators in momentum space as

$$
\hat{a}_k^{(1)} = \frac{1}{\sqrt{N_l}} \sum_l e^{-ikl} \hat{a}_l, \quad \hat{a}_k^{(2)} = \frac{1}{\sqrt{N_l}} \sum_l e^{-i(k+\pi)l} \hat{a}_l
$$

(3.59)

with corresponding definitions for $\hat{b}_k^{(1)}$ and $\hat{b}_k^{(2)}$. The sums run over all lattice sites $l$, $N_l$ denotes the total number of sites and the quasi-momentum lies in the reduced Brillouin zone, $k \in [0, \pi)$. Note that we introduced a dimensionless quasi-momentum $k$ via $k = d k_{\text{phys}}$ with respect to the physical quasi-momentum $k_{\text{phys}}$ and the lattice spacing $d$ here. The last equality shows that $\hat{a}_k^{(1)}$ ($\hat{a}_k^{(2)}$) correspond to the symmetric (anti-symmetric) combination of the Fourier components on the even (2$l$) and odd (2$l + 1$) sublattices. Thus, in anticipation of restoring tunnelling between the sublattices, we have chosen a basis reflecting this. In contrast, the operators $1/\sqrt{2} \left( \hat{a}_k^{(1)} \pm \hat{a}_k^{(2)} \right)$ would correspond to states on either sublattice.

One obtains the Hamiltonian in momentum space as

$$
\hat{H}_0(\tau) = \sum_k \epsilon_k^{(a)} \hat{a}_k^{(1)}\hat{a}_k^{(1)\dagger} + \epsilon_{k+\pi}^{(a)} \hat{a}_k^{(2)}\hat{a}_k^{(2)\dagger} + \sum_k V_c(\tau) \left( \hat{a}_k^{(1)}\hat{a}_k^{(2)\dagger} + \hat{a}_k^{(2)}\hat{a}_k^{(1)\dagger} \right) + (a \rightarrow b)
$$

$$
+ \sum_k \Delta_g \left( \hat{b}_k^{(1)}\hat{b}_k^{(1)\dagger} + \hat{b}_k^{(2)}\hat{b}_k^{(2)\dagger} \right)
$$

(3.61)
3.4. Applications

with \( V_c(\tau) = 1/2 [V_2 + V_\omega \cos(\omega \tau)] \) and \( \epsilon_k^{(n)} = 2 \sum_l l t_{l,n}^{(n)} \cos(lk) \) and \( l = |i - j| \). The staggering of the lattice is now seen to induce a coupling between the two momentum components at \( k \) and \( k + \pi \).

We proceed to diagonalise this Hamiltonian by the use of a rotating wave like approximation for the case of resonant modulation \( \hbar \omega = V_2 \). Details of the derivation are given in Appendix B.2. The Floquet modes turn out to be

\[
\Phi_{\sigma,k}^{(n),m}(\tau) = 1/2 \left[ (f(\tau) + \sigma e^{i\omega \tau} \tilde{f}(\tau)) \hat{c}_{k,n}^{(1)\dagger} + (f(\tau) - \sigma e^{i\omega \tau} \tilde{f}(\tau)) \hat{c}_{k,n}^{(2)\dagger} \right] e^{i m \omega \tau} |\text{vac}\rangle,
\]

where we denote by \( \hat{c}_{k,n}^{(i)\dagger} \) the creation operator for a Bloch state in band \( n = a \) or \( b \) with quasi momentum \( k \) in either momentum state \( i = 1(2) \). The states are characterised by an additional subband index \( \sigma = \pm \), and the time-periodic function \( f(\tau) = \exp[i \kappa \sin(\omega \tau)] \) with \( \kappa = V_\omega / (\hbar \omega) \) was defined. The corresponding quasi-energies are

\[
\begin{align*}
\epsilon_{\sigma,k}^{a,0} &= \sigma \epsilon_k^a J_{-1}(\kappa), \\
\epsilon_{\sigma,k}^{b,0} &= \sigma \epsilon_k^b J_{-1}(\kappa) + \Delta_g.
\end{align*}
\]

where \( J_{-1} \) denotes the Bessel function of the first kind. Note that the quasi-energies are not reduced to a Floquet BZ here, but rather defined to keep the association with the original lowest first (a) and second (b) bands that are gapped in energy by \( \Delta_g \) in the static Hamiltonian. The resulting band structure is depicted in Fig. 3.10.

The modulation of the lattice now shows its effect in two ways. Firstly, the tunnelling is restored with a modified strength of \( \epsilon_k^b J_{-1}(\kappa) \). Secondly, the population of momentum components oscillates in time between \( k \) and \( k + \pi \) with equal amplitudes as the energy gap of \( V_2 \) is bridged by the energy of the modulation \( \hbar \omega = V_2 \).

Following the definitions in Section 3.2.1 scattering processes in which particles change the band from \( a \) to \( b \) and those for which particles stay within a band, but scatter into higher energy single-particle states in the same band will be called inelastic. The first process leads to loss of particles from the lowest band, whereas the second process may lead to heating within the band.
3. Scattering Theory for Floquet-Bloch States

Figure (3.10) Quasienergies of the resonantly modulated lattice, Eq. (3.63) and Eq. (3.64), as a function of the quasi-momentum $k$ in arbitrary energy units. The two lowest bands of the original lattice (a) and (b) both split into two subbands $\tau = \pm$ which are degenerate at the Brillouin zone boundaries. Depicted is a typical situation in which the energy of the periodic modulation $\hbar \omega$ is larger than the bandwidth of the lowest band and smaller than the bandgap $\Delta_g$. The balls show our initial state with two particles in the lowest band and a possible final state with two particles in the upper band after scattering. For this plot a nearest neighbour tight-binding dispersion $e^{(n)}(k) = t^{(n)} \cos(k)$ is assumed with parameters $t^a = 1.1$, $t^b = 2.3$ and $\hbar \omega = 4.8$, $\Delta_g = 10$ and $\kappa = 1$. 

![Figure 3.10](image_url)
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Two-Particle Scattering

To consider the effects of the collisions of the atoms given by the interaction Hamiltonian, Eq. (3.55), we will treat them to first order within the FFGR. This will preclude the discussion of strongly correlated many-body phases, but is still sufficient to see the relevant 2-particle physics and their relevance to heating.

The scattering processes we consider are illustrated in Fig. 3.10. We apply FFGR (Eq. (3.22)) for an initial state consisting of two particles in the lowest band with the same subband index \( \sigma_i = \pm \) with crystal-momentum \(+k\) and \(-k\) respectively, i.e.

\[
\Psi_i = \hat{\Psi}_{\sigma_i,k}^a \hat{\Psi}_{\sigma_i,-k}^a |\text{vac}\rangle
\]  

(3.65)

and a final state containing two particles in the upper band in subbands \( \sigma_1, \sigma_2 \) with momenta \( q_1 \) and \( q_2 \)

\[
\Psi_f = \hat{\Psi}_{\sigma_1,q_1}^b \hat{\Psi}_{\sigma_2,q_2}^b |\text{vac}\rangle.
\]  

(3.66)

This is the only relevant inelastic scattering process allowed within FFGR for the case in which \( \hbar \omega > 4 \epsilon_{k} J_{-1}(\kappa) \) which forbids the absorption of a quantum of energy \( \hbar \omega \) within the lowest band. Because of the resonance condition \( \hbar \omega = V_2 \), this corresponds to strong suppression of tunnelling for which \( V_2 \) was assumed to be large compared to the bandwidth.

As a first step we again derive stability regions implied by kinematic constraints, these are shown in the \( (V_\omega, \omega) \)-plane in Fig. 3.11. Due to the structure of the single-particle states that contain two momentum components at \( k \) and \( k + \pi \) scattering is allowed into states with momenta \( q_1 = q, q_2 = -q \) and \( q_1 = q + \pi, q_2 = -q \). Within the reduced BZ, the second case \( (\sigma_1, q + \pi) \) actually corresponds to \( (-\sigma_1, q) \). As we consider the case in which the bands are well separated, i.e. \( 4(t_{1,\text{eff}} + t_{2,\text{eff}}) < \Delta_g \), transitions from the lower to the upper band require the absorption of a non-zero number \( m_0 \) of photons. Specifically, the conservation of quasi-energy in the FFGR then picks the representative state \( \Phi_{1}^m \) with \( m = -m_0 \) and energy conservation reduces to

\[
2 \epsilon_{k} J_{-1}(\kappa) = \epsilon_{q} J_{-1}(\kappa) [\sigma_1 \pm \sigma_2] + (2 \Delta_g - m_0 \hbar \omega)
\]  

(3.67)
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![Stability diagram of the lowest band in a time-periodically modulated one-dimensional lattice of depth $V_1 = 6E_r$ for which the band gap is $4.75E_r$. Shaded regions correspond to energetically allowed scattering from the ground state into the first excited band. Different lobes correspond to different orders of the instability $m$ starting with $m = 1$ at the top and increasing downwards. In (a) only the first 4 such lobes are shown for clarity, in (b) the region $1 \leq \omega h/E_r \leq 3$ with the $m = 4, 5, 6, 7$ lobes which overlap the $m = 5$ lobe are shown. The dashed lines of constant $\omega h/E_r$ correspond to the cuts along which the scattering rate is shown in Fig. 3.12.](image)

Figure (3.11) Stability diagram of the lowest band in a time-periodically modulated one-dimensional lattice of depth $V_1 = 6E_r$ for which the band gap is $4.75E_r$. Shaded regions correspond to energetically allowed scattering from the ground state into the first excited band. Different lobes correspond to different orders of the instability $m$ starting with $m = 1$ at the top and increasing downwards. In (a) only the first 4 such lobes are shown for clarity, in (b) the region $1 \leq \omega h/E_r \leq 3$ with the $m = 4, 5, 6, 7$ lobes which overlap the $m = 5$ lobe are shown. The dashed lines of constant $\omega h/E_r$ correspond to the cuts along which the scattering rate is shown in Fig. 3.12.

where the $+$ ($-$) sign corresponds to the cases $q_1 + q_2 = 0$ ($q_1 + q_2 = \pi$) described above. This equation fixes the momentum $q_f$ of the final state depending on the band gap $\Delta_g$, the amplitude of the driving $V_\omega$ and the driving frequency $\omega$. Assuming for the moment that an arbitrary number of photons may be absorbed within FFGR, which we will confirm below, Eq. (3.67) implies the stability diagram displayed in Fig. 3.11. Depending on the modulation strength $\kappa = V_\omega / (\hbar \omega)$ and frequency $\omega h/E_r$, there are stable regions in which no energy absorption takes place, regions where a single transition with a unique $m$, and regions where multiple transitions with different photon numbers $m$ are allowed.

Next we turn to the computation of the scattering rates. For this we require the matrix elements appearing in the FFGR

$$I^m_{\sigma_1, \sigma_2, k; q} = \langle \Phi^m_{\sigma_1, q, \sigma_2, -q} | \hat{H}_{\text{int}} / g | \Phi^0_{\sigma_1, k, -k} \rangle.$$  

(3.68)
To obtain these, we expand the field operators in the basis of Bloch functions $\psi_n(x, k)$ of band $n$ as

$$\hat{\Psi}_n(x) = \sum_k \hat{\phi}_n(k) \psi^k_n(x).$$  \hspace{1cm} (3.69)$$

Thus, the interaction Hamiltonian, Eq. (3.55), becomes

$$\hat{H}_{\text{int}} = \frac{g}{2} \sum_{\{n_i\}} \int_0^L dx \, \hat{\Psi}^{\dagger}_{n_1}(x) \hat{\Psi}^{\dagger}_{n_2}(x) \hat{\Psi}_{n_3}(x) \hat{\Psi}_{n_4}(x)$$

$$= g \sum_{\{n_i, k_i\}} W^{k_1 k_2 k_3 k_4}_{n_1 n_2 n_3 n_4} \hat{\phi}_{n_1}^{\dagger}(k_1) \hat{\phi}_{n_2}^{\dagger}(k_2) \hat{\phi}_{n_3}(k_3) \hat{\phi}_{n_4}(k_4),$$  \hspace{1cm} (3.70)$$

where we defined the matrix elements of the interaction between Bloch waves

$$W^{k_1 k_2 k_3 k_4}_{n_1 n_2 n_3 n_4} = \frac{1}{2} \int_0^L dx \, \hat{\phi}_{n_1}^{k_1}(x) \hat{\phi}_{n_2}^{k_2}(x) \hat{\phi}_{n_3}^{k_3}(x) \hat{\phi}_{n_4}(x).$$  \hspace{1cm} (3.71)$$

The explicit expressions for the coupling matrix elements $I^m_{\sigma_i, \sigma_1, \sigma_2, k}$, Eq. (3.68), are given in the Appendix B.3. If one assumes that the matrix element between Bloch functions $W^{k_1 k_2 k_3 k_4}_{n_1 n_2 n_3 n_4}$ defined in Eq. (3.71) is completely momentum-independent, then the matrix element $I^m_{\sigma_i, \sigma_1, \sigma_2, k}$ in Eq. (3.68) vanishes for $m \neq 0$ and there is no inelastic scattering. This occurs in the case of an infinitely deep lattice, then tunnelling vanishes, the Hamiltonian becomes local and all terms commute. This implies that heating vanishes as discussed in Section 3.2. Thus, for sufficiently deep lattices there is no inelastic scattering and no coupling to the higher-band within the FFGR. Generically, $I^m_{\sigma_i, \sigma_1, \sigma_2, k}$ is non-vanishing for any $m$. This implies the possibility of absorption of arbitrary integer numbers of energy $\hbar \omega$ during scattering and thus justifies the assumption made in deriving the stability diagram.
3. Scattering Theory for Floquet-Bloch States

To obtain the total inelastic scattering rate one integrates over all allowed final states

\[
\frac{dn}{d\tau} = \frac{L}{\hbar} \sum_{\sigma_1, \sigma_2} \int \frac{dq}{\Delta_0} g^2 \left| \frac{r^m}{\sigma_1, \sigma_2; k, q} \right|^2 \delta(\epsilon_i - \epsilon_f(q) + m\hbar\omega)
\]

\[
= \frac{g^2 L}{\hbar} \sum_{\sigma_1, \sigma_2} \int \frac{dq}{\Delta_0} \left| \frac{r^m}{\sigma_1, \sigma_2; k, q} \right|^2 \delta(\epsilon_i - \epsilon_f + m\hbar\omega)
\]

\[
= \frac{g^2}{\hbar E_r L d} \int \frac{dq}{\Delta_0} \left| \frac{r^m}{\sigma_1, \sigma_2; k, q} \right|^2 \delta(\epsilon_i - \epsilon_f + m\hbar\omega)
\]

\[
= \frac{g^2}{\hbar E_r L d} \Gamma^{1D}
\]

which defines the intensive dimensionless scattering rate \(\Gamma^{1D}\) for scattering into the higher band. \(\Gamma^{1D}\) depends on the lattice via the band structure \(\epsilon_k\) and the gap \(\Delta_0\), and the modulation strength and frequency which determine both the effective band structure \(\epsilon_k J_{-1}(V_0/\hbar\omega)\) and the eigenstates via their dependence on \(f(\tau) = \exp[i\kappa \sin(\omega \tau)] = \sum_n J_n(\kappa) \exp[\iota n \omega \tau]\) with the Bessel functions of the first kind \(J_n\) introduced above. Therefore, the scattering rate will show a complicated behaviour, possibly with zeros inherited from the Bessel functions. Moreover, the rate will diverge at the thresholds for scattering, i.e. at the envelop functions of the shaded areas in Fig. 3.11, where the momentum of the final state is at the edges of the BZ and the dispersion is flat yielding a diverging 1-D density of states. These expectations are confirmed in Fig. 3.12 which shows the scattering rate \(\Gamma^{1D}\) for transitions of particles in the lower band \((a)\) into the higher band \((b)\) along the cuts indicated in Fig. 3.11.

As an order of magnitude estimate for the decay of particles starting in the lower band, consider a gas of \(N\) particles with density \(N/L \approx 1/d\), \(a_s = 5\) nm, \(d_\perp = 100\) nm, \(M = 100\) u and take \(\Gamma^{1D} \approx 0.05\) to obtain \(N/(dN/d\tau) \approx 40\) ms. From this estimate, experiments in the unstable region would be seriously affected by the scattering into higher bands and a single-band approximation would not be valid. We can conclude that experiments using modulated lattices need to take care to work in regions of parameter space where transitions are not allowed to avoid rapid scattering into higher bands. From Fig. 3.11 this corresponds to avoiding single \((m = 1)\) and multi-photon \((m > 1)\) resonances in which the gap \(2\Delta_0\) to lift two particles into the higher band is bridged by \(m\) photons. Multi-photon
3.4. Applications

Figure (3.12) Dimensionless scattering rate $\Gamma_{a\rightarrow b}^{1D}$ defined in Eq. (3.72), along the cuts $\hbar \omega / E_r = \text{const.}$ as indicated in Fig. 3.11 for particles in the first band $a$ with momentum $k = 0$ scattering into the second band $b$. (a) $\hbar \omega / E_r = 10$ for which $m = 1$ is the only scattering channel. (b) $\hbar \omega / E_r = 2$ for which $m = 5$ transitions are allowed for $0.6 \leq V_\omega / E_r \leq 6.9$ and both $m = 4, 5$ for $2.1 \leq V_\omega / E_r \leq 5.3$.

scattering processes may also be reduced by keeping the modulation amplitude $V_\omega$ small compared to $\hbar \omega$. However, for this specific model there is parameter space available to avoid any resonant scattering into the higher bands while still keeping within the limits of the approximations made. An example for such suitable parameter values would be given by working at $\hbar \omega / E_r \approx 4$ which allows modulation strengths $\kappa = V_\omega / (\hbar \omega)$ sufficiently high to explore both the maximum and the first zero of $J_{-1}(\kappa)$, thus, completely tuning the effective dispersion of the resulting bands.

Extension to weakly-confined system

We now discuss the inclusion of an additional free degree of motion. Such a model is relevant for experiments in which the confinement in the transverse direction is relatively weak. In this case particles may absorb energy during collisions from the driving fields and may scatter into states with fast motion in the transverse direction, which may either lead to heating or to loss from the experimentally relevant region. We will be referring to this as the $z$ direction in the following. We emphasise that in the experimental setups the gauge field is actually simulated in a 2D setting (in the $xy$-plane) which we simplified...
3. Scattering Theory for Floquet-Bloch States

to a 1D lattice in the $x$-direction for our model. We therefore only consider motion in one additional direction which is also relevant for comparison to the experiments in Ref. [81].

We assume that the motion in the $z$-direction is free, so the previous discussion generalises straightforwardly by including the additional energy $E_z = 2E_r(dk_z)^2$ and integrating over the plane-wave states of the transverse direction. The scattering into the higher band still requires a minimal energy and the additional degree of freedom does not change the stability regions. However, as the energy in the transverse direction is unbounded, arbitrarily high energy may be absorbed from the driving fields, which corresponds to the presence of non-zero terms for all $m$ in FFGR higher than the minimal $m$ required to scatter into the higher band.

Additionally, inelastic scattering within the same band now becomes possible which was forbidden by the smallness of the bandwidth compared to the modulation energy before, as any amount of energy can be absorbed in the transverse direction irrespectively of how small or high the driving frequency is. For these processes any scattering with $m \neq 0$ corresponds to inelastic scattering following the definitions made at the end of Section 3.2.1. Therefore, the system is always susceptible to inelastic scattering if motion in the transverse direction is free.

The inelastic scattering rate is now given by

$$\frac{dn_{a,\tilde{a}}}{d\tau} = \frac{2\pi}{\hbar} \sum_{\sigma_1,\sigma_2} \left( \frac{L}{2\pi d} \right)^2 \int dq_z \int dq \, g^2 \left| m_{a,\sigma_1\sigma_2;\tilde{a},k,q} \right|^2 \delta(\epsilon^a_q - \epsilon^\tilde{a}_q(q, q_z) + m\hbar\omega)$$

$$= \frac{c^2}{2 \pi \hbar E_r} \frac{1}{L^2 d^2} \sum_{\sigma_1,\sigma_2} \left( \frac{L}{2\pi d} \right)^2 \int dE_z \frac{dE_z}{dE_z/E_r} \int dq \, d\epsilon_q \frac{d\epsilon_q}{d(\epsilon_q/E_r)} \left| m_{a,\sigma_1\sigma_2;\tilde{a},k,q} \right|^2 \delta(\epsilon^a_q - \epsilon^\tilde{a}_q - E_z + m\hbar\omega)$$

$$= \frac{c^2}{2 \pi \hbar E_r} \frac{1}{L^2 d^2} \sum_{a,\tilde{a}} \frac{1}{4\pi^2}$$

where we split the final state energy into the part due to the motion in the lattice and the free part via $\epsilon_q(q) = \epsilon_k(q, k_z) - E_z(k_z)$ and defined the generalised matrix element $m_{a,\sigma_1\sigma_2;\tilde{a},k,q}$ for transitions with two particles initially in band $a$ to a final state with two particles in band $\tilde{a}$. 

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The dimensionless rate constants $\Gamma^{2D}_{a\rightarrow b}$ and $\Gamma^{2D}_{a\rightarrow a}$ are shown in Fig. 3.13(a) and (b) and Fig. 3.13(c) and (d) respectively. For the scattering into the higher band $\Gamma^{2D}_{a\rightarrow b}$ the rates are of the same order as in the 1D-case. The inelastic rate $\Gamma^{2D}_{a\rightarrow a}$ for particles remaining in the lower band depends strongly on $\hbar \omega$. For high oscillation frequencies most of the energy must be absorbed in the transverse direction for which the density of states decreases as $1/\sqrt{E_z}$ and consequently the total rate remains small.
Figure (3.13)  Dimensionless scattering rate $\Gamma_{a \rightarrow \tilde{a}}^{2D}$ for the extension to a weakly-confined system with a free transverse degree of motion defined in Eq. (3.73), along the cuts $\hbar \omega / E_r = \text{const.}$ as indicated in Fig. 3.11 for particles in the first band with quasi-momentum $k = 0$ and relative momentum $k_y = 0$ scattering into band $\tilde{a}$, integrated over the final states with crystal momentum $q$ and relative momentum $q_y$. (a) and (b) $\tilde{a} = b$, i.e. particles scatter into the second band. (c) and (d) $\tilde{a} = a$, i.e. particles stay in the first band. (a) $\hbar \omega / E_r = 10$ for which $m \geq 1$ are the available inelastic scattering channel (b) $\hbar \omega / E_r = 2$ for which $m \geq 5$ transitions are allowed for $0.6 \leq V_\omega / E_r \leq 6.9$ and $m \geq 4$ for $2.1 \leq V_\omega / E_r \leq 5.3$. (c) $\hbar \omega / E_r = 10$ (d) $\hbar \omega / E_r = 2$. For (c) and (d) all processes with $m \geq 1$ are inelastic and allowed as the particles remain in the same band and the energy in $y$ direction is not gapped.
To relate these considerations to recent experiments in Ref. [81] we provide a rough estimate of the relevant inelastic scattering processes. The experiment simulates the Hofstadter model in a two-dimensional driven optical lattice. The flux per cell is $\pi/2$, so the lowest Wannier band splits into four Hofstadter subbands. Firstly, based on the experimental parameters, we conclude that the restriction to the lowest Wannier band is justified as scattering into the higher Wannier bands should be forbidden by quasi-energy conservation or very highly suppressed. Thus, the dominant process should be the absorption of energy within the same Wannier band and into weakly confined transverse directions, i.e. inelastic scattering between the 4 Hofstadter subbands. The results of Ref. [81] indeed show repopulation dynamics in which particles from the lowest Hofstadter subband are transferred to the higher subbands. The rate of transfer into the highest subband is observed to be approximately $\gamma^{\text{exp}} \approx 10 \text{ Hz per particle}$. In our model, the collision of two particles in the lowest subband can lead to both being transferred to the highest subband, for a total number $N$ of particles we get a rate

$$\gamma^{\text{model}} = 2 \frac{d n_{a \rightarrow a}}{d t} N \text{ per particle.}$$

To connect to the experimental 2D setup, we extend our 1D model to 2D by assuming that particles collide and remain in the lowest Wannier band of the optical lattice. Based on the optical lattice depth of $V_g = 10 E_r$ this leads to $g_{2D} = 2 g_{3D}/d$. Further we assume confinement in the transverse direction, i.e. $L_z = \sqrt{\pi} a_z$ with $a_z$ the oscillator length in the transverse direction. The rate in our model then is

$$\gamma^{\text{model}} = \left( g_{2D}^2 / (d L_z h E_r) \Gamma_{a \rightarrow a}^{2D} \right) \rho$$

where we introduced the two dimensional particle density $\rho = N / (L_x L_y)$. For the experimental parameters of $\rho d^2 \approx 20$ and with $\Gamma_{a \rightarrow a}^{2D} = 0.25$ this yields $\gamma^{\text{model}} \approx 9 \text{ Hz}$. These simple considerations show that Floquet scattering might provide a viable explanation for the experimentally observed behaviour. We will give a more detailed account of the scattering processes for this experimental setup in Chapter 4.

Inelastic scattering within the same subband can be reduced by either working at larger $\hbar \omega / E_r$ as this then requires a large amount of energy to be absorbed in the $z$-direction or by working in sufficiently deep lattices in which the inelastic processes of the type discussed become strongly suppressed. Such inelastic scattering processes can also be eliminated by adding an additional optical confining potential in the transverse direction which depending on the parameters of the experiment might be required to avoid losses and heating.
3. Scattering Theory for Floquet-Bloch States

3.5. Summary

We have studied the scattering processes of Floquet-Bloch waves in periodically driven systems in the weakly interacting regime, as relevant to recent experiments creating artificial gauge fields for gases of cold atoms. We have demonstrated how "inelastic" scattering by static potentials can emerge in the Floquet framework as the potential is seen to be periodically-time dependent in the reference frame of the Floquet states. We have illustrated these general considerations in a simple toy model showing all the described properties.

We have developed a formalism that allows the computation of elastic and inelastic two-body scattering rates of particles in Floquet-Bloch states, and have illustrated the consequences for model systems that are representative of experimental situations: where energy can be absorbed through transitions into other Floquet-Bloch bands or to motion in weakly-confined directions. Notably we have shown that, in general, the scattering cannot be understood in terms of some effective time-independent Hamiltonian even for rapid modulation. Our results provide a framework by which the relative sizes of elastic and inelastic two-body scattering processes can be determined. As experiments move towards the realization of strongly correlated phases of matter in artificial gauge fields, it will be crucial to determine the parameter regions in which the elastic interactions which are responsible for the emergence of the interesting physics remain dominant compared to the inelastic processes which can limit the experimentally achievable temperatures through particle loss or heating.

The formalism we described relies on using the FFGR, the result of the Born approximation in first order in the interactions. Therefore, the results are limited to a regime in which this first order approximation is applicable. In particular, in the case of a strongly correlated phase interactions cannot be described in this way. However, the FFGR is still applicable in the case where $V$ are not the interactions leading to the strongly correlated phase, but rather a different additional interaction potential, and one may consider the stability of the (Floquet) phase under this perturbation within the FFGR.

A different approach is given by the interaction in the Floquet frame of reference Eq. (3.11). One might start by solving the non-interacting time-dependent problem and compute
the interactions in this basis. The interaction is seen to contain both static and oscillating parts, and if the static part is large compared to the time-dependent parts, one may try to treat them as a perturbation of a correlated state. In this way, one could build a many-body theory starting from the interactions in the Floquet frame, possibly treating the static part as leading to strong correlations and the time-dependent parts to Floquet scattering processes.

However, it should be noted that the application of the FFGR relies on being able to efficiently compute the matrix elements between all relevant states. In a strongly interacting (and time-dependent) system this is generically not possible.
3. Scattering Theory for Floquet-Bloch States

In this chapter we study the recent Floquet-realisation of the Harper-Hofstadter model in a gas of cold bosonic atoms [78, 81]. We study in detail the scattering processes in this system in the weakly interacting regime due to the interplay of particle interactions and the explicit time dependence of the Floquet states that lead to band transitions and heating. We focus on the experimentally used parameters and explicitly model the transverse confining direction. Based on transition rates computed within the FFGR we obtain band population dynamics which are in agreement with the dynamics observed in experiment. Finally, we discuss whether and how photon-assisted collisions that may be the source of heating and band population dynamics might be suppressed in the experimental setup by appropriate design of the transverse confining potential. The
suppression of such processes will become increasingly important as the experiments progress into simulating strongly interacting systems in the presence of artificial gauge fields.

4.1. Introduction

In Chapter 3 we described how within a perturbative treatment of interacting Floquet systems inelastic scattering associated with the absorption of quanta $\hbar \omega$ becomes possible which can lead to heating and band transitions. For heating due to two-particle collisions independent of the specific lattice and driving protocol considered, we found that the rates scale with the square of the corresponding interaction strength and scale linearly in the density of particles, and in the case of scattering into transverse dimensions can be further modified by changing the transverse density of states. Thus, appropriate design of the Hamiltonian might be used to suppress these processes, of paramount importance for experiments as deleterious heating and band transitions can limit the achievable lifetimes. Depending on the specific setup the microscopic processes leading to such energy absorption are slightly different. In all cases they can be understood as arising from the explicit time-dependence of the Floquet-states and the non-commutativity of the interaction with the time-evolution operator of the non-interacting system, see the discussion in Chapter 3. If in addition to the perturbative treatment of the interactions, the time-dependence is treated approximately, e.g. in a rotating wave approximation, or the time-evolution is further expanded in small parameters, e.g. the hopping on the lattice, the heating rates can be associated with a microscopic process, e.g. a particle hopping to a lower energy site and converting that potential energy into kinetic energy, which would be possible in a time-independent system, or a genuine Floquet process in which the particles absorb energy from the driving field and convert that into energy of motion [176]. For the system we consider below it is the second process which will be of most interest as it uniquely occurs in Floquet systems. This process will naturally scale with the amplitude of the driving field, quadratically within perturbation theory in the driving fields for small amplitudes, and as a complicated function for stronger driving.
4.2. Model and Single-Particle Physics

In this chapter we study the specific setup of the experiments which recently simulated the Harper-Hofstadter Hamiltonian [78, 81]. We apply the perturbative formalism we described in Chapter 3 to study heating and band transition processes in the experimentally used periodically modulated superlattice potential. We will treat the non-interacting time-dependent Hamiltonian exactly within Floquet theory and treat the particle-interactions perturbatively. Focusing on the effects of two-particle scattering processes, we identify the heating processes that arise from weak two-body interactions and the corresponding intra- and inter-band transition rates. We begin by introducing the model in Section 4.2 and obtain the single particle Floquet spectrum for the experimentally used parameters in Section 4.2.2. We proceed by introducing the Floquet scattering processes computed within the FFGR in Section 4.3.1. In Section 4.3.2 we obtain band population dynamics based on the Floquet scattering rates for the experimentally used parameters. Finding good agreement with the experimentally observed dynamics we then discuss in Section 4.3.3 whether these processes can be suppressed by appropriate design of the transverse confining potential. We show that strong suppression can be achieved under sufficiently strong confinement, suggesting a possible way to enable experiments to access strongly correlated quantum phases without the deleterious heating and repopulation dynamics demonstrated to be present in this Floquet system at weak confinement.

4.2. Model and Single-Particle Physics

4.2.1. Model

We study bosons described by a field-operator $\hat{\Psi}(x)$ loaded into a two-dimensional (2D) optical lattice with both time-dependent and static parts with additional transverse
confinement. The Hamiltonian is given by \( \hat{H} = \hat{H}_0(\tau) + \hat{H}_{\text{int}} \).

\[
\hat{H}_0(\tau) = \int \, d^3x \, \frac{-\hbar^2}{2M} \nabla^2 \Psi^\dagger(\mathbf{x}) \left( \partial_x^2 + \partial_y^2 + \partial_z^2 \right) \hat{\Psi}(\mathbf{x}) + \int \, d^3x \, \hat{\Psi}^\dagger(\mathbf{x}) [V(x, y, \tau) + V^z(z)] \hat{\Psi}(\mathbf{x}),
\]

\[
\hat{H}_{\text{int}} = \frac{g}{2} \int \, d^3x \, \hat{\Psi}^\dagger(\mathbf{x}) \hat{\psi}(\mathbf{x}) \hat{\Psi}(\mathbf{x}),
\]

where the first line of Eq. (4.1) describes the kinetic energy of the atoms moving in the optical lattice and the second line gives the time-dependent in-plane optical potential \( V(x, y, \tau) \) and the static transverse confining potential \( V^z(z) \) experienced by the atoms. The last part, Eq. (4.2), gives the contact interaction between atoms of strength \( g \). For the weak contact interactions considered here, \( g = 4\pi \hbar^2 a_s / M \) describes collisions with \( s \)-wave scattering length \( a_s \).

The in-plane optical lattice \( V(x, y, \tau) \) is a dynamical superlattice [200], which in the experiments of [81] can be written as \( V(x, y, \tau) = V_{\text{sl}}(x, y) + V_{\text{mod}}(x, y, \tau) \) with

\[
V_{\text{sl}}(x, y) = V_x \sin^2(k_r x) + V_{x\ell} \sin^2(k_r x/2) + V_y \sin^2(k_r y)
\]

where the static superlattice \( V_{\text{sl}}(x, y) \) consists of a short lattice in \( x(y) \) direction of strength \( V_x(V_y) \) and the long lattice with strength \( V_{x\ell} \) that creates the staggering along the \( x \)-direction with respective wave-vectors \( k_r \) and \( k_r/2 \). The time-dependent part \( V_{\text{mod}}(x, y, \tau) \) is

\[
V_{\text{mod}}(x, y, \tau) = \kappa \left[ \sin(\pi/4 + k_r x/2) \cos(\phi_0 + \omega \tau - k_r y/2) - \cos(\pi/4 + k_r x/2) \sin(\phi_0 - \omega \tau - k_r y/2) \right]
\]

where \( \kappa \) denotes the magnitude of the modulation oscillating with frequency \( \omega \), which is fixed to be on resonance with the energy staggering along the \( x \)-direction. Is is chosen such that the first and second line respectively restore tunnelling along each other bond in the staggered \( x \)-direction, see Fig. 4.2 for an illustration of the modulation pattern. We refer to the first and second line as the blue and red part respectively for two reasons. Firstly, as the modulations address each other bond respectively, the blue (red) modulation pattern is seen to restore tunnelling along bonds with a negative (positive) energy-offset.
4.2. Model and Single-Particle Physics

Figure (4.2) In the left panel modulation pattern $V_{\text{mod}}(x, y = 0, \tau)$, split into the blue (top-panel) and red (bottom panel) part, corresponding to the first and second line of Eq. (4.4) respectively. Right panels show $V_{\text{mod}}(x_i, y = 0, \tau)$ at the lattice sites $x_i = i d$ of the static potential corresponding to the colour-coded sites in the left panels. The blue-laser induces a differential modulation between sites 0 and 1 (and periodically at every other bond) and restores tunnelling between these sites, sites 1 and 2 are modulated in phase and tunnelling is thus not affected. The modulation pattern of the red-laser is offset by one site in space and a quarter period in time, and addresses the other bonds, e.g. sites 1 and 2 are differentially modulated. The blue (red) modulation pattern therefore restores tunnelling along bonds with a negative (positive) energy-offset of the static superlattice.
of the static superlattice. Secondly, in the experiment the laser beams creating the red and blue potential are actually realised as the red and blue sidebands around the original laser frequency of a single beam.

The phase $\phi_0$ is not controlled in the experiment. Physically, it corresponds to the phase of the running laser beams in the $y$-direction, i.e. changing $\phi_0$ moves the time-dependent potential along $y$ in relation to the underlying static lattice. The phase $\phi_0$ changes the physics of the effective time-independent model only in higher orders in $\kappa/(\hbar\omega)$ and leads to an inhomogeneous hopping along the $y$ direction as discussed in [81], with the conclusion that the effects are within the experimental uncertainties. For simplicity, we use $\phi_0 = \pi/4$ in the following; we have checked that the results are not changed significantly for a different choice.

The transverse confinement potential is taken to be either an optical lattice $V_z^{\text{lat}} = V_z \cos^2(k_z^x z)$ or a harmonic trap $V_z^{\text{osc}} = \frac{1}{2} m \omega_{\text{osc}}^2 z^2$ which is the potential actually used in the experiment.

In the tight-binding description the time-dependent model can be mapped to the Harper-Hofstadter model via the use of the high-frequency approximation as outlined in [81] with the result

$$\hat{H}_{\text{eff}} = t_x^{\text{eff}} \sum_{m,n} \hat{a}^\dagger_{m+1,n} \hat{a}_{m,n} e^{i(\pi/2(m+n) - \phi_0)} + \text{h.c.} \quad (4.5)$$

$$- t_y \sum_{m,n} \hat{a}^\dagger_{m,n+1} \hat{a}_{m,n} + \text{h.c.} \quad (4.6)$$

$$+ \hat{H}_{\text{int}} \quad (4.7)$$

where $\hat{a}_{m,n}$ creates a boson at lattice-site $(m, n)$ defined with respect to the short lattice, i.e. $x_{m,n} = (md, nd)$ with $d = \pi/k_r$. Tunnelling along the $x$-lattice was restored by the time-periodic modulation pattern with an effective strength $t_x^{\text{eff}} = t_x \frac{\kappa}{\sqrt{2 \hbar \omega}}$, and $t_x$ ($t_y$) are the original tunnelling couplings along $x$ ($y$) directions. We also see that the time-modulation leads to complex hopping phases in the $x$-direction corresponding to a uniform flux $\Phi = 2\pi/4 = \pi/2$ per plaquette. The band structure of the model turns out to consist of 4 topological bands, two each with Chern-numbers $C = 1, -1$. The groundstate band has Chern number $C = 1$ and is the one targeted in the experiment. In
4.2. Model and Single-Particle Physics

Figure (4.3) Resulting Floquet band structure $E_n(k_x, k_y)$ in units of the recoil-energy $E_r = \hbar^2 k^2_r / (2M)$ as a function of momentum $k_x$ and $k_y$ in the reduced BZ of the non-interacting model, Eq. (4.1), for the parameters $V_x = 6E_r$, $V_{xl} = 0.8E_r$, $V_y = 10E_r$, $\kappa = 0.58 \hbar \omega$ and $\hbar \omega = 0.72E_r$. The Floquet band structure shows 4 bands of which the middle two are touching at the borders of the reduced BZ and combined into a single superband.

In the following we will treat the system beyond the tight-binding description and discuss the experimentally observed bandpopulation dynamics in terms of our theory of Floquet scattering.

4.2.2. Single-Particle States and Band Structure

We proceed to obtain the single-particle Floquet spectrum of the non-interacting time-dependent Hamiltonian $\hat{H}_0(\tau)$. Due to the separability of the non-interacting Hamiltonian we may focus on the particle spectrum of the in-plane ($x\text{-}y$) motion, i.e. wavefunctions take the form $\Psi(x, y, z, \tau) = \Psi^{2D}(x, y, \tau) \Psi^z(z)$ and energies are given by $E_{n,k,n^z} = E_{n,k}^{2D} + E_{n^z}^z$. As the Hamiltonian is invariant under discrete temporal and spatial translations the solutions take the form of Floquet-Bloch waves.

We note that the static potential has the following symmetries, $V_{st}(x + 2d, y) = V_{st}(x, y + d) = V_{st}(x, y)$ with the lattice spacing $d = \pi / k_r$. We may choose a unit cell of $2 \times 2$ sites and each Bloch-band will split into 4. However, the time-dependent part has a lower symmetry, $V_{\text{mod}}(x + 4d, y, \tau) = V_{\text{mod}}(x, y + 4d, \tau) = V_{\text{mod}}(x, y, \tau)$, and naively, this would
lead to a real space unit cell of $4 \times 4$ sites and to a splitting into 16 bands. However, the unit cell can be reduced by rewriting $V_{\text{mod}}$ as

$$V_{\text{mod}}(x, y, \tau) = e^{i\omega\tau} F(x, y) + e^{-i\omega\tau} F^*(x, y)$$

(4.8)

with quasi-periodic $F(r + R_j) = e^{iG \cdot R_j} F(r)$ where $G = (\pi/(2d), \pi/(2d))$. This allows us to perform a unitary gauge-transformation in Floquet-space as done in [200] and obtain a Hamiltonian invariant under translations by 2 lattice sites in both $x$- and $y$-directions which is described in detail in Appendix C.1. Consequently, we may keep the unit cell consisting of $2 \times 2$ sites with each band split into 4 and exactly expand the time-dependent problem in the Bloch-states of the time-independent problem as they now share the same periodicity. We project the full time-dependent Schrödinger equation on the set of the 4 lowest Bloch-bands of $V_{\text{st}}$ which are resonantly coupled by the time-dependent optical potential $V_{\text{mod}}$. Moreover, in the expansion of the Floquet-states, $\Psi_c(\tau) = e^{i\epsilon t} \Phi_c(\tau) = e^{i\epsilon t} \sum_m \phi_m e^{im\omega\tau}$, we keep only a finite number of frequency components $-M \leq m \leq M$ with sufficiently high $M$ to ensure convergence of both the spectrum and wavefunctions.

A plot of the resulting band structure is shown in Fig. 4.3 which shows the 4 Harper-Hofstadter bands in the reduced Brillouin zone corresponding to the $2 \times 2$ real-space unit-cell. Following the convention in [78] we refer to the middle two bands as a single band as they are not separated by an energy gap. We emphasise that this calculation does not rely on the tight-binding limit or on a high-frequency approximation, but is the solution of the full non-interacting time-dependent Schrödinger equation.

### 4.3. Interaction Effects

#### 4.3.1. Floquet-Scattering

We treat the effects of the collisions of the atoms described by the interaction Hamiltonian (Eq. (4.2)) in the framework of the scattering theory for Floquet states we developed
4.3. Interaction Effects

in Chapter 3. We employ the FFGR to compute transition rates from an initial state \( \Psi_i \) to final state \( \Psi_f \) given by

\[
\gamma_{i\rightarrow f} = \sum_{\Delta m} \frac{2\pi}{\hbar} \delta(e_i^0 - e_f^0 - \Delta m \hbar \omega) |\langle \Phi_f^{\Delta m} | \hat{H}_{\text{int}} | \Phi_i^0 \rangle|^2
\]  

(4.9)

Using the FFGR will preclude the discussion of strongly correlated many-body phases, but is appropriate for the regime of weakly-interacting particles considered here and sufficient to explore the two-particle physics that are a potential source of heating and band repopulation.

We take the initial state to contain particles in any bands \( n_1 \) and \( n_2 \) with in-plane quasi-momentum \( k_1 \) and \( k_2 \) of the 2D band structure in states \( n_1^z \) and \( n_2^z \) of the transverse potential, i.e. they are of the form

\[
|\Psi_i \rangle = \hat{\Psi}^{a\dagger}_{n_1,k_1,n_1^z} \hat{\Psi}^{a\dagger}_{n_2,k_2,n_2^z} |\text{vac} \rangle.
\]  

(4.10)

The interaction couples these to final states containing two particles in bands \( n_3 \) and \( n_4 \) with quasi-momentum \( k_3 \) and \( k_4 \) in states \( n_3^z \) and \( n_4^z \)

\[
|\Psi_f \rangle = \hat{\Psi}^{a\dagger}_{n_1,k_1,n_3^z} \hat{\Psi}^{a\dagger}_{n_4,k_4,n_4^z} |\text{vac} \rangle.
\]  

(4.11)

In the calculations of the population dynamics in Section 4.3.2 we only keep transitions with emission and absorption of up to a single energy quantum \( \hbar \omega \), i.e. \( \Delta m = 0, \pm 1 \) in the FFGR as transitions with higher energy transfers are successively suppressed as shown in Fig. 4.4. Note that we still have to keep a high number \( M \) of Floquet modes in the expansion of the Floquet states used to compute the rates.

The exponential decay of these transition-matrix elements also justifies our restriction to the lowest 4 Harper-Hofstadter bands. Whereas transitions into the higher bands are allowed within the FFGR, for the experimental parameters they correspond to a transition with \( \Delta m \approx 11 \) and are thus negligible on the time-scales we are interested in. This argument applies rather generally and does not rely on the precise form of the wavefunctions, but only on the fact that the higher bands are gapped in the static Hamiltonian and that the Floquet states are exponentially localised in the frequency

\[ I_{\Delta m} = |\langle \langle \Phi_{\Delta m}^{f}(x, y) | \hat{H}_{\text{int}} | \Phi_{0}^{i}(x, y) \rangle \rangle|^{2} \]

\[ \Delta m \]

Figure (4.4) Overlap matrix element \( I_{\Delta m} = |\langle \langle \Phi_{\Delta m}^{f}(x, y) | \hat{H}_{\text{int}} | \Phi_{0}^{i}(x, y) \rangle \rangle|^{2} \) of the wavefunctions of the two-dimensional model for a band-transition \((1, 1) \rightarrow (3, 3)\) summed over the final state momenta and averaged over the initial state momenta as a function of the photon transfer \( \Delta m \) normalised to the element at \( \Delta m = 0 \).

domain, thus, leading to the observed exponential suppression of the matrix elements. In addition, it establishes that the elastic \((\Delta m = 0)\) rates are stronger than the Floquet \((\Delta m \neq 0)\) rates in this system. We emphasise that this exponential decay allows to greatly reduce Floquet scattering by suppressing transitions with \( \Delta m = \pm 1 \) and achieve a regime in which Floquet scattering rates become negligible compared to the elastic rates.

4.3.2. Band Population Dynamics

We proceed to compute the resulting band population dynamics based on the Floquet transition rates, Eq. (4.9), for the experimental parameters, i.e. \( V_{x} = 6E_{r}, V_{xl} = 0.8E_{r}, V_{y} = 10E_{r}, \kappa = 0.58\hbar\omega \) with \( E_{r} = \frac{\hbar^{2}k_{r}^{2}}{2M} \), \( k_{r} = \pi/d \) and \( d = 0.5 \times 767 \text{ nm} \), the modulation frequency is \( \hbar\omega = 0.72E_{r} \) and the experimentally used harmonic confinement given by \( V_{osc}^{z} = \frac{1}{2}M\omega_{osc}^{2}z^{2} \) with \( \omega_{osc} = 12\text{Hz} \). We use the value of the scattering length for \(^{87}\text{Rb}\) and the experimental density for which \( Nd^{2}/(L_{x}L_{y}) \approx 20 \) with the number of particles \( N \) and the lattice size \( L_{x} \) \((L_{y})\) in the \( x \) \((y)\)-direction. We assume that the distribution of atoms in the bands is incoherent and that the particles are homogeneously spread over the full BZ. This assumption has been verified explicitly in the experiment [81]. Thus, we will average all rates over the initial state momenta. In addition, we will not consider
4.3. Interaction Effects

Figure (4.5) Data with errorbars: experimental data from [81] supplied by the corresponding author, solid lines: results of the rate model. Dynamics of the fractional band populations $n_{\mu} = \sum_{n_z} \frac{N_{\mu,n_z}}{N_{\text{total}}}$ in the Floquet realization of the Harper-Hofstadter model for the experimental parameters with a transverse harmonic confinement summed over the $n_z$ oscillator quantum number. Colours correspond to the bands shown in Fig. 4.3.

the effects of elastic scattering, as the initial state is already completely spread over each band and elastic scattering is not expected to change the distribution further. Finally, the assumption of an incoherent distribution and scattering justifies to model the dynamics via a rate model of band populations, rather than considering coherent scattering of (condensed) Bogoliubov quasi-particles.

We start from the transition rate $\gamma_{i\rightarrow f}$ given by the FFGR (Eq. (4.9)) where the states are characterised by $(\mu_1, k_1, n_1^z, \mu_2, k_2, n_2^z)$ giving the band-index $\mu_i$ of the 2D band structure, the two-dimensional in-plane momentum $k_i$ and the oscillator state label $n_i^z$ of the transverse confinement. As described above, the rate is exponentially suppressed in $\Delta m$ and we only keep the terms with $\Delta m = 0, 1$. We define a superindex $\alpha = (\mu, n_z)$ combining the band-index of the 2D band structure and the oscillator state label, and define the band-averaged transition rates as

$$
\gamma^{\text{av}}_{(\alpha,\beta)\rightarrow(\gamma,\delta)} = \left(\frac{2d}{\pi}\right)^4 \left(\frac{L_x L_y}{(2\pi)^2}\right)^2 \int_{BZ} d^2k_1 d^2k_2 d^2k_3 d^2k_4 \gamma_{i\rightarrow f} \quad (4.12)
$$
Then, we can write a rate-model for the single-particle state populations \( n_{\alpha} \) of the form

\[
\frac{dn_{\alpha}}{d\tau} = \sum_{\alpha', \beta', \gamma', \delta'} V^{\alpha\alpha'}_{(\alpha', \beta', \gamma', \delta')} \left[ (\delta_{\alpha, \gamma'} + \delta_{\alpha, \delta'}) - (\delta_{\alpha, \alpha'} + \delta_{\alpha, \beta'}) \right] n_{\alpha'} n_{\beta'} .
\]  

(4.13)

The dynamics for the fractional band occupations \( n_{\mu} = \sum_{n^z} n_{\mu, n^z} / N_{\text{total}} \) summed over the states of the transverse confining harmonic potential are shown in Fig. 4.5. We compare the experimental results shown as circles with errorbars to our theoretical predictions shown as the solid lines, based on a calculation with initial fractional occupations of \( n_1 = 0.6, n_2 = 0.3 \) and \( n_3 = 0.1 \), all assumed to be initially in the \( n^z = 0 \) state. Our results are seen to compare favourably with the experimental results. The mean summed absolute differences between the experimental data and the theory curves \( 1/N_{\tau} \sum_{i} |n^{\text{th}}_{\mu}(\tau_i) - n^{\exp}_{\mu}(\tau_i)| \), where the sum runs over a total of \( N_{\tau} \) times \( \tau_i \), are 0.03, 0.02 and 0.02 for the first, second and third band respectively. In the calculation the population in the first band remains slightly too high, whereas the population in the third band is slightly too low compared to the experimental data. Given the approximations made in reducing the scattering and dynamics to a simple rate model, and that the model does not contain any fitting parameters, the agreement is surprisingly good.

We observe two time scales for the population dynamics. On a fast time-scale elastic \((\Delta m = 0)\) collisions of the type \((1, 3) \rightarrow (2, 2)\) and the reverse process redistribute particles between the bands while conserving the in-plane motion energy, i.e. the transverse motion quantum numbers \( m^z_i = m^z_f \) are conserved. As expected from Fig. 4.4 these occur considerably faster than the Floquet \( \Delta m \neq 0 \) transitions. This initially leads to an increase of the population in band 2 and the corresponding decrease of populations in band 1 and 3, while keeping all particles in the \( n^z = 0 \) states of the transverse potential. For the initial conditions, these processes achieve a quasi-equilibrium on a very short time-scale stopping further redistribution. For longer times Floquet transitions \((\Delta m = \pm 1)\), changing both the Hofstadter bands and allowing transfer into higher energy states of the tranverse direction \( m^z_i \neq m^z_f \), become relevant. The interplay of the elastic and the inelastic collisions is seen to reverse the initial decrease in population of band 3. As the higher states of the transverse potential are occupied the reverse scattering processes become important and slow down the population dynamics after a time scale of about 10
4.3. Interaction Effects

Figure (4.6) Total absorbed energy $\Delta E(\tau) = E(\tau) - E(\tau = 0)$ per particle in units of $E_r$ in the Floquet realization of the Harper-Hofstadter model for the experimental parameters with a transverse harmonic confinement.

ms. The further dynamics is seen to be slower explained by the fact that the higher states of the transverse potential are less strongly interacting. Finally, the system approaches a state in which all Harper-Hofstadter bands are equally populated over a timescale of 200 ms.

We remark that even though the Harper-Hofstadter band populations approach a steady state, the system slowly continues to heat up in the transverse direction. The total absorbed energy $\Delta E(\tau) = E(\tau) - E(\tau = 0)$ per particle in units of $E_r$ is shown in Fig. 4.6. After an initial period of fast energy absorption the rate flattens out. This is due to the fact that the interactions become weaker as the particles are transferred to higher $n^z$ states.

In the beginning all particles occupy $n^z = 0$ states and are strongly interacting. The $\Delta m = \pm 1$ photon transitions then establish an equilibrium between states at $n^z = 0$ and $n^z = n^z_\omega = \hbar \omega / E_{osc}$. Consequently, particles in the $n^z_\omega$ states would be scattered to states in the $n^z = 2n^z_\omega$ state. The timescale for this to happen is controlled by the square of the ratio of the matrix elements $\langle \Psi_{n^z_\omega/2}^z \Psi_{n^z_\omega/2}^z | \hat{H}_{int} | \Psi_{n^z_\omega/2}^z \Psi_{n^z_\omega/2}^z \rangle$ and $\langle \Psi_0^z \Psi_0^z | \hat{H}_{int} | \Psi_{n^z_\omega/2}^z \Psi_{n^z_\omega/2}^z \rangle$ which is approximately 0.06, yielding transition rates 3 orders of magnitude lower. We observe that the total absorbed energy per particle remains small compared to the bandgaps of the undriven system, thus, being consistent with only considering the 4 lowest bands for these time scales.

We conclude that the strong inter-band population dynamics and the associated heating stemming from $\Delta m = \pm 1$ transitions would make the realization of strongly interacting
phases exceedingly difficult unless proper care is taken to suppress the corresponding processes.

### 4.3.3. Stability Regions and Scattering Rates

Based on the conservation of quasi-energy in the FFGR (Eq. (4.9)) and the specific experimental parameters, one can readily envisage ways in which the transverse density of states can be adapted in order to make the system stable to the two-particle scattering processes with \( \Delta m = \pm 1 \) which cause band transfer and lead to heating.

We keep the optical lattice potential in the \( x-y \) plane the same as in the experimental setup as discussed above. In particular, we keep \( \hbar \omega = 0.72E_r \). We consider the cases in which the transverse potential in the \( z \)-direction is either an optical lattice \( V_{\text{lat}}^z = V_z \cos^2(k_z r_z) \) of depth \( V_z \) with associated energy scale \( E_r^z = \frac{(k_z^2)^2}{2M} \) or a harmonic trap \( V_{\text{osc}}^z = \frac{1}{2}M\omega_{\text{osc}}^2z^2 \) with associated energy \( E_{\text{osc}} = \hbar \omega_{\text{osc}} \). For both cases we investigate whether particles in the ground state band\(^1\) of the Harper-Hofstadter model can possibly undergo transitions with \( \Delta m = \pm 1 \) depending on the strength of the transverse potential and compute the resulting scattering rates.

The results for confinement by an optical lattice are shown in Fig. 4.7 and Fig. 4.8 respectively showing the stability diagram and the rates, and both the stability diagram and the rates for the case of the harmonic trap are shown in Fig. 4.9. The stability diagrams are based purely on kinematic constraints on the scattering process and is therefore valid for two-particle scattering beyond the applicability of the FFGR. We conclude that by sufficiently strong transverse potential the inelastic two-particle single-photon-transfer scattering processes can be completely suppressed.

For the discussion of the scattering rates in this section we assume an initial state in the unique lowest energy state of the transverse direction, i.e. \( n_1^z = n_2^z = 0 \) for harmonic confinement, and define a total dimensionless rate for transitions \( \Gamma_{(n_1,n_2) \rightarrow (n_3,n_4)} \) taking the initial state to be \( (n_1,k_1,0; n_2,k_2,0) \), summing over the final state momenta \( k_3 \) and \( k_4 \)

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\(^1\)While generically there is no preferred ordering of the bands in the Floquet BZ and therefore no ground state we use this notion based on the character of the bands in terms of bands of the undriven Hamiltonian.
4.3. Interaction Effects

Figure (4.7) In (a) stability of the groundstate band of the Harper-Hofstadter model to different inelastic transitions as indicated in the figure in the case of transverse confinement by an optical lattice \( V_{\text{lat}} = V_z \cos^2(k_z z) \) of strength \( V_z/E_r \) with \( E_r = E_r \). A jump from 0 to 1 indicates the change of allowed to forbidden for the respective transition. In (b) the critical confinement strength \( V_z/E_r \) required to suppress the \( \Delta m = \pm 1 \) transitions as a function of \( E_r/E_r \). In all cases \( \hbar \omega = 0.72 E_r \).

We begin by discussing the case in which the transverse potential is an optical lattice shown in Fig. 4.7. For vanishing depth, \( V_z = 0 \), we recover the situation of free particles where the system can always absorb energy and is therefore unstable. As we increase the lattice depth \( V_z \), the transition with the smallest energy transfer, the intraband scattering transition \((1, 1) \rightarrow (1, 1)\), is suppressed first, and those with higher energy transfer are consecutively suppressed until finally the last transition, \((1, 1) \rightarrow (3, 3)\), becomes energetically forbidden and the system is stable to single photon (\(\Delta m = \pm 1\)) transitions. This happens when the density of states in the transverse direction vanishes for the

Figure (4.8) Scattering rates $\Gamma_{(n_1,n_2)\rightarrow(n_3,n_4)}$ for the band indicated in the figure in the case of transverse confinement by an optical lattice $V_{\text{lat}}^z = V_z \cos^2(k_r^2 z)$ for $E_r^z = E_r$ in panel (a) and $E_r^z = 0.36E_r$ in (b) corresponding to the minimum of $V_z^z$ observed in Fig. 4.7. The modulation frequency is $\hbar \omega = 0.72E_r$.

required energy transfer, i.e. for these parameters when the bandwidth of the lowest band in the transverse direction becomes smaller than $\hbar \omega - 2[\max(E_3) - \min(E_1)]$. Additionally, we may change the ratio $E_z^r/E_r$ which determines the critical value of the confinement strength as shown in the right panel of Fig. 4.7 which is minimised at $V_z = 1.5E_r^z$ for $E_z^r/E_r = 0.36$.

The corresponding transition rates for $E_z^r = E_r$ are shown in Fig. 4.8. These start from the finite non-zero value at $V_z = 0\) expected for free particles, and increase with increasing $V_z$ to reach a maximum. This maximum occurs at the point at which there is a closing of the channel for scattering into higher transverse modes, and arises from the characteristic singular density of states of the transverse lattice at the edges of the BZ. Thus, we see that the transverse optical lattice at first increases the scattering rates until it finally completely suppresses two-particle single-photon scattering for sufficiently deep lattices.

In addition to the lattice depth $V_z/E_r^z$ which determines the form of the density of states in the transverse direction, changing the ratio $E_z^r/E_r$ which effectively rescales the energy axis of the transverse direction compared to the 2D Harper-Hofstadter model can be used to control the scattering rates. This effect can be understood by the fact that at fixed $V_z/E_r^z$ reducing $E_z^r/E_r$ implies that the particles in the transverse direction are less strongly localised and thus subject to weaker interactions.

For the harmonic trap the behaviour is slightly more complicated as seen in Fig. 4.9.
4.3. Interaction Effects

**Figure (4.9)** Stability of the groundstate band of the Harper-Hofstadter model to different inelastic transitions as indicated in the figure in the case of transverse confinement by a harmonic potential \( V_{\text{osc}} = \frac{1}{2} M \omega_{\text{osc}}^2 z^2 \) in panel (a) and corresponding scattering rates in panel (b) both as a function of the oscillator energy \( E_{\text{osc}} = \hbar \omega_{\text{osc}} \) in terms of the recoil energy \( E_r \). The modulation frequency is \( \hbar \omega = 0.72E_r \).

Again for no transverse potential, \( E_{\text{osc}} = \hbar \omega_{\text{osc}} = 0 \), we recover the behaviour of the free system. As we increase the confinement energy \( E_{\text{osc}} \) transitions become possible and forbidden whenever the required transition energy matches an integer number of the oscillator energy. For weak confinement, this typically includes a range of possible final oscillator states for a given band-transition which shrinks with increasing confinement. The system is stable to single-photon \( (\Delta m = \pm 1) \) transitions when the energy balance equation \( 2n\hbar \omega_{\text{osc}} = \hbar \omega - E_{\text{trans}} \) has no solution with integer \( n \) for all band transitions. Here we obtain two stability regions, one in the intermediate regime around \( \omega_{\text{osc}} \approx \omega/3 \) and one for strong confinement \( \omega_{\text{osc}} \gtrapprox \omega/2 \).

In both cases, by sufficiently strong modifications of the transverse density of states, the single photon \( (\Delta m = \pm 1) \) transitions can be completely suppressed. However, in that regime the next to leading order processes of transitions with \( \Delta m = \pm 2 \) may still be present. Due to the localisation of the Floquet modes observed in the overlap matrix elements seen in Fig. 4.4 and the suppression due to the interaction matrix elements they are at least 2 orders of magnitude smaller than the elastic \((\Delta m = 0)\) rates.

4.4. Conclusions

We have studied the two-particle scattering processes occurring in the Floquet-realisation of the Harper-Hofstadter Hamiltonian focusing on the experimental setup used in [78, 81] involving a dynamically modulated superlattice potential. Using the FFGR we have calculated scattering rates due to particle interactions. Importantly, we observe an exponential localisation in Floquet space of the wavefunctions and consequently an exponential decay of the scattering rates with photon transfer $\Delta m$ seen in Fig. 4.4. Fundamentally, this is the reason why one may hope to achieve a regime in which elastic scattering is strongly dominant over inelastic Floquet processes.

Based on the Floquet transition rates we obtain the resulting band population dynamics and compare to the experimental results of [81]. The agreement between the experimental result and the predictions of this rate model suggests that two-particle processes and the Floquet scattering rates might play an important role in establishing the band dynamics and the heating rates in this system. Of particular relevance to the stability of a Bose-Einstein condensate (BEC) in one of the Harper-Hofstadter bands, we observe that the scattering rates do not depend strongly on the final state momenta. Consequently, an initial BEC quickly spreads over the BZ and into other subbands. We remark that in a different experimental realisation of the Harper-Hofstadter model [118] heating processes have been investigated very carefully and two-particle scattering was found not to be the limiting factor for the lifetimes in that setup. The reported lifetimes of the order of 70ms seem to be limited by technical noise in the experiment.

More generally, our study provides insight into the heating dynamics of a closed quantum system with an unbounded dispersion subject to periodic driving. We find a timescale over which the system approaches an infinite temperature state for the bounded degrees of freedom of the in-plane motion and a generically different time-scale over which the system then continues to heat up in the transverse direction.

Having established these processes in the Floquet system with the geometry of [78, 81], we discussed how these rates can be influenced by additional transverse confinement. We studied transverse confinement by both an optical lattice and a harmonic potential and concluded that by choosing a sufficiently strong confinement inelastic single photon
4.4. Conclusions

transitions with the absorption or emission of $\hbar \omega$ can be suppressed completely. Moreover, in the case of confinement by an optical lattice, the scattering rates can be further controlled by choosing an optimal values for the ratio $E_z/E_r$ in addition to the lattice depth $V^z$. By suppressing the single-photon $\Delta m = \pm 1$ rates one can achieve a regime in which the next order Floquet processes $\Delta m = \pm 2$ are at least two orders of magnitude smaller than the elastic $\Delta m = 0$ rates which are responsible for establishing the strongly correlated behaviour of the quantum system. This possibility to strongly suppress the two-particle inelastic scattering rates provides one possible route towards the design of future experiments aiming to access strongly interacting regimes without deleterious scattering and heating.
5. Synthetic Dimensions in the Strong-Coupling Limit: Supersolids and Pair-Superfluids

**Figure (5.1)** Sketch of a gas of ultracold atoms with spin $I = 3/2$ with internal states $m_z = -3/2, -1/2, 1/2, 3/2$ confined in a one-dimensional optical lattice. Spin states are coupled via Raman transitions of strength $\Omega$ endowed with a running phase $\phi(x)$. Particles can hop along the lattice with amplitude $t$ and particles interact via a SU($2I + 1$)-invariant density-density on-site interaction $U$.

In this chapter we study the many-body phases of bosonic atoms with $N$ internal states confined to a 1D optical lattice under the influence of a synthetic magnetic field and strong repulsive interactions. The $N$ internal states of the atoms are coupled via Raman transitions creating the synthetic magnetic field in the space of internal spin states corresponding to recent experimental realisations. The system for the case of $N = 4$ internal states is sketched in Fig. 5.1. We focus on the case of strong SU($N$) invariant local density-density interactions in which each site of the 1D lattice is at most singly occupied, and strong Raman coupling, in distinction to previous work which has focused on the weak Raman coupling case. This allows us to keep only a single state per site and derive a low energy effective spin $1/2$ model. The effective model contains first-order nearest neighbour tunnelling terms, and second-order nearest neighbour interactions and correlated next-nearest neighbour tunnelling terms. By adjusting the
flux $\phi$ one can tune the relative importance of first-order and second-order terms in the effective Hamiltonian. In particular, first-order terms can be set to zero, realising a novel model with dominant second-order terms. We show that the resulting competition between density-dependent tunnelling and repulsive density-density interaction leads to an interesting phase diagram including a supersolid (SS) and a phase with long-ranged pair-superfluid correlations. The method can be straightforwardly extended to higher dimensions and lattices of arbitrary geometry including geometrically frustrated lattices where the interplay of frustration, interactions and kinetic terms is expected to lead to even richer physics.

5.1. Introduction

We will focus on one-dimensional systems with a finite synthetic dimension composed of $N = (2I + 1)$ spin states coupled by laser beams in such a way as to create an artificial magnetic field as described in Section 1.2.5. Thus, they can alternatively be considered as frustrated $N$-leg ladders. Optical lattice experiments with cold atoms motivate the study of both bosonic [201–206] and fermionic systems [127–129, 207–213]. The predicted behaviour includes chirally ordered phases [202], vortex phases [204], magnetic crystals and quasi-1D analogues of fractional Quantum Hall states [127, 128, 212]. At the centre of these phenomena is the interplay of the gauge fields and the SU$(2I + 1)$ symmetric interactions [59–62]. The natural SU$(2I + 1)$ symmetry of the interactions between the spin states implies, in the interpretation of a ladder, that the interactions are infinitely ranged along the synthetic dimension and short-ranged along the real dimension in contrast to the situation usually considered in the solid-state context. We remark that therefore the limit of hardcore interactions of bosonic particles does not correspond to a Tonks-Girardeau gas [28, 214, 215] and the system does not reduce to free fermions.

Prior studies have focused on the weak Raman coupling case in which one obtains helical states and edge currents [127]. In contrast we will study the case of strong Raman coupling and strong interactions, focusing on an effective model of hardcore bosons/spinless fermions in these limits which can alternatively be understood in terms
of an effective pseudo spin-1/2 system. Our main focus will be on a regime in which the physics is dominated by the interplay of density-density interactions and correlated tunnelling terms. This will lead to a competition between phase-separation and charge-order, and normal superfluidity and pair-superfluidity.

In 2D pair-superfluids can be realised using the long-range interactions of dipolar quantum gases [216, 217] and confining them in bi-layer geometries [218–220]. In a mean field analysis the presence of correlated tunnelling allows the condensation of pairs of particles described by an operator $\hat{b}$, i.e. $(\langle \hat{b}_i \hat{b}_j \rangle \neq 0)$, in the absence of single-particle condensation $(\langle \hat{b}_i \rangle = 0)$ [221] Generically, correlated tunnelling can be understood to act as an attractive interaction between the bosons favouring pair formation, and the repulsive nearest neighbour interaction is required to avoid collapse [222] or phase-separation [223]. Correlated tunnelling has been shown to lead to pair-superfluidity for bosons in 2D [223] and in 1D [224, 225] in theoretical studies, but the required models are hard to realise experimentally.

We propose a way to realise a (quasi) pair-condensed phase of ultracold atoms starting from an experimentally realised system. We do not require special (long-range) interactions or complicated lattice geometries. The proposed scheme is applicable to both fermions and bosons, but we will limit the discussion to the bosonic case here. We do not assume specially engineered Raman couplings of the spin states to obtain homogeneous couplings along the synthetic dimension or periodic boundary conditions which are hard to realise experimentally for large number of internal spin states, but consider the highly non-homogeneous couplings and open boundary conditions along the synthetic dimension which occur naturally for $I > 1$ due to the nature of the atom-light interaction.

We introduce the full model and the effective model derived in the limits of large Raman coupling and strong interactions in Section 5.2. Importantly, the coupling constants will turn out to depend on the flux $\phi$, and the freedom in tuning both the flux and the number of spin states $2I + 1$ allows great control and freedom in engineering the resulting effective Hamiltonian. In Section 5.3 we will focus on the special case of flux $\phi = \pi$ in which the first order terms vanish and investigate the behaviour resulting from the dominant second order terms in the effective model. By employing Density-Matrix-Renormalization Group
(DMRG) calculations [226] the phase-diagram of the effective model is obtained, and described in Section 5.3.1. Based on the analysis of correlation functions and the von-Neumann entropy we establish a phase-diagram containing a charge-density wave (CDW) at half-filling, a supersolid phase (SS) with simultaneous charge-density wave order and superfluid correlations, and a (quasi) pair-superfluid phase.

5.2. Model

\[ \hat{H} = \hat{H}_1 + \hat{H}_2 + \hat{H}_{\text{int}}. \]

\[ \hat{H}_1 \]

\[ m_z = 3/2 \]

\[ m_z = 1/2 \]

\[ m_z = -1/2 \]

\[ m_z = -3/2 \]

\[ j = 1 \]

\[ j = 2 \]

\[ j = 3 \]

\[ \sqrt{3}\Omega e^{i\phi} \]

\[ \sqrt{3}\Omega e^{2i\phi} \]

\[ \sqrt{3}\Omega e^{3i\phi} \]

\[ 2\Omega e^{i\phi} \]

\[ 2\Omega e^{2i\phi} \]

\[ 2\Omega e^{3i\phi} \]

\[ U \]

\[ \Phi \]

Figure (5.2) Graphical illustration of the original model Hamiltonian for atoms with \( I = 3/2 \) in the interpretation of a ladder system. Note the highly inhomogeneous couplings along the spin direction, and the dependence of the complex hopping phase on the site index \( j \) in the \( x \)-direction. The interaction \( U \) is infinite-range along the spin-direction, but of contact type along the real \( x \) direction. The phase-pattern shown here corresponds to a gauge-invariant flux of \( \Phi = \phi/(2\pi) \) through each plaquette.

We consider spinful bosons with \( N = 2I + 1 \) internal spin states loaded into a one-dimensional optical lattice described by a Hamiltonian \( \hat{H} = \hat{H}_1 + \hat{H}_2 + \hat{H}_{\text{int}}. \hat{H}_1 \) describes
the bosonic hopping along the lattice,

$$\hat{H}_1 = -t \sum_j \sum_{m_z=-I}^I \left( \hat{c}_{j+1,m_z}^{\dagger} \hat{c}_{j,m_z} + h.c \right)$$  \hspace{1cm} (5.1)

where $\hat{c}_{j,m_z}^{(\dagger)}$ are bosonic operators annihilating (creating) bosons in spin state $m_z$ at site $j$ and $t$ is the hopping amplitude. $\hat{H}_2$ describes the Raman coupling of the internal spin states via

$$\hat{H}_2 = -\sum_j \sum_{m_z=-1}^{I-1} \Omega_{m_z+1} \left( e^{i\phi} \hat{c}_{j,m_z+1}^{\dagger} \hat{c}_{j,m_z} + h.c \right)$$  \hspace{1cm} (5.2)

where $\Omega_{m_z} = \sqrt{\Omega g_{m_z}}$ with $g_{m_z} = \sqrt{I(I+1) - m_z(m_z-1)}$ and $\phi$ is the running phase of the Raman beams (set by the wavevector transfer $\Delta k$ and the lattice constant $d$). $\hat{H}_{int}$ is taken to be an SU($2I+1$) invariant interaction of contact form, i.e. $\hat{H}_{int} = U \sum_{j,m,m'} \hat{N}_{j,m} (\hat{h}_{j,m} - \delta_{m_z,m'_z})$. The full model is illustrated in the interpretation of a ladder system in Fig. 5.2. We derive it from the underlying atom-light coupling via Raman lasers in Appendix D. In the next section we will consider an effective spin-1/2 model describing the dynamics in the strong coupling limit.

### 5.2.1. Effective Model at strong Coupling

We will consider the parameter regime $t \ll \Omega, U$ and work with the resulting low-energy effective Hamiltonian in the following. In the limit $t \ll \Omega$ only the lowest of the eigenstates of $\hat{H}_2$ remains in the effective description coupled via direct and virtual hoppings induced by $\hat{H}_1$. The interaction $\hat{H}_{int}$ takes the same form in the eigenbasis of $\hat{H}_2$ due to its SU($2I+1$)-invariance and in the limit of $t \ll U$ leads to a hardcore constraint in the effective basis. In Appendix E.1 we derive the effective second-order model describing spinless particles interacting via a nearest neighbour interaction and hopping with nearest neighbour, next-nearest neighbour and correlated next-nearest neighbour tunnelling terms.
Figure (5.3) Second order virtual processes in the effective Hamiltonian (Eq. (5.3)) illustrated in the case of $I = 2$. The left shows a particle hopping into an excited state on an unoccupied site and back to the ground state and leads to a normal and a correlated NN neighbour hopping term $t_2$ and $t_{\text{cor}}$, hopping via an occupied site gives an additional contribution to $t_{\text{cor}}$, the right corresponds to hopping back and forth via an excited state and leads to an effective NN interaction $V$ of particles on neighbouring sites. The hopping is described by a matrix $T_{s_1,s_2}(\phi)$ between different states $s_1$ and $s_2$ that depends on the phase $\phi$ as described in Appendix E.1.

The effective Hamiltonian takes the form

$$\hat{H}_{\text{eff}}/t = -t_1(\phi) \sum_j (\hat{d}_{j+1}^\dagger \hat{d}_j + h.c.) + \kappa V(\phi, \tilde{u}) \sum_l \hat{n}_l \hat{n}_{l+1}$$

$$- \kappa t_2(\phi, \tilde{u}) \sum_j (\hat{d}_{j+2}^\dagger \hat{d}_j + h.c)$$

$$+ \kappa t_{\text{cor}}(\phi, \tilde{u}) \sum_j (\hat{d}_{j+2}^\dagger \hat{n}_{j+1} \hat{d}_j + h.c).$$

(5.3)

where $\hat{d}_j = \hat{d}_{j,I}$ is the creation operator for a particle in the $s_x = I$ (after the unitary transformation explained in Appendix E.1) eigenstate at site $j$, $\kappa = t/\Omega$, and $\tilde{u} = U/(4\Omega I)$. The explicit form and functional dependence of the coupling constants on the flux $\phi$, the interaction strength $\tilde{u}$ and the number of spin states $I$ is provided in Appendix E.1, Eqs. (E.4) to (E.6).

The first term describes the direct hopping between the $s_x = I$ spin state on neighbouring lattice sites, with an energy scale that is reduced from the bare hopping $t$ by the factor $t_1(\phi) = (\cos\phi/2)^2$ (Appendix E.1). The remaining terms describe virtual hopping processes, with energy scale proportional to $\kappa t = t^2/\Omega$. The nearest neighbour repulsion $V$ contains three contributions, originating from nearest neighbour hopping.
and returning to the original site via an excited spin state on a neighbouring site which is either empty or occupied or hopping onto an occupied site in the lowest energy spin state. The correlated tunnelling term $t_{\text{cor}}$ arises from the corresponding processes with the particle not returning to the original site. These processes are illustrated in Fig. 5.3.

Importantly, the virtual hopping between the different Raman eigenstates is controlled by $\kappa = t/\Omega$. To avoid double occupancy we only require $tt_1(\phi) \ll U$, which can be achieved even if the bare coupling $t$ is large by making $t_1(\phi)$ small through a judicious choice of $\phi$. This allows us to work at relatively high energy scales using shallow lattices with high bare tunnelling rates $t$, in contrast to the induced interactions in the Mott regime of the Hubbard model scaling with $t/U$ requiring deeper lattices and lowering the overall energy scale. Further, the dependence of the coupling constants on the flux $\phi$ allows one to eliminate the first order tunnelling terms and obtain an effective model with dominant second order terms even for relatively shallow lattices where all energy scales remain large.

5.3. Model at $\phi = \pi$

In the following we focus on the model at flux $\phi = \pi$. Then, the first order nearest neighbour tunnelling term $t_1(\phi)$ vanishes identically and the effective model is determined by the second order terms only. The model reduces to

$$\hat{H}_{\text{eff}}/(t\kappa) = V \sum_j \hat{n}_j \hat{n}_{j+1} - t_2 \sum_j \left( \hat{c}_j^\dagger \hat{c}_{j+2} + \text{h.c.} \right) + V/2 \sum_j \left( \hat{c}_j^\dagger \hat{n}_{j+1} \hat{c}_{j+2} + \text{h.c.} \right) \quad (5.4)$$

where $c_j^\dagger$ is the creation operator for hard-core bosons or spinless fermions at site $j$ and $n = c_j^\dagger c_j$ the corresponding density and the couplings are the ones defined below Eq. (5.3) for $\phi = \pi$. Note that in these limits $t_{\text{cor}} = V/2$. Since the NN tunnelling term has dropped out, particles now only hop on their respective $A/B$ sublattices, the model can therefore also be understood to live on a “zigzag” lattice as shown in Fig. 5.4a.
To gain some understanding of the effective model, we first consider the more general case in which all coupling constants can be tuned independently, i.e. we consider the model with couplings $t_2$, $t_{cor}$ and $V$. Note that those correspond to to 2-body, 3-body and 4-body terms respectively. For $t_{cor} = V = 0$ the model is non-interacting and describes free hardcore bosons living separately on each sublattice. For $t_{cor} = 0$ the model corresponds to the $t_2 - V$-model [227]. It has been shown to undergo a quantum phase-transition from a superfluid (SF) phase to a supersolid (SS) at non-half filling and to a charge-density-wave (CDW) at exactly half-filling as a function of $t_2/V$. For $V = 0$ the model is integrable and known as Bariev’s model [228], in this limit we have two NNN hopping terms, a normal hopping $t_2$ and a correlated hopping $t_{cor}$ for which hopping between sites depends on the occupation of the intermediate site on the other sublattice. Depending on $t_{cor}/t_2$ the model has a finite CDW amplitude, i.e. different sublattice populations, in the groundstate. The fermionic spin 1/2 version of this model has recently been studied in Ref. [229]. For $V = 0$ and $t_{cor} = -t_2$, the model admits an exact solution via mapping to free spinless particles moving on a charge lattice. This solution becomes possible, because for $t_{cor} = -t_2$ particles cannot pass each other, and the sequence of particles remains preserved throughout the dynamics. The groundstate of the model is found to be a paired-hole superconductor with hidden string order and algebraically decaying 2-particle correlations.
For our model, we are not free to choose these couplings independently. The dependence of the couplings in the effective model Eq. (5.4) on the rescaled interaction strength $\tilde{u} = U/(4\Omega I)$ is shown in Fig. 5.4b. In these limits we obtain $t_{\text{cor}}/V = 0.5$ and $t_2/V = (1 + \tilde{u})/(2\tilde{u})$. Thus, the model depends only on a single free parameter, $\tilde{u}$, which determines the ratio $t_2/V$, or we can alternatively consider the model as a function of $t_2/V$. Hardcore interactions correspond to $t_2/V = 0.5$ and we will consider the region of repulsive interactions corresponding to $t_2/V \geq 0.5$ in Section 5.3.1. We note that with these parameters we are outside of the integrable limits described above and it will be interesting to see what remains of the physics of these limits in our model.

### 5.3.1. Phase Diagram

To characterise the ground state phases we perform DMRG simulations using the ALPS MPS framework [230, 231]. We consider system sizes of $L = 80, 120, 160, 240$ with open boundary conditions keeping a maximal number of states of $m = 400, 600, 800$, extrapolating results for fixed system size in $1/m$. To characterise the ground state and obtain the phase-diagram we study two- and four-point correlation functions and the structure factors for CDW, superfluid and pair-superfluid order. To reduce the effects of the open boundary conditions correlators are measured from the middle of the system and averaged over a window of 10 sites around the central site. We perform finite-size scaling of the corresponding correlation-lengths, decay exponents and structure factors to obtain the phase-boundaries. In addition we characterise the phases via their entanglement entropy and central charge.

On a bipartite lattice, due to the vanishing of the nearest neighbour tunnelling, the sublattice populations $n_{A(B)} = \sum_{i \in A(B)} n_i$ are separately conserved, and we focus on equal populations on both sublattices $n_A = n_B$. The phase diagram of the model as a function of $t_2$ in the range $0.5 \leq t_2/V \leq 0.64$ and density $0 \leq n \leq 1$ is shown in Fig. 5.5. Three distinct phases are observed in this parameter range, a charge-density wave (CDW) with a period of two lattice sites, a supersolid (SS) with simultaneous (quasi-) superfluid
5. Synthetic Dimensions in the Strong-Coupling Limit: Supersolids and Pair-Superfluids

Figure (5.5) Phase-diagram of the effective model Eq. (5.4) obtained from the DMRG calculations as a function of coupling $t_2$ and density $n$. Three distinct phases are observed, a CDW at $n = 0.5$ and $t_2 \leq 0.6$ with central charge $c = 0$, a supersolid phase (SS) with superfluid order on one of the sublattices with the other sublattice being empty with central charge $c = 1$ below half-filling $n < 0.5$, and a homogeneous phase with dominant superfluid ($SF_{A+B}$) order on both lattices with $c = 2$ for high densities $n$ and high $t_2$ which also shows strong pair-superfluid correlations. Above half-filling at low $t_2$ we find phase-separation (PS) as indicated by a jump in the density-chemical potential curve $n(\mu)$. 
and maximal CDW order with a period of 2 lattice sites\(^1\), and a homogeneous phase with (quasi-) superfluidity on both sublattices (SF\(_{A+B}\)) with pair-superfluid correlations. (Since we consider the case of \(n_A = n_B\), both the CDW and the SS phases are additionally separated into a left/right region with vanishing density on one of the sublattices in both regions.)

Exactly at half-filling \(n = 0.5\) the CDW phase is stabilised and persists up to \(t_2/V = 0.6\). Below half-filling \(n < 0.5\) at low coupling \(t_2\) the effects of the nearest neighbour repulsion are still dominant, resulting in a phase where one of the sublattices is empty and the other is filled and becomes (quasi-)superfluid, thus forming a supersolid state. We remark that if one sublattice is empty, the model reduces to free particles hopping on the other sublattice with amplitude \(t_2\). Above half-filling \(n > 0.5\) at low \(t_2\) particles cannot avoid the cost of the interaction energy \(V\) and the system phase-separates. At sufficiently high \(t_2\) the effect of the repulsion \(V\) can be overcome and a homogeneous phase with superfluid order on both lattices emerges. In this regime all of \(t_2\), \(t_{\text{cor}}\) and \(V\) are relevant.

An important tool to characterise the ground state behaviour of strongly correlated systems in one dimension is the von Neumann block entropy [232]. This is defined as 
\[
S^N_A = \text{Tr} \rho_A \ln \rho_A
\]
where \(\rho_A = \text{Tr}_B \rho\) obtained by dividing the chain into the block \(A\) consisting of sites \(i = 1, \cdots, l\) and \(B\) of sites \(i = l + 1, \cdots, L\). In particular, for a gapped state the entropy saturates whereas it diverges for a gapless state [233, 234]. For a 1D system of size \(L\) with open boundary conditions the von Neumann block entropy behaves as 
\[
S^N_L(l) = s_1 + \frac{c}{6} \ln \left[ \frac{2L}{\pi} \sin \left( \frac{\pi l}{L} \right) \right]
\]
where \(c\) is the central charge of the associated conformal field theory (CFT) and \(s_1\) is a non-universal constant [235–237]. By fitting \(S^N_L\) linearly in the conformal distance \(\lambda = \ln \left[ \frac{2L}{\pi} \sin \left( \frac{\pi l}{L} \right) \right]\) we obtain the central charge \(c\) of the phase. The behaviour of the central charge \(c\) as a function of the coupling \(t_2\) at density \(n = 0.5\) is shown Fig. 5.6a. The results indicate a transition close to \(t_2/V = 0.6\).

The state for \(t_2/V \leq 0.6\) is gapped with \(c = 0\) as expected for the CDW phase and the transition occurs into a state with with central charge of \(c = 2\) in the SF\(_{A+B}\). Finally

---

\(^1\)Since the continuous translational symmetry is explicitly broken by the optical lattice, interactions only break the remaining discrete symmetry and the situation is fundamentally different to the continuum case. One might as well simply refer to this phase as a CDW with simultaneous superfluid order. We follow the convention to call it a SS as in [227].
5. Synthetic Dimensions in the Strong-Coupling Limit: Supersolids and Pair-Superfluids

![Graph showing synthetic dimensions](image)

**Figure (5.6)** (a) The central charge $c$ determined from fitting the von Neumann block entropy via $S^N_L(l) = \frac{c}{6} \ln \left( \frac{2l}{\pi} \sin \left( \frac{\pi l}{L} \right) \right)$ for different system sizes as a function of the coupling $t_2$ at density $n = 0.5$. The CDW is gapped with $c = 0$ and the transition occurs into the SF$_{A+B}$ phase with central charge $c = 2$. (b) Extrapolated CDW order parameter $\Delta_{CDW} = \lim_{L \to \infty} \sqrt{\frac{1}{L} \sum_l e^{i\pi l} G(l)}$ at density $n = 0.5$ as a function of coupling $t_2$ showing the vanishing of CDW order at $t_2/V = 0.61$.

below half-filling we find a central charge $c = 1$ (not shown), which is consistent with superfluidity on one of the sublattices in the SS phase.

The CDW order can be directly extracted from the density-density correlation and the static structure factor. We measure $G(l) = \langle \hat{n}_i \hat{n}_{i+l} \rangle - n^2_{av}$ with $n_{av} = 1/L \sum_i \langle \hat{n}_i \rangle$. The static structure factor is defined as $S_L(q) = 1/L \sum_l e^{iql} G(l)$. The CDW order parameter is given by the square root of the structure factor at $q = \pi$, $\Delta_{CDW}(L) = \sqrt{S_L(\pi)}$ and its infinite system size limit, $\Delta_{CDW} = \lim_{L \to \infty} \sqrt{S_L(\pi)}$. The finite system results $\Delta_{CDW}(L)$ are extrapolated via a quadratic fit in $1/L$ to infinite system size. The results of this extrapolation are shown in Fig. 5.6b. The CDW order parameter vanishes at $t_2/V = 0.61$ signalling the transition into the superfluid state.

To characterise the degree of (quasi-)superfluid order we consider the following two point correlation function $C_{\alpha}(2l) = \langle \hat{c}^\dagger_{L/2-l+\alpha} \hat{c}^\dagger_{L/2+\alpha} \rangle$ on either sublattice ($\alpha = 0, 1$) measured symmetrical around the middle of the system. This correlation function is shown in Fig. 5.7a for a system of size $L = 240$ on sublattice A ($\alpha = 0$) displaying a transition from short-ranged to long-ranged correlations around $t_2/V = 0.61$; the other sublattice (not shown) exhibits the same behaviour. In contrast to CDW there is no order parameter
5.3. Model at $\phi = \pi$

(a) Two-point correlation function $C_\alpha(l)$ as a function of $l$ on sublattice $A$ ($\alpha = 0$) for a system of size $L = 240$ at density $n = 0.5$ for $t_2/V = 0.61, 0.6, 0.59$ (top to bottom) showing the transition from short-ranged to long-ranged correlations at $t_2/V = 0.61$. (b) System size $L$ divided by superfluid correlation length $\xi_{sf}$ for sublattice $A$ vs coupling $t_2$ for $L = 240, 160, 120, 80$ (top to bottom). Coalescence of data points for different $L$ at $t_2/V = 0.61 \pm 0.05$ signals transition to SF state.

Figure (5.7) (a) Two-point correlation function $C_\alpha(l)$ as a function of $l$ on sublattice $A$ ($\alpha = 0$) for a system of size $L = 240$ at density $n = 0.5$ for $t_2/V = 0.61, 0.6, 0.59$ (top to bottom) showing the transition from short-ranged to long-ranged correlations at $t_2/V = 0.61$. (b) System size $L$ divided by superfluid correlation length $\xi_{sf}$ for sublattice $A$ vs coupling $t_2$ for $L = 240, 160, 120, 80$ (top to bottom). Coalescence of data points for different $L$ at $t_2/V = 0.61 \pm 0.05$ signals transition to SF state.

for superfluidity in one dimension, and the whole superfluid phase is critical. Still, the superfluid phase is characterised by a diverging correlation length [238]. To determine the transition point we perform finite-size scaling of the correlation length defined as $\xi_{sf} = \sqrt{\sum_l l^2 C_\alpha(l)/\sum_l C_\alpha(l)}$ [239, 240]. In Fig. 5.7b $L/\xi_{sf}$ on sublattice $A$ ($\alpha = 0$) is shown as a function of $t_2$ at $n = 0.5$ for different system sizes, the correlations on sublattice $B$ show the same behaviour. The coalescence of the data signals the transition to the superfluid state at $t_2/V = 0.61$. In the superfluid phase we find strong correlations between the superfluids on the sublattices. To characterise this phase further we also consider possible condensation of pairs via $P(2l) = \langle \hat{c}^\dagger_{L/2-l} \hat{c}^\dagger_{L/2+1-l} \hat{c}_{L/2+1+l} \hat{c}_{L/2-l} \rangle - \langle \hat{c}^\dagger_{L/2-l} \hat{c}^\dagger_{L/2+1-l} \rangle \langle \hat{c}_{L/2+1+l} \hat{c}_{L/2-l} \rangle$ and its corresponding correlation length $\xi_{pf} = \sqrt{\sum_l l^2 P(l)/\sum_l P(l)}$. The pair-superfluid correlator is shown in Fig. 5.8a and the finite size scaling of the correlation length in Fig. 5.8b. We observe very strong pair-superfluid correlations in the SF$A+B$ phase consistent with quasi-condensation of pairs as the system becomes superfluid. However, single-particle superfluidity persists alongside pair-superfluidity in the parameter regime we have studied.

In Fig. 5.9(a) and (b) we display the momentum distribution of particles on sublattice...
Figure (5.8)  (a) Four-point correlation function \( P(l) \) as a function of \( l \) for a system of size \( L = 240 \) at density \( n = 0.5 \) for \( t_2/V = 0.61, 0.6, 0.59 \) (top to bottom) showing the transition from short-ranged to long-ranged correlations at \( t_2/V = 0.61 \). (b) System size \( L \) divided by pair-superfluid correlation length \( \xi_{pf} \) vs coupling \( t_2 \) for \( L = 240, 160, 120, 80 \) (top to bottom). Coalescence of data points for different \( L \) at \( t_2/V = 0.61 \pm 0.05 \) signals transition to PSF state.

\[ A, n(q) = \sum e^{iql} C_A(l), \text{ and in (c) and (d) the momentum distribution of pairs of particles} \]
\[ n_{pf}(q) = \sum e^{iql} P(l). \] As for hardcore bosons \( n(q = 0) \) is expected to scale with \( \sqrt{L} \) [241], both quantities are normalised by this factor. We focus on the transition from the SS phase in (a) and (c) to the SF\(_{A+B}\) phase in (b) and (d). Whereas in the single-particle momentum distribution a quasi-coherent peak is observed in both phases, pairs only quasi-condense in the SF\(_{A+B}\) phase as seen in (d).
5.3. Model at $\phi = \pi$

Figure (5.9) (a)-(b) Single-particle momentum-distribution $n(q) = \sum e^{iql} C_A(l)$ on sublattice A. (c)-(d) Momentum distribution for pairs of particles $n_{pl}(q) = \sum e^{iql} P(l)$. All at density $n = 0.25$ and (a) and (c) at $t_2/V = 0.51$ in the SS phase and (b) and (d) at $t_2/V = 0.55$ in the $SF_{A+B}$ phase. The single-particle momentum distribution shows a quasi-coherent peak in both phases (a) and (b). In contrast, for pairs in the SS phase in (c) no quasi-coherent peak is observed, whereas a peak forms in the $SF_{A+B}$ phase in (d).
5.4. Conclusions

In summary, in this work we have shown that the interplay of (synthetic) gauge fields and interactions in ultracold gas systems leads naturally to effective Hamiltonians with correlated hopping terms. We start from an experimentally feasible set-up for the creation of artificial magnetic field using synthetic dimensions. We consider this model in the limits of strong Raman coupling of the spin states and strong interactions where it reduces to an effective model with first order nearest neighbour tunnelling, and second order next-nearest neighbour correlated tunnelling terms and nearest neighbour repulsion. Importantly, the additional degree of freedom given by adjusting the flux $\phi$ allows to engineer effective models dominated by second-order processes with large energy scales.

By working at flux $\phi = \pi$, the first order nearest neighbour tunnelling term is eliminated, and we obtain a novel model with dominant second-order terms. This is a natural route to a large density-dependent tunnelling term, so the proposed scheme is directly relevant to the realisation and study of models with interaction-assisted hopping and kinetic frustration [242–248].

The physics of our effective model involves the competition between the correlated tunnelling which favours pair formation, and the nearest neighbour repulsion which favours local CDW order. We find three distinct phases: a CDW phase; a supersolid (SS) with simultaneous quasi-superfluidity on either sublattice and maximal CDW order; and a quasi-superfluid on both sublattices with strong pair-superfluid correlations $\text{SF}_{\text{A}+\text{B}}$.

The model can be directly generalised to fermionic species and higher dimensional lattices of arbitrary geometry. In the case of fermions, the study of attractive interactions seems particularly relevant for the study of paired phases. The extension to higher dimensions promises even more interesting physics, e.g. BKT transitions to novel superconducting states and geometrically frustrated magnetism. We reserve the discussion of the resulting phases for future work.
6. Conclusions

6.1. Summary

In this thesis, we have explored some of the novel and fascinating physics arising from the interplay of interactions, time-dependence and artificial gauge fields in systems of ultracold atomic gases. We have focused on two key approaches to creating artificial gauge fields based on current experimental research, coherent time-periodic driving of quantum systems and Floquet Theory, and the method of synthetic dimensions. For both of these distinct methods we have explored the consequences of interactions and the resulting novel physics.

This research has been motivated by current experiments and new experimental techniques. Tools to create artificial gauge fields are of great interest to extend the ability of ultracold atomic systems to serve as quantum simulators of solid state systems, and to explore genuinely new phenomena not found in solid state materials. Interactions are naturally present for atomic gases, and are of crucial importance to many of the most intriguing physics expected to be present in these systems. This led us to study, in Chapter 3, the two-body scattering properties of particles in time-periodically driven closed quantum systems. We have established a general framework to obtain scattering rates of Floquet-Bloch waves, the eigenstates of time-periodically driven and translationally invariant Hamiltonians, in presence of weak, i.e. perturbative, interactions. We have demonstrated that quasi-energy spectra of non-interacting systems do not provide sufficient information to understand the effect of even perturbatively weak interactions, in contrast to the time-independent case, and have to be interpreted with care when...
including interactions. We carefully defined the notions of “elastic” and “inelastic” scattering processes when only quasi-energy is conserved. We identified the fundamental underlying mechanism by which the Floquet nature of the eigenstates in presence of interactions leads to non-energy conserving or photon-assisted scattering as the non-commutativity of the interactions and the Floquet modes. Finally, we studied two schemes related to Floquet realisations of artificial gauge fields for cold atomic gases in detail, the optical dressing of internal states, and the time-periodic modulation of tight-binding lattices. We have derived the generic scaling of scattering rates of “elastic” and “inelastic” components with system parameters and their dependence on dimensionality and the density of states. We have derived stability regions in which “inelastic” scattering can be suppressed by judicious choice of parameters. This is particularly important to enable future experiments to work in a regime in which “elastic” scattering responsible for many-body physics remains dominant compared to the “inelastic” scattering leading to heating and particle loss.

In Chapter 4 we applied the developed framework to an experimental Floquet realisation of the Harper-Hofstadter model in a gas of cold bosonic atoms. Using the experimental parameters we have obtained scattering rates within the FFGR. We have demonstrated that the observed population dynamics can be explained by (non-energy conserving) scattering processes due to the particle-interactions and the time-dependence of the Floquet states. This work also provides some insight into the wider field of heating dynamics of closed quantum systems with an unbounded dispersion subject to periodic driving. We have found a fast time scale over which the system approaches an infinite temperature state for the bounded degrees of freedom of the in-plane motion and a longer time-scale over which the system then continues to heat up in the transverse direction. Finally, we have shown how the photon-assisted scattering processes, responsible for heating and band transfer, can be suppressed in the experimental setup by proper design of a confining transverse lattice potential. Therefore, we have established a route for future experiments aiming to access the strongly interacting regime requiring the suppression of deleterious heating processes.

In the final chapter of this thesis, Chapter 5, we have studied the many-body phases of bosonic atoms with \( N \) internal states confined to a one-dimensional optical lattice under the influence of a synthetic magnetic field and strong repulsive interactions. We
have focused on the physics of an effective model in the limits of strong Raman coupling and strong SU(N)-invariant contact interactions. We obtained the phase-diagram of the effective model at flux $\phi = \pi$, including charge-density wave, supersolid and pair-superfluid phases. In particular, we demonstrated the presence of a quasi-pair-superfluid phase within an experimentally realised setup. More generally, the additional freedom of adjusting the flux allows to obtain novel effective models with dominant second-order terms with large energy scales. Thus, we establish a natural method towards models with dominant density-dependent tunnelling terms. These types of models are particularly interesting in the context of interaction-assisted hopping and kinetic frustration.

### 6.2. Outlook

Based on the work described in this thesis, there are a number of extensions that naturally follow, and which relate to wider concerns in the field.

The treatment of two-particle scattering within the FFGR in Chapter 3 and its application to the Floquet-realisation of the Harper-Hofstadter model in Chapter 4 are restricted to the weakly interacting regime and are fundamentally based on few-particle physics. One is led to ask what the role of strong, non-perturbative interactions in the Floquet setting might turn out to be, both from a fundamental point of view, but also from the point of direct relevance to experiments as they progress to study many-body physics in artificial gauge fields. Additionally, the application of the FFGR, in principle, limits the applicability to short time-scales, and the infinite-time behaviour can certainly not be inferred from it. Thus, what happens on longer time-scales and what the coherent many-body dynamics are remains an intriguing question. Another crucial issue that we have so far completely neglected concerns the preparation of Floquet states [249]. The idealisation of an infinitely long lasting, perfectly periodic driving scheme can clearly never be realised in an experiment. This raises the question what the effect of finite time parameter ramps and driving schemes would be in Floquet systems.

These specific questions point to more general lines of inquiry in the wider field, such
6. Conclusions

as adiabaticity and transient dynamics in Floquet systems [163, 250, 251] and the thermodynamics of periodically driven interacting quantum systems [252–254]. Whereas the situation seems to be broadly understood for bounded closed Hamiltonians, with an infinite temperature long-time state in absence of many-body localisation, and bounds on the heating time scales have been established [164, 165], the situation for unbounded Hamiltonians which one naturally needs to consider both for lattice and continuum models is less clear.

A direct extension of the work in Chapter 5 would be the study of the corresponding physics in the case of fermionic species. Experimentally, synthetic gauge fields have already been realised for fermions [124]. Specifically, an interesting avenue of research distinct from the bosonic case we considered would be attractive interactions and the potentially resulting (exotic) paired phases of fermions.

In a more general direction, another strand of research would be to explore the consequences and opportunities in combining synthetic dimensions and artificial gauge fields with their associated topological properties in higher-dimensional, i.e. more than one-dimensional, settings in the presence of interactions in cold atomic systems. Already two-dimensional systems allow a large variety of lattice geometries which in presence of gauge fields can lead to frustration and highly degenerate groundstates, and generally much richer physics than in one dimension. In particular, in one dimension possible phases are severely limited by quantum fluctuations, whereas in 2D the BKT mechanism allows the breaking of continuous symmetries and existence of superfluidity. Specifically, in 2D one could expect (exotic) superfluid and quantum spin-liquid phases to be present in models similar to those discussed in Chapter 5, as demonstrated in two-dimensional SU(N) Hubbard models in presence of gauge fields [255, 256]. Thus, the study of higher dimensions seems particularly relevant both to explore theoretically challenging and novel physics, but also to connect with experimental setups which are easily extended to two (or more) dimensions.

The role of interactions both within the context of time-dependent Hamiltonians and within the context of artificial gauge fields remains an intriguing and in many ways open field of research. There still are many natural future directions of research based on the
work described in this thesis. Further, there still are many questions of fundamental and practical importance for theory and experiment in the wider field.
6. Conclusions
Appendix A.

Atom-Light Interactions and Optical Potentials

In this appendix we describe the interactions of atoms with light in far off-resonant laser fields. We will consider the interaction of atoms with light via the dipole Hamiltonian coupling a groundstate manifold to electronically excited states. As the main result we will obtain an effective Hamiltonian containing optically induced potentials describing the dynamics of atoms in the ground state manifold.

A.1. Atom-Light Interactions

We consider atom-light interaction via

\[ \hat{H}_{\text{dip}} = \hat{d} \cdot \mathbf{E}, \]  

(A.1)

with the electric field \( \mathbf{E}(\tau) \) and the dipole operator \( \hat{d} = q \mathbf{r} \), where \( q \) is the electronic charge and \( \mathbf{r} \) the position operator. We consider the lowest energy dipole transition in an alkali atom, between the ground state S electron orbital with energy \( E_g \) and an electronically excited P orbital with an energy \( E_e \). The atomic Hamiltonian is then given by

\[ \hat{H}_{\text{at}} = E_g \hat{P}_g + E_e \hat{P}_e + \frac{A_{FS}}{\hbar^2} \hat{L} \cdot \hat{\mathbf{S}}, \]  

(A.2)
Appendix A. Atom-Light Interactions and Optical Potentials

with the fine structure constant $A_{\text{FS}}$, the projectors onto the ground state (excited state) manifold $\hat{P}_g(e)$, the electronic orbital angular momentum operator $\hat{L}$ and the electron spin operator $\hat{S}$. In the following we set $E_g = 0$. Note that we neglect the hyperfine structure here, as the resulting splitting is considerably smaller, $A_{\text{hf}} \ll A_{\text{FS}} \ll E_e$, and of no relevance for the transition driven by strongly off-resonant laser fields we will be considering.

As a first step we transform into a rotating frame via $\hat{U}(\tau) = \hat{P}_e + e^{-i\omega \tau} \hat{P}_g e^{i\omega \tau}$. In the atomic Hamiltonian this will lead to an energy shift $E_e \rightarrow E_e - \hbar \omega$.

The dipole Hamiltonian in the rotating frame takes the form

$$\hat{H}_{\text{dip}} = E_e e^{-i\omega \tau} \hat{P}_g \hat{d} \hat{P}_e + E_e e^{i\omega \tau} \hat{P}_e \hat{d} \hat{P}_g.$$  \hspace{1cm} (A.3)

Assuming a time-dependence of the electric field as $E(\tau) = \tilde{E} e^{-i\omega \tau} + \tilde{E}^* e^{i\omega \tau}$, we will drop terms rotating with $\pm 2\omega \tau$ and obtain

$$\hat{H}_{\text{dip.}RW} = \tilde{E} \hat{P}_g \hat{d} \hat{P}_e + \tilde{E}^* \hat{P}_e \hat{d} \hat{P}_g.$$  \hspace{1cm} (A.4)

We emphasise that this rotating wave approximation is on the level of the laser-frequency and between the groundstate and excited state manifold. Unless we include additional terms in the Hamiltonian that couple them, it does not affect the rest of the Hamiltonian. In particular, considering interactions we may reasonably exclude scattering by contact interactions between the S and P orbitals which implies that the interactions do not pick up a time-dependence by this transformation.

The total Hamiltonian is then given by

$$\hat{H}_{\text{RW}} = (E_e - \hbar \omega) \hat{P}_e + \frac{A_{\text{FS}}}{\hbar^2} \hat{L} \cdot \hat{S} + \hat{H}_{\text{dip.}RW}.$$  \hspace{1cm} (A.5)

We may now derive an effective Hamiltonian for the atom in the ground state manifold via

$$\hat{H}_{\text{eff}} = \hat{P}_g \hat{H}_{\text{dip.}RW} \hat{P}_e \hat{H}_{\text{at}}^{-1} \hat{P}_e \hat{H}_{\text{dip.}RW} \hat{P}_g.$$  \hspace{1cm} (A.6)
The effective Hamiltonian turns out to be [70]

\[
\hat{H}_{\text{eff}} = \left[ u_s \hat{E}^* \cdot \hat{E} + \frac{iu_v \left( \hat{E}^* \times \hat{E} \right)}{\hbar} \cdot J \right] \hat{P}_g ,
\]

(A.7)

where \( u_s \) and \( u_v \) are the scalar and vector polarizabilities. Importantly, they contain the reduced matrix element for the dipole transitions, \( \langle |d| |l = 0 \rangle |d| |l = 1 \rangle \), between the ground state and the excited state manifold. They take the explicit form

\[
u_s = \frac{\langle |d| \rangle^2}{36} \left( \frac{2}{E_e - A_{FS} - \hbar \omega} + \frac{1}{E_e + A_{FS}/2 - \hbar \omega} \right) , \tag{A.8}\]

\[
u_v = \frac{u_s A_{FS}}{E_e - A_{FS}/2 - \hbar \omega} . \tag{A.9}\]

This now allows us to comment on the ratio of off-resonant light scattering, which is detrimental to the experiment, to the intended effects characterised by \( u_s \) and \( u_v \). The scattering of off-resonant light is proportional to the population of the eliminated excited states. If the detuning is large compared to the hyperfine splitting, \( \Delta_e = E_e - \hbar \omega \gg A_{FS} \), the population will scale as \( 1/\Delta_e^2 \). In contrast, the scalar polarizability behaves as \( u_s \sim 1/\Delta_e \). Therefore working at sufficiently large detuning allows to suppress spontaneous emission and effectively realise a conservative scalar optical potential. For the vector polarizability the situation is unfortunately worse. For \( \Delta_e \gg A_{FS} \), it decreases as \( 1/\Delta_e^2 \) as well. Therefore, the ratio of the vector coupling to the off-resonant scattering is bounded and cannot be improved by working at larger detunings.
Appendix B.

Scattering Theory

In Chapter 3 we discussed scattering theory for Floquet systems and its applications to specific experimental setups used to create artificial gauge fields for neutral atoms. In Section 3.4.1 we studied a model of Raman dressed states for the creation of artificial gauge fields in the continuum. In Appendix B.1 we provide the derivation of the effective two-level system given in the main part of the thesis. In Section 3.4.2 we considered a lattice system with periodically time-modulated on-site energies. In Appendix B.2 we derive the single-particle Floquet-modes of the modulated lattice in a rotating-wave like approximation required for the computation of the scattering rates and life-times.

B.1. Derivation of the Effective Two-Level System for Raman Dressed States

We start from a three level description of the dynamics of an atom under the influence of laser fields. The Hamiltonian in the basis of internal states (|1⟩, |2⟩, |0⟩) is given by

\[
\hat{H} = \frac{\hbar}{2} \begin{pmatrix}
\Delta/2 & 0 & \Omega_1 \cos(\omega_1 \tau + k_1 x) \\
0 & \Delta/2 & \Omega_2 \cos(\omega_2 \tau + k_2 x) \\
\Omega_1^* \cos(\omega_1 \tau + k_1 x) & \Omega_2^* \cos(\omega_2 \tau + k_2 x) & \omega_c
\end{pmatrix}.
\] (B.1)
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We assume the splitting $\hbar \Delta$ between $|1\rangle$ and $|2\rangle$ to be small compared to the splitting $E_e = \hbar \omega_e$ between the two low lying states and the excited state $|0\rangle$. The atom is additionally illuminated by two pairs of Raman lasers of frequency $\omega_1 = \omega_L + \delta_\omega$ and $\omega_2 = \omega_L + \delta_\omega$ and $\omega_2 = \omega_L - \delta_\omega$ with wavevectors $k_1$ and $k_2$ respectively. The laser beams are propagating along the $x$-direction and have orthogonal polarisations. The frequency difference $\delta_\omega \ll \omega_L$ and therefore $|k_1| \approx |k_2|$. Finally $\Omega_1$ and $\Omega_2$ are the Rabi frequencies for the atomic transitions given by $\Omega_1 = \frac{q}{\hbar} \langle 0 | E_1 \cdot r | 1 \rangle$ and $\Omega_2 = \frac{q}{\hbar} \langle 0 | E_2 \cdot r | 2 \rangle$ where $q$ is the charge of the electron, $r$ is the position operator and $E_i$ is the amplitude of the electric field of the respective laser where the space and time-dependence has been explicitly factored out.

The states $|1\rangle$ and $|2\rangle$ could be two $m_F$ levels in the ground-state manifold of an alkali atom, for example, the $F=1$ manifold of $^{87}\text{Rb}$, and $|0\rangle$ an electronically excited state. The splitting $\hbar \delta$ between $|1\rangle$ and $|2\rangle$ can then be induced by a physical magnetic field by the linear Zeeman shift which is the situation discussed in [108].

We now transform into a frame in which the excited state $|0\rangle$ is rotating with the mean laser frequency $\omega_L$ via $\hat{U}(\tau) = \hat{P}_g + e^{-i\omega_L \tau} \hat{P}_0$ where $\hat{P}_g$ is the projector onto $|1, 2\rangle$ and $\hat{P}_0$ the projector onto $|0\rangle$ and obtain the transformed Hamiltonian $\tilde{H} = \hat{U}^\dagger(\tau) \hat{H} \hat{U}(\tau) - i\hbar \hat{U}^\dagger(\tau) \partial_\tau \hat{U}(\tau)$ given by

$$
\begin{pmatrix}
  -\Delta/2 & 0 & \Omega_1 \cos[(\omega_L + \delta_\omega)\tau + k_1 x] e^{-i\omega_L \tau} \\
  0 & \Delta/2 & \Omega_2 \cos[(\omega_L - \delta_\omega)\tau + k_2 x] e^{i\omega_L \tau} \\
  \Omega_1^* \cos[(\omega_L + \delta_\omega)\tau + k_1 x] e^{i\omega_L \tau} & \Omega_2^* \cos[(\omega_L - \delta_\omega)\tau + k_2 x] e^{-i\omega_L \tau} & \omega_e - \omega_L
\end{pmatrix}.
$$

As we assume $\delta_\omega \ll \omega_L$ we can now perform a rotating wave approximation and drop terms oscillating with $2\omega_L \pm \delta_\omega$ to obtain the Hamiltonian in rotating wave form

$$
\hat{H}_{\text{RWA}} = \hbar/2 \begin{pmatrix}
  -\Delta & 0 & \Omega_1 e^{i(\delta_\omega \tau + k_1 x)} \\
  0 & \Delta & \Omega_2 e^{i(\delta_\omega \tau - k_2 x)} \\
  \Omega_1^* e^{-i(\delta_\omega \tau + k_1 x)} & \Omega_2^* e^{i(\delta_\omega \tau - k_2 x)} & \omega_e - \omega_L
\end{pmatrix}.
$$

We emphasise that we perform the rotating wave approximation on the level of the frequency $\omega_L$ which is of the order of the ground-state manifold to excited state splitting.
\( \omega_e \). In particular, this frequency is large compared to \( \delta \omega \) and the splitting \( \Delta \) of the low-lying states.

Finally, we will adiabatically eliminate the excited state \(|0\rangle\). Working in the regime in which \(|\Delta| \ll |\omega_e - \omega_L|\) and with large detuning from atomic resonance \(|\Omega_{1(2)}| \ll |\omega_e - \omega_L|\), such that the population in \(|0\rangle\) is negligible, we obtain the second order effective Hamiltonian for the reduced dynamics of \(|1\rangle, |2\rangle\) as

\[
H_{\text{eff}} = \frac{\hbar}{2} \begin{pmatrix}
-\Delta + \frac{|\Omega_1|^2}{\omega_k - \omega_L} e^{-[2\delta \omega + (k_1-k_2)x]} & \frac{\Omega_1 \Omega_2^*}{\omega_k - \omega_L} e^{i[2\delta \omega + (k_1-k_2)x]} \\
\frac{\Omega_1 \Omega_2^*}{\omega_k - \omega_L} e^{-[2\delta \omega + (k_1-k_2)x]} & \Delta + \frac{|\Omega_2|^2}{\omega_k - \omega_L}
\end{pmatrix},
\]

(B.4)

Assuming equal Rabi frequencies \( \Omega_1 = \Omega_2 \) and counter propagating Raman beams with \( k_1 = -k_2 = k_r \), we define \( \Omega = \frac{\Omega_1^2}{\omega_k - \omega_L}, \omega = 2\delta \omega \) and drop the diagonal energy shift \( \frac{|\Omega_2|^2}{\omega_k - \omega_L} \) to arrive at

\[
H_{\text{eff}} = \frac{\hbar}{2} \begin{pmatrix}
-\Delta & \Omega e^{i(\omega \tau + 2k_r x)} \\
\Omega e^{-i(\omega \tau + 2k_r x)} & \Delta
\end{pmatrix},
\]

(B.5)

which is the Hamiltonian given in Eq. (3.37).

**B.2. Derivation of the Floquet-Modes in the Modulated Lattice**

We start from the non-interacting Hamiltonian given in momentum space in Eq. (3.61)

\[
\hat{H}_0(\tau) = \sum_k e_k^{(a)} \hat{a}_k^{(1)\dagger} \hat{a}_k^{(1)} + e_k^{(a)} \hat{a}_k^{(2)\dagger} \hat{a}_k^{(2)} + \sum_k V_c(\tau) \left( \hat{a}_k^{(1)\dagger} \hat{a}_k^{(2)} + \hat{a}_k^{(2)\dagger} \hat{a}_k^{(1)} \right) + (a \rightarrow b) + \sum_k \Delta_g \left( \hat{b}_k^{(1)\dagger} \hat{b}_k^{(1)} + \hat{b}_k^{(2)\dagger} \hat{b}_k^{(2)} \right),
\]

(B.6)
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Figure (B.1) Schematic quasienergies of the lower band of the staggered superlattice, Eq. (B.7), in the case of a tight-binding dispersion $\epsilon(k) = -t \cos(k)$ with $V_2 = \hbar \omega = 5t$ as a function of the quasi-momentum $k/k_r$ in arbitrary energy units. (a) Static lattice, $\kappa = V_\omega / (\hbar \omega) = 0$, with a bandgap of magnitude $V_2$ (b) dispersion within rotating wave approximation, see Eq. (B.18), for $\kappa = V_\omega / (\hbar \omega) = 0.6$, with a closed band-gap at $k/k_r = \pm 0.5$ and effective bandwidth $2t_{\text{eff}} = 2J_{-1}(\kappa)t$.

Recalling that $\hat{a}_k^{(1)\dagger} = \hat{a}_k^\dagger$ and $\hat{a}_k^{(2)\dagger} = \hat{a}_{k+\pi}^\dagger$ we write the Hamiltonian in the basis of coupled momentum states at $k$ and $k + \pi$ as

$$\hat{H}_0(\tau) = \sum_k \left( \begin{array}{cc} \hat{a}_k^\dagger & \hat{a}_{k+\pi}^\dagger \end{array} \right) \left( \begin{array}{cc} e_k^a & V_c(\tau) \\ V_c(\tau) & -e_k^a \end{array} \right) \left( \begin{array}{c} \hat{a}_k \\ \hat{a}_{k+\pi} \end{array} \right) + \sum_k \left( \begin{array}{cc} \hat{b}_k^\dagger & \hat{b}_{k+\pi}^\dagger \end{array} \right) \left( \begin{array}{cc} e_k^b + \Delta_g & V_c(\tau) \\ V_c(\tau) & -e_k^b + \Delta_g \end{array} \right) \left( \begin{array}{c} \hat{b}_k \\ \hat{b}_{k+\pi} \end{array} \right),$$

where $k$ is restricted to lie in the reduced BZ $-\pi/2 < k \leq \pi/2$ corresponding the supercell of two inequivalent sites in the real space lattice.

Without the modulation term $V_\omega$, this model can be easily solved exactly. The result will be a ground-state of bosons with two momentum components at $k = 0$ and $k = \pi$ with a relative occupation that depends on the strength of $V_2$. In the limit of strong staggering $V_2 \gg \epsilon_k^{(n)}$, both components are equally occupied, corresponding in real space to occupation of the lower-energy sites, and the excited states correspond to occupation of the higher-energy sites gapped by an energy difference of $V_2$ and both subbands are flat as a function of $k$. The undriven band structure is given by $E_{\pm}(k) = \pm \sqrt{\epsilon(k)^2 + (V_2/2)^2}$ with $\epsilon(k)$ corresponding to either the $a$ or $b$ band. Assuming a nearest neighbour tight-
binding dispersion $\epsilon(k) = -t \cos(k)$ the band structure displays a gap of $V_2$ for $k = \pm \pi/2$ between the $\pm$ subbands and the bandwidth of the subbands is suppressed by a factor of $t/V_2$ compared to the case of vanishing $V_2$. This is shown schematically in Fig. B.1a.

As tunnelling should be strongly suppressed, i.e. $V_2 > \epsilon_k^{(n)}$, we first change basis to the eigenstates for $\epsilon_k^{(n)} = 0$, $\hat{a}_k^\pm = 1/\sqrt{2}(\hat{a}_k \pm \hat{a}_{k+\pi})$, and treat the resulting off-diagonal terms as a small coupling. With this definition one obtains

$$\tilde{H}_0(\tau) = \sum_k \begin{pmatrix} \hat{a}_k^\dagger & \hat{a}_k^\dagger \\ \hat{a}_k^- & \hat{a}_k^- \end{pmatrix} \begin{pmatrix} \epsilon_k^a(\tau) \\ \epsilon_k^a(\tau) \end{pmatrix} \begin{pmatrix} \hat{a}_k^+ \\ \hat{a}_k^- \end{pmatrix}$$

$$+ \sum_k (\beta_k^\dagger \beta_k^-) \begin{pmatrix} \epsilon_k^b(\tau) \\ \epsilon_k^b(\tau) \end{pmatrix} \begin{pmatrix} \hat{b}_k^\dagger + V_c(\tau) \\ \hat{b}_k^\dagger - V_c(\tau) \end{pmatrix} \begin{pmatrix} \hat{b}_k^+ \\ \hat{b}_k^- \end{pmatrix}. \tag{B.8}$$

We now perform a unitary transformation to eliminate the diagonal terms via

$$U_\nu(\tau) = \begin{pmatrix} \exp[-i\kappa \sin(\omega \tau)/2] & 0 \\ 0 & \exp[i\omega \tau + \kappa \sin(\omega \tau)/2] \end{pmatrix} \tag{B.9}$$

where we defined $\kappa = V_\omega/(\hbar \omega)$ and use the resonance condition $V_2 = \hbar \omega$ to get

$$\tilde{H}_0(\tau) = \sum_k \begin{pmatrix} \hat{a}_k^\dagger & \hat{a}_k^- \\ \hat{a}_k^\dagger & \hat{a}_k^- \end{pmatrix} \begin{pmatrix} 0 \\ \epsilon_k^a(\tau) \end{pmatrix} \begin{pmatrix} \hat{a}_k^+ \\ \hat{a}_k^- \end{pmatrix}$$

$$+ \sum_k (\beta_k^\dagger \beta_k^-) \begin{pmatrix} \epsilon_k^b(\tau) \\ \epsilon_k^b(\tau) \end{pmatrix} \begin{pmatrix} \Delta_g + V_c(\tau) \\ \Delta_g - V_c(\tau) \end{pmatrix} \begin{pmatrix} \hat{b}_k^+ \\ \hat{b}_k^- \end{pmatrix}. \tag{B.10}$$

where $\epsilon_k^{(n)}(\tau) = \epsilon_k^{(n)} \exp[i(\omega \tau + \kappa \sin(\omega \tau))]$ and an overall constant energy shift of $\hbar \omega/2$ was dropped. The exponential is expanded in terms of Bessel functions of the first kind $J_n$ as

$$\epsilon_k^{(n)}(\tau) = \epsilon_k^{(n)} e^{i \omega \tau} \sum_n J_n(\kappa)e^{i n \omega \tau}, \tag{B.11}$$

and we see that this contains a term constant in time and oscillating terms. In particular, for a nearest neighbour tight-binding dispersion $\epsilon_k^{(n)} = -t^{(n)} \cos(k)$, the time-dependent dispersion simplifies to $\epsilon_k^{(n)}(\tau) = -t^{(n)} \cos(k)e^{i \omega \tau} \sum_n J_n(\kappa)e^{i n \omega \tau} = -t^{(n)}(\tau) \cos(k)$ and the
modulation is seen to lead to a time-dependent hopping strength $t^{(n)}(\tau)$. Finally, we perform a rotating wave-approximation and only keep the constant term $\epsilon^{(n)}_{k} (\tau) \approx \epsilon^{(n)}_{k} J^{-1}(\kappa)$, which can alternatively be interpreted as approximating the Hamiltonian by the first order term of the high-frequency expansion. Thus, one obtains the eigenstates as

$$\hat{\Psi}^a_{\sigma,k} |\text{vac}\rangle = \frac{1}{\sqrt{2}}(\tilde{a}^{\dagger}_{k+} + \sigma \tilde{a}^{\dagger}_{k-})|\text{vac}\rangle, \quad \hat{\Psi}^b_{\sigma,k} |\text{vac}\rangle = \frac{1}{\sqrt{2}}(\tilde{b}^{\dagger}_{k+} + \tau \tilde{b}^{\dagger}_{k-})|\text{vac}\rangle,$$

with $\tau = \pm$. Abbreviating $f(\tau) = \exp[i\kappa \sin(\omega \tau)]$ these states read in the original basis as

$$\hat{\Phi}^{a,m}_{\sigma,k}(\tau) = 1/2 \left[ (f(\tau) + \sigma e^{i\omega \tau} \tilde{f}(\tau)) \hat{a}^\dagger_{k} + \sigma e^{im\omega \tau} |\text{vac}\rangle, \right.$$

$$\hat{\Phi}^{b,m}_{\sigma,k}(\tau) = 1/2 \left[ (f(\tau) + \tau e^{i\omega \tau} \tilde{f}(\tau)) \hat{b}^\dagger_{k} + \sigma e^{im\omega \tau} |\text{vac}\rangle, \right.$$  

and the corresponding quasi-energies are

$$\epsilon^{a,0}_{\sigma,k} = \sigma \epsilon^{a}_{k} J^{-1}(\kappa),$$

$$\epsilon^{b,0}_{\sigma,k} = \sigma \epsilon^{b}_{k} J^{-1}(\kappa) + \Delta_g.$$  

Again turning to the discussion of the nearest neighbour tight-binding dispersion $\epsilon(k) = -t \cos(k)$ with hopping strength $t$ where the subbands were gapped by $V_2$ and the hopping was suppressed by a factor of $t/V_2$ in the case of an undriven lattice, we note that the hopping is now modified by $J^{-1}(\kappa)$ instead and the gap between the subbands is closed at $k = \pm \pi/2$ as shown in Fig. B.1b.
In this section we provide the explicit expressions for the matrix element

\[ I^m_{\sigma_1, \sigma_2; k, q} = \langle \Phi_0^{\sigma_1, q; \sigma_2, -q} | \hat{H}_{\text{int}} / g | \Phi_0^0 \rangle. \]  

(B.20)

appearing in the FFGR for the scattering in the modulated lattice, see Eq. (3.68) and the following discussion for details.

As a first step we compute

\[ I^m_{\sigma_1, \sigma_2; k, q} = \langle \langle \Phi_{-m, \sigma_1, q; \sigma_2, -q} | \hat{H}_{\text{int}} / g | \Phi_0^{0, \sigma_1, k; \sigma_2, -k} \rangle \rangle \]

\[ = \frac{1}{T} \int_0^T d\tau \langle \Phi_{-m, \sigma_1, q; \sigma_2, -q} | \hat{H}_{\text{int}} / g | \Phi_0^{0, \sigma_1, k; \sigma_2, -k} \rangle \]

\[ = \frac{1}{T} \int_0^T d\tau e^{im \omega \tau} \langle \Phi_{0, \sigma_1, q; \sigma_2, -q} | \hat{H}_{\text{int}} / g | \Phi_0^{0, \sigma_1, k; \sigma_2, -k} \rangle \]

\[ = \frac{1}{T} \int_0^T d\tau e^{im \omega \tau} I_0^{0, \sigma_1, \sigma_2; k, q}, \]

(B.21)

where

\[ I_0^{0, \sigma_1, \sigma_2; k, q} = \langle \Phi_{0, \sigma_1, q; \sigma_2, -q, 0} | \hat{H}_{\text{int}} / g | \Phi_0^{0, \sigma_1, k; \sigma_2, -k, 0} \rangle \]  

(B.22)

was defined. This implies that \( I^m_{\sigma_1, \sigma_2; k, q} \) is just the Fourier component of \( I_0^{0, \sigma_1, \sigma_2; k, q} \) oscillating at \( e^{im \omega \tau} \) and \( I_0^{0, \sigma_1, \sigma_2; k, q} \) contains all the relevant information.

We expand the single particle Floquet mode \( \hat{\Phi}_n^{\sigma, k} \) in the basis of Bloch functions \( \psi_n^k(x) \) of band \( n \) as

\[ \hat{\Phi}_n^{\sigma, k}(x, \tau) = \sum_{\tau_n} c_{\sigma, \tau_n}^n(\tau) \psi_n^k(x). \]  

(B.23)

By Eq. (B.14) \( c_n^{\sigma, k} \) do not depend either on the band (\( a \) or \( b \)) or on the momentum \( k \), but only on which subband (\( \sigma = \pm \)) the particles are in. However, the interaction matrix elements \( W_{bbaa}^{k_1; k_2; k_3; k_4} \) do depend on the momenta of the particles.
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(\begin{align*}
(a, k, +; a, -k, +) \rightarrow (b, q, +; b, -q, +) & : \quad 4M_1 \cos \left[ \frac{1}{2}(\omega \tau - 2V_\alpha/(\hbar \omega \sin(\omega \tau))) \right]^4 \\
& + 2(-M_1 - M_4 + M_5 + M_6 - M_7 - M_8) \sin \left[ \frac{1}{2}(\omega \tau - 2V_\alpha/(\hbar \omega \sin(\omega \tau))) \right]^2 \\
& + 2(-M_1 - M_4 + M_5 + M_6 + M_7 - M_8) \cos \left[ \frac{1}{2}(\omega \tau - 2V_\alpha/(\hbar \omega \sin(\omega \tau))) \right] \\
& \times \sin \left[ \frac{1}{2}(\omega \tau - 2V_\alpha/(\hbar \omega \sin(\omega \tau))) \right]^2 \\
(a, k, +; a, -k, +) \rightarrow (b, q, -; b, -q, -) & : \quad 1/2(-M_1 + 3M_3 - M_4 + M_5 + M_6 + M_7 - M_8) \\
& + 4M_2 \cos \left[ \frac{1}{2}(\omega \tau - 2V_\alpha/(\hbar \omega \sin(\omega \tau))) \right]^4 - 8M_1 \cos \left[ \frac{1}{2}(\omega \tau - 2V_\alpha/(\hbar \omega \sin(\omega \tau))) \right] \\
& + 1/2(\omega \tau - 2V_\alpha/(\hbar \omega \sin(\omega \tau))) \\
(a, k, +; a, -k, +) \rightarrow (b, q, +; b, -q, -) & : \quad (M_4 + M_2 - M_1 - M_4 + M_5 + M_6 - M_7 - M_8) \sin \left[ \frac{1}{2}(\omega \tau - 2\kappa \sin(\omega \tau)) \right] \\
& + 1/2(\omega \tau - 2\kappa \sin(\omega \tau)) \\
\end{align*})

\textbf{Table (B.1)} Matrix-elements \( I_{a_1, a_2; b_1, b_2; q, -q; \tau_{mi} = \pm} \) as defined in Eq. (B.22) for transitions from an initial state with particles starting in the lower band \( a \) in subband \( \tau_{mi} \) into the state with two particles in the upper-band \( b \) in subbands \( \sigma_1 \) and \( \sigma_2 \) with momenta \( q \) and \(-q\), abbreviated as \((a, k, +; a, -k, +) \rightarrow (b, q, \sigma_1; b, -q, \sigma_2)\).

With the definition of the following abbreviations

\begin{align*}
M_1 & = W_q^{q-k,-k} \\
M_2 & = W_q^{q+k,-k+\pi} \\
M_3 & = W_q^{q+k,-k} \\
M_4 & = W_q^{q+k,-k+\pi} \\
M_5 & = W_q^{q+k,-k+\pi} \\
M_6 & = W_q^{q+k,-k} \\
M_7 & = W_q^{q+k,-k+\pi} \\
M_8 & = W_q^{q+k,-k+\pi} \\
\end{align*}

the matrix-elements for transitions from an initial state with particles starting in the lower band \( a \) in subband \( \tau_{mi} = \pm \) into the state with two particles in the upper-band \( b \) in subbands \( \sigma_1 \) and \( \sigma_2 \) with momenta \( q \) and \(-q\), abbreviated as \((a, k, +; a, -k, +) \rightarrow (b, q, \sigma_1; b, -q, \sigma_2)\), are given in Table B.1.

To better understand the general behaviour of these matrix elements with regard to their Fourier-structure and justify the statements made in their discussion, we will consider more closely the \((a, k, +; a, -k, +) \rightarrow (b, q, +; b, -q, -)\) element given by

\begin{equation}
I_{+,-k,q} = f_1(\{M_i\}) \sin \left[ \omega \tau - 2\kappa \sin(\omega \tau) \right] + f_2(\{M_i\}) \sin \left[ 2(\omega \tau - 2\kappa \sin(\omega \tau)) \right] / 2 \quad \text{(B.32)}
\end{equation}
with

\[ f_1(\{M_i\}) = M_1 + M_2 - M_3 - M_4 - M_5 + M_6 - M_7 + M_8 , \]
\[ f_2(\{M_i\}) = M_1 + M_2 + M_3 + M_4 - M_5 - M_6 - M_7 - M_8 . \]  
(B.33)

If the interaction matrix elements are momentum-independent, \( M_i = M \), we have that \( f_1(\{M_i\}) = f_2(\{M_i\}) = 0 \) and the time-dependent terms vanish, and therefore no inelastic scattering occurs.

Using the usual expansion in terms of Besselfunctions, \( \exp \left[ iz \sin(\omega \tau) \right] = \sum_n J_n(z)e^{in\omega \tau} \), the term given in Eq. (B.32) is seen to in fact contain all frequency components allowing the absorption of an arbitrary integer number of energy quanta \( \hbar \omega \). Moreover, for small \( \kappa = V_\omega / (\hbar \omega) \) higher order processes are suppressed by powers of \( \kappa \). Specifically, for this matrix element, in a given order \( (\kappa)^n \), frequency components \( \exp[im\omega \tau] \) from \( m = -n - 2 \) up to \( m = n + 2 \) are present. Or put differently, an \( m \)-photon transition is at least suppressed by a power of \( (\kappa)^{n_0} \) with \( n_0 = \max \{ |m| - 2, 0 \} \).
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Appendix C.

Floquet Calculation for the Dynamical Superlattice

In Chapter 4 we studied the specific experimental setup used to simulated the Harper-Hofstadter Hamiltonian with ultracold atoms [78, 81]. In this appendix we provide the details on the calculation of the full non-interacting Floquet states and spectrum for this model.

C.1. Structure of the Floquet Matrix and Floquet States

The model, Eq. (4.2), was given by

\[ \hat{H}_0(\tau) = \int d^2x \frac{-\hbar^2}{2M} \hat{\Psi}^\dagger(x) \left[ \frac{\partial_x^2 + \partial_y^2}{y} \right] \hat{\Psi}(x) + \int d^2x \hat{\Psi}^\dagger(x) V(x, y, \tau) \hat{\Psi}(x) \]  

(C.1)

where we restricted to the two-dimensional plane since the transverse dynamics separates in the non-interacting problem.

To obtain the Floquet states we first split the Hamiltonian into its static and time-dependent contributions

\[ \hat{H}_0(\tau) = \hat{H}_{\text{stat}} + \hat{V}_{\text{mod}}(\tau) \]  

(C.2)
where $\hat{H}_{\text{st}} = \hat{H}_{\text{kin}} + \hat{V}_{\text{st}}$ is given by the kinetic energy and the static potential

$$\hat{V}_{\text{st}}(x, y) = V_x \sin^2(k_r x) + V_x l \sin^2(k_r x/2) + V_y \sin^2(k_r y).$$  \hspace{1cm} (C.3)

The static part has translational symmetry under $x \rightarrow x + 2d$ and $y \rightarrow y + d$. We artificially reduce the BZ to $k \in [\pi/(2d), \pi/(2d)] \times [\pi/(2d), \pi/(2d)]$ with $d = \pi/k_r$, i.e. only consider $y \rightarrow y + 2d$. The time-dependent part is

$$\hat{V}_{\text{mod}}(x, y, \tau) = \kappa \left[ \sin(\pi/4 + k_r x/2) \cos(\phi_0 + \omega \tau - k_r y/2) - \cos(\pi/4 + k_r x/2) \sin(\phi_0 - \omega \tau - k_r y/2) \right].$$  \hspace{1cm} (C.4)

We can rewrite this as $\hat{V}_{\text{mod}}(x, y, \tau) = e^{i\omega \tau} F(x, y) + e^{-i\omega \tau} F^*(x, y)$ with a quasi-periodic function $F(r) = e^{iG \cdot r} f(r)$, where $r = (x, y)$ and $G = (\pi/(2d), \pi/(2d))$, with respect to the BZ defined above. This means $f(r)$ is periodic under translations by two lattice sites in $x$ and $y$. For $\phi_0 = \pi/4$ it takes the form

$$f(x, y) = \kappa \left(-i - e^{-ik_r x} + e^{-ik_r y} + ie^{-ik_r (x+y)}\right)/4.$$  \hspace{1cm} (C.5)

Expanding the Floquet states as $|\Psi_e(\tau)\rangle = e^{i\omega \tau/\hbar} \sum_m e^{im\omega \tau} |\phi_m\rangle$ the time-dependent Schrödinger equation becomes an infinite-dimensional matrix eigenvalue equation $\hat{H}_F \Phi = \epsilon \Phi$ with $\Phi = (\cdots, \phi_{-1}, \phi_0, \phi_1, \cdots)$ and

$$\hat{H}_F = \begin{pmatrix} \cdots & \cdots & \cdots & \cdots \\ \cdots & \hat{H}_{\text{st}}(r) - \omega & F(r) & \cdots \\ & F^*(r) & \hat{H}_{\text{st}}(r) & F(r) \\ & & F^*(r) & \hat{H}_{\text{st}}(r) + \omega & \cdots \\ & & & \cdots & \cdots & \cdots \\ & & & & & \cdots \end{pmatrix}$$

We can now perform a unitary gauge-transformation in Floquet space defined via

$$\hat{U} \Phi = (\cdots, e^{-iG \cdot \phi_{-1}}, \phi_0, e^{iG \cdot \phi_1}, \cdots).$$  \hspace{1cm} (C.6)
for which the transformed Hamiltonian \( \tilde{H}_F = \hat{U} \hat{H}_F \hat{U}^\dagger \) turns out to be

\[
\tilde{H}_F = \begin{pmatrix}
\ddots & \ddots & \ddots \\
\ddots & e^{-iG \cdot r} \hat{H}_{st}(r) e^{iG \cdot r} - \omega & f(r) \\
& \hat{H}_{st}(r) & f(r) \\
& \hat{H}_{st}(r) & e^{iG \cdot r} \hat{H}_{st}(r) e^{-iG \cdot r} + \omega \\
\ddots & \ddots & \ddots 
\end{pmatrix}
\]

We emphasise again that \( \hat{H}_{st}(r) \) and \( f(r) \) are both periodic under translations by two lattice-sites. Exploiting further that \( 2G \) is a reciprocal lattice vector, and thus,

\[
e^{-iG \cdot r} \hat{H}_{st}(r) e^{iG \cdot r} = \hat{H}_{st}(k - G) = \hat{H}_{st}(k - G + 2G) = \hat{H}_{st}(k + G) \quad (C.7)
\]

we can write the Hamiltonian in momentum space as

\[
\tilde{H}_F(k) = \begin{pmatrix}
\ddots & \ddots & \ddots \\
\ddots & \hat{H}_{st}(k + G) - \omega & f(k) \\
& \hat{H}_{st}(k) & f(k) \\
& \hat{H}_{st}(k) & \hat{H}_{st}(k + G) + \omega \\
\ddots & \ddots & \ddots 
\end{pmatrix}
\]

where \( k \) is restricted to lie in the Brillouin Zone, \( k \in [\pi/(2d), \pi/(2d)] \times [\pi/(2d), \pi/(2d)] \). Since the Hamiltonian still contains operators at \( k \) and \( k + G \) this BZ would have to be further reduced. However, there is another symmetry under \( \tilde{H}_F \rightarrow \tilde{H}_F + \omega \mathbb{1}, k \rightarrow k + G \) which just shifts the spectrum by \( \hbar \omega \), thus, leaving it invariant. We can now project all operators onto the 4 lowest bands of \( \hat{H}_{st} \) at \( k \) and \( k + G \) which are resonantly coupled by the oscillating potential. By further restricting to a finite number of frequency modes, \(-M \leq m \leq M\), we obtain a finite-dimensional matrix equation which can be solved by standard methods. We remark that the spectrum and the Floquet states will appear in copies of the desired Floquet band structure spaced by \( \hbar \omega \) and shifted in Floquet space due to the freedom in defining the quasi-energy, up to boundary effects due to truncating the matrix. To keep these boundary effects minimal, the representative states have to be taken from the middle of the spectrum, and a sufficient number of frequency modes.
$M$ has to be kept such that this symmetry of the spectrum and the Floquet modes is observed within the desired accuracy.

We finish by pointing out the consequences for the structure of the Floquet states of the non-interacting problem. Due to the additional symmetry described above, the Hamiltonian will have 4 distinct Floquet states. Each Floquet state at momentum $k$ will contain 8 bands of the static Hamiltonian, 4 bands at $k$ and a further 4 at $k + G$. In addition, due to the unitary gauge transformation we performed, components at even/odd frequencies will be shifted relatively by $G$. As we already observed in the simpler toy model in Appendix B.2, the relative population of these momentum-states will be periodically time-dependent as well.
Appendix D.

Synthetic Dimensions and Synthetic Magnetic Fields

In this appendix we provide a derivation of the time-independed Hamiltonian for the dynamics of atoms under the influence of Raman beams in an optical lattice used in Section 5.2, Eqs. (5.1) to (5.2).

In Appendix D.1 we explain how to use Raman lasers to create synthetic magnetic fields. We follow Ref. [70] with the difference that we will comment on the rotating wave approximation in relation to Floquet scattering. The rotating wave approximation is performed on the level of the frequency of the linear Zeeman splitting and between atoms in different states in the groundstate manifold. We will consider whether this leads to Floquet scattering in this system. Specifically, we will see below that it does not lead to Floquet scattering if the interactions do conserve the spin projection as already seen in Section 3.4.1. In Appendix D.2 we will connect the general theory with the explicit model we studied in Chapter 5.

D.1. Synthetic Magnetic Fields through Raman beams

We consider an atom in its groundstate manifold subject to a physical magnetic field and Raman beams.
Appendix D. Synthetic Dimensions and Synthetic Magnetic Fields

The atomic Hamiltonian in the groundstate manifold is

\[ \hat{H} = A_{hf} \hat{I} \cdot \hat{J} + \frac{\mu_B}{\hbar} g_J \mathbf{B} \cdot \hat{J}, \]  

where we include the hyperfine splitting proportional to \( A_{hf} \), coupling the nuclear spin \( \hat{I} \) to the combined angular momentum of electron spin and angular motion, \( \hat{J} = \hat{L} + \hat{S} \), and the effects of a physical magnetic field \( \mathbf{B} \) coupling to \( \hat{J} \) where \( \mu_B \) is the Bohr magneton and \( g_J \) the Landé factor.

We consider interactions with a light field \( \mathbf{E}(\tau) \) of the same form as in Appendix A, i.e. \( \mathbf{E}(\tau) = \hat{E} e^{-i \omega \tau} + \hat{E}^* e^{i \omega \tau} \). We may now include the effect of the coupling by the Raman lasers to the excited state manifold by the dipole-Hamiltonian via the effective Hamiltonian Eq. (A.7) derived in Appendix A, and obtain

\[ H_{B+R} = u_s \hat{E}^* \cdot \hat{E} + \frac{\mu_B}{\hbar} g_J (\mathbf{B} + \mathbf{B}_{\text{eff}}) \cdot \hat{J} + A_{hf} \hat{I} \cdot \hat{J} \]  

where the vector coupling is seen to lead to an effective magnetic field defined as \( \mathbf{B}_{\text{eff}} = \frac{iu_s (\hat{E}^* \times \hat{E})}{\mu_B g_J} \) and \( u_s \) and \( u_v \) are the scalar and vector polarizabilities.

Finally, we will assume that the linear Zeeman shifts are small compared to the hyperfine splitting \( A_{hf} \). In this case the total angular momentum \( \hat{F} = \hat{J} + \hat{I} \) is a good quantum number and we obtain

\[ H_{B+R} = u_s \hat{E}^* \cdot \hat{E} + \frac{\mu_B}{\hbar} g_F (\mathbf{B} + \mathbf{B}_{\text{eff}}) \cdot \hat{F} + A_{hf} \hat{I} \cdot \hat{J} \]  

where \( g_F \) is the hyperfine Landé factor and we may drop the last term as it is constant in a fixed hyperfine manifold.

We may decompose the magnetic field coupling term

\[ \mathbf{B} \cdot \hat{F} = B_x \hat{F}_x + B_- \hat{F}_+ + B_+ \hat{F}_- \]  

with respect to the raising and lowering operators \( \hat{F}_\pm = \hat{F}_x \pm i \hat{F}_y \) and \( B_\pm = \frac{B_x \pm B_y}{2} \) which will prove useful in the following.
Starting from D.3 we may now analyse the experimental settings of interest. We assume atoms in a physical magnetic field $B = B_0 e_z$ in a hyperfine manifold, the $m_F$ states will consequently be split in energy by $\mu_B B_0$. The atoms will then in addition be illuminated by two lasers of frequencies $\omega_1$ and $\omega_2 = \omega_1 + g_F \mu_B B_0 / \hbar + \delta$ where the additional detuning $\delta$ is small compared to the linear Zeeman shift and the frequency difference $\delta = \omega_2 - \omega_1$.

The electric field is then given by $E = E_1 e^{-i\omega_1 \tau} + E_2 e^{-i\omega_2 \tau} + E_1^* e^{i\omega_1 \tau} + E_2^* e^{i\omega_2 \tau}$. This leads to an effective magnetic field of the form

$$B_{\text{eff}} = B^{(0)} + B^{(12)} e^{-i\delta \omega \tau} + B^{(21)} e^{+i\delta \omega \tau}$$  \hspace{1cm} (D.5)

with

$$B^{(0)} = \frac{i u_\omega}{\mu_B g_f} (E_1^* \times E_1 + E_2^* \times E_2)$$  \hspace{1cm} (D.6)

$$B^{(12)} = \frac{i u_\omega}{\mu_B g_f} E_1^* \times E_2$$  \hspace{1cm} (D.7)

$$B^{(21)} = \frac{i u_\omega}{\mu_B g_f} E_2^* \times E_1$$  \hspace{1cm} (D.8)

Using the decomposition introduced above, we obtain the corresponding terms $B_z$, $B_+$, and $B_-$ for each of these magnetic fields.

The final step consists in another rotating wave approximation, we now additionally assume that $\delta = \omega_1$ is large compared to all energy scales we are interested in. Therefore, we perform a unitary transformation via $\hat{U}(\tau) = \exp \left[ -i \frac{\delta \omega}{\hbar} \hat{F}_z \tau \right]$ with the transformed Hamiltonian $\hat{U}(\tau)^\dagger \hat{H}_{B+} \hat{U}(\tau) - i \hbar \hat{U}(\tau)^\dagger \partial_\tau \hat{U}(\tau)$.

This is the rotating wave approximation mentioned in the beginning. Since it is defined via $\hat{F}_z$ it will only affect the interactions if they contain terms changing the total spin projection of the particles, e.g. terms of the form $\hat{c}_{m_1}^\dagger \hat{c}_{m_2}^\dagger \hat{c}_{m_3} \hat{c}_{m_4}$ with $m_1 + m_2 \neq m_3 + m_4$ where $c_{m_i}^\dagger$ are creation operators for particles in the $\hat{F}_z$ eigenbasis. In particular, for the interactions considered in Chapter 5 of the form $\hat{n}_{m_2} \hat{n}_{m_2}'$ with $\hat{n}_{m_2} = \hat{c}_{m_2}^\dagger \hat{c}_{m_2}$ this is manifestly not the case, i.e. the unitary transformation commutes with the interactions and they do not become time-dependent in the rotating frame.

We consider the effects of this on the Hamiltonian in parts:
Firstly, terms coupling to $\hat{F}_z$ will be unaffected, $\hat{U}(\tau)^\dagger \hat{F}_z \hat{U}(\tau) = \hat{F}_z$, whereas for the raising/lowering operators we obtain, $\hat{U}(\tau)^\dagger \hat{F}_\pm \hat{U}(\tau) = \hat{F}_\pm e^{i\pm \delta_\omega \tau}$. Eliminating any terms in the transformed Hamiltonian rotating with $\pm \delta_\omega$ and $\pm 2 \delta_\omega$, the only terms remaining are $B^{(12)}_\pm \hat{F}_\pm$, $B^{(21)}_+ \hat{F}_-^*$ and $B^{(0)}_\pm \hat{F}_z$.

Secondly, we will obtain an energy shift $-i\hbar \hat{U}(\tau)^\dagger \partial_\tau \hat{U}(\tau) = -(g_F \mu_B B_0 / \hbar + \delta) \hat{F}_z$ which cancels the linear Zeeman shift up to $\delta$.

Thus, we obtain the transformed Hamiltonian as

$$\hat{H}_{B+R,RW} = \Omega_z \hat{F}_z + \Omega_- \hat{F}_- + \Omega_+ \hat{F}_+ + V, \quad (D.9)$$

with

$$\Omega_z = \frac{\mu_B g_F \hat{F}_z^{(0)}}{\hbar} - \delta \quad (D.10)$$
$$\Omega_+ = \frac{\mu_B g_F \hat{F}_z^{(21)}}{\hbar} \quad (D.11)$$
$$\Omega_- = \frac{\mu_B g_F \hat{F}_z^{(12)}}{\hbar} \quad (D.12)$$

and the scalar potential

$$V = u_s (E_1^* \cdot E_1 + E_2^* \cdot E_2). \quad (D.13)$$

We recall that the induced effective magnetic fields are proportional to $u_s$. Therefore, as discussed in Appendix A.1, spontaneous emission cannot be completely suppressed by working at large detunings from the atomic resonance. Consequently, these systems are always subject to some level of off-resonant light-scattering which cannot be improved by increasing the detuning beyond the hyperfine splitting.

**D.2. Experimental Setup for Synthetic Dimensions**

This now allows us to consider a specific experimental setup used to simulate synthetic dimensions. We assume counter propagating Raman lasers aligned along $x$.
D.2. Experimental Setup for Synthetic Dimensions

with wavenumber \( k_R = 2\pi/\lambda \) and crossed linear polarisations, i.e. \( E_1 = E e^{i k_R x} e_y \) and \( E_2 = E e^{-i k_R x} e_z \).

We obtain \( \Omega_x = -\delta \) and

\[
\Omega_{\pm} = \Omega_R \pm i(2k_R x - \pi/2)
\]

with \( \Omega_R = \frac{q e u_x}{g} E^2 \). The scalar potential is given by \( V = 2u_x E^2 \).

To make the connection to the model studied in the main text explicit, we now expand the operator \( \hat{F}_\pm \) in the basis \( |m_z\rangle \) of the eigenstates of \( \hat{F}_z \). The only non-vanishing matrix elements are given by

\[
\hat{F}_\pm = \langle m_z | \hat{F}_\pm | m_z \mp 1 \rangle = g_{m_z} = \sqrt{F(F+1) \mp m_z(m_z - 1)}.
\]

Thus, we can write the Hamiltonian as

\[
\hat{H}(x) = \Omega_+ \hat{F}_- + \Omega_- \hat{F}_+
\]

\[
= \frac{\Omega_R}{2} \sum_{m_z=-F}^{F-1} e^{-i\phi(x)} g_{m_z+1} \hat{c}^\dagger_{x,m_z+1} \hat{c}_{x,m_z} + \frac{\Omega_R}{2} \sum_{m_z=-F+1}^{F} g_{m_z} e^{i\phi(x)} \hat{c}^\dagger_{x,m_z} \hat{c}_{x,m_z-1}
\]

\[
= \frac{\Omega_R}{2} \sum_{m_z=-F}^{F-1} \left( e^{-i\phi(x)} g_{m_z+1} \hat{c}^\dagger_{x,m_z+1} \hat{c}_{x,m_z} + h.c. \right)
\]

with \( \phi(x) = 2k_R x - \pi/2 \) and the creation operator \( \hat{c}^\dagger_{x,m_z} \) for an atom in the \( m_z \) state at position \( x \). In arriving at this Hamiltonian we set \( \delta = 0 \) and neglected the effect of the scalar potential \( V \), as we are about to add a stronger optical potential in the following.

We consider an additional optical lattice along \( x \) of the form \( V_{\text{lat}} = V_L \sin^2(k_L x) \) of depth \( V_L \) created by two counter propagating laser beams with wavenumber \( k_L \) and we assume a regime in which \( V_L \gg V \). This optical lattice confines the atoms to the lattice-sites \( x_j = j d \) with \( d = \pi/k_L \). In the tight-binding approximation for hopping along the optical lattice we obtain the Hamiltonian of Section 5.2, Eqs. (5.1) to (5.2), with \( \phi = 2k_R d \) and \( \Omega = \Omega_R/2 \).
Appendix E.

Effective Model for Synthetic Dimensions in Strong Coupling Limit

In Chapter 5 we discussed the many-body phases of bosonic atoms with \( N \) internal states confined to a 1D optical lattice under the influence of a synthetic magnetic field and repulsive interactions. By considering the case of strong SU\((N)\) invariant local density-density interactions and strong Raman coupling we simplified the full problem to the study of an effective spin 1/2 model. In this appendix we provide the explicit derivation leading to the effective Hamiltonian in Eq. (5.3).

E.1. Derivation of the Effective Model

We start from the Hamiltonian of bosons with \( N = 2I + 1 \) internal spin states loaded into a one-dimensional optical lattice described by \( \hat{H} = \hat{H}_1 + \hat{H}_2 + \hat{H}_{\text{int}} \).

\( \hat{H}_1 \) describes the bosonic hopping along the lattice,

\[
\hat{H}_1 = -t \sum_j \sum_{m_z = -I}^I \left( \hat{c}^\dagger_{j+1,m_z} \hat{c}_{j,m_z} + h.c. \right) \tag{E.1}
\]

where \( \hat{c}^{(\dagger)}_{j,m_z} \) are bosonic operators annihilating (creating) bosons in spin state \( m_z \) at site \( j \) and \( t \) is the hopping amplitude.
Figure (E.1) Illustration of the position-dependent spin-orientation $\langle \hat{U} \hat{S} \hat{U}^\dagger \rangle$ in the $s_x = l$ eigenstate when transformed back to the original basis, see the discussion after the unitary transformation Eq. (E.3).

In addition the internal spin states are coupled by Raman lasers described by the Hamiltonian

$$\hat{H}_2 = -\sum_j \sum_{m_z=-l}^{l-1} \Omega_{m_z+1} \left( e^{i\phi j} \hat{c}_{j,m_z+1}^\dagger \hat{c}_{j,m_z} + h.c. \right)$$  \hspace{1cm} (E.2)$$

where $\Omega_{m_z} = \Omega_{g_{m_z}}$ with $g_{m_z} = \sqrt{l(l+1) - m_z(m_z-1)}$ and $\phi = \Delta k_R d$ is the running phase of the Raman beams given by the wave-vector transfer $\Delta k_R$ and the lattice spacing $d$. $\hat{H}_{\text{int}}$ is taken to be a SU($2l+1$) invariant interaction of contact form, i.e. $\hat{H}_{\text{int}} = U \sum_{j,m_z,m'_z} \hat{n}_{j,m_z} (\hat{n}_{j,m'_z} - \delta_{m_z,m'_z})$.

For open boundary conditions in the synthetic direction using the unitary transformation $\hat{U}$ defined by $\hat{U} \hat{c}_{j,m_z} \hat{U}^\dagger = e^{i\phi_m} \hat{c}_{j,m_z}$ the Hamiltonian is transformed to

$$\hat{U} \hat{H} \hat{U}^\dagger = -t \sum_j \sum_{m_z=-l}^{l-1} \left( e^{-i\phi_{m_z}} \hat{c}_{j+1,m_z}^\dagger \hat{c}_{j,m_z} + h.c. \right)$$

$$- \sum_j \sum_{m_z=-l}^{l-1} \Omega_{m_z} \left( \hat{c}_{j,m_z+1}^\dagger \hat{c}_{j,m_z} + h.c. \right) + \hat{H}_{\text{int}}$$  \hspace{1cm} (E.3)$$

As we consider $t \ll \Omega$ we now transform to the eigenstates of the Raman coupling Hamiltonian $\hat{H}_2$. After the unitary transformation this is just $\hat{H}_2 = -2\Omega \sum_j \hat{S}_{x,j}$, where $\hat{S}_{x,j}$ is the $\hat{S}_x$ operator for spin $l$ for particles at site $j$. Note in particular that it is now site-independent due to gauging the Raman phase into the hopping part of the Hamiltonian. Consequently, the eigenfunctions are just the $s_x$ eigenstates and the spectrum at each site
is given by \( E_s = -2\Omega s \) with \( s = -1, \ldots, I \). Due to the gauge-transformation we performed, this actually corresponds to a rotating spin-orientation in the original basis. In Fig. E.1 we show the expectation values of \( \langle \hat{U}\hat{S}_s\hat{U}^\dagger \rangle \), \( \langle \hat{U}\hat{S}_y\hat{U}^\dagger \rangle \) in the \( s = I \) eigenstate transformed to the original basis, \( \langle \hat{U}\hat{S}_z\hat{U}^\dagger \rangle \) vanishes for this state.

\[ \hat{H}_1 \] in the new basis reads as \( \hat{H}_1 = -t \sum_{s,s'} \left( T_{s,s'}(\phi)\hat{d}_{j+1,s}^\dagger\hat{d}_{j,s} + \text{h.c.} \right) \) where \( \hat{d}_{j+1,s}^\dagger \) creates a particle in the \( s' \) eigenstate at site \( j \) and we defined the hopping matrix \( T_{s,s'}(\phi) = \langle s_x | e^{-i\phi\hat{S}_z} | s'_x \rangle \) which now couples states \( s \) and \( s' \). As the interaction Hamiltonian is SU(2I+1) invariant it takes the same form in the transformed basis, \( \hat{H}_{\text{int}} = U \sum_{j,s,s'} \hat{n}_{j,s}(\hat{n}_{j,s'} - \delta_{s,s'}) \) where now the sum runs over the \( s_x \) eigenstates. In the limit of strong interactions this restricts the occupation at each site to be 0 or 1.

We see that \( \hat{H}_2 + \hat{H}_{\text{int}} \) is diagonal in the occupation number basis of \( s_x \) eigenstates. In the limit \( t \ll \Omega, U \) we treat \( \hat{H}_1 \) as a perturbation and derive an effective model keeping only the lowest energy eigenstate at each site, i.e. the \( s = I \) state, and consider the sector with empty and singly occupied sites. To second order we obtain a model describing spinless particles interacting via a nearest neighbour interaction and hopping with nearest neighbour, next-nearest neighbour and correlated next-nearest neighbour tunnelling terms. The effective Hamiltonian takes the form

\[
\hat{H}_{\text{eff}} / t = -f^I_1(\phi) \sum_j \left( \hat{d}_{j+1}^\dagger \hat{d}_j + \text{h.c.} \right) + 2\kappa \left[ f^I_1(\phi, \tilde{u} = 0) - f^I_1(\phi, \tilde{u}) - \frac{f^I_1(\phi)^2}{2I\tilde{u}} \right] \sum_l \hat{n}_l \hat{n}_{l+1}
+ \kappa \left[ f^I_{\text{cor}}(\phi, \tilde{u} = 0) \sum_j \left( \hat{d}_{j+2}^\dagger (1 - \hat{n}_{j+1})\hat{d}_j + \text{h.c.} \right) + f^I_{\text{cor}}(\phi, \tilde{u}) \sum_j \left( \hat{d}_{j+2}^\dagger \hat{n}_{j+1} \hat{d}_j + \text{h.c.} \right) \right]
- \frac{f^I_1(\phi)^2}{2I\tilde{u}} \sum_j \left( \hat{d}_{j+2}^\dagger \hat{n}_{j+1} \hat{d}_j + \text{h.c.} \right)
\]

where \( \hat{d}_j = \hat{a}_{j,I} \) is the creation operator for a particle in the \( s_x = I \) eigenstate at site \( j \), \( \kappa = t / \Omega \) and \( \tilde{u} = U / (4I\Omega) \).

The functions \( f^I_1(\phi) \) depend on the flux \( \phi \), the interaction strength \( \tilde{u} \) and parametrically on the number of spin states \( I \). The first term describes the diagonal hopping between the \( s = I \) spin states and the remaining terms describe virtual hopping processes. The nearest neighbour repulsion \( V \) originates from nearest neighbour hopping and returning to the original site via an excited spin state on a neighbouring site which is either empty (first
term) or occupied (second term) or hopping onto an occupied site in the lowest energy
spin state (third term). The correlated tunnelling term \( t_{\text{cor}} \) arises from the corresponding
processes with the particle not returning to the original site. The functions \( f_i^{(l)}(\phi) \) take
the explicit form

\[
f_i^{(l)}(\phi) = \cos(\phi/2)^{2l}
\]

(E.4)

\[
f_{\text{cor}}^{(l)}(\phi, \tilde{u}) = -\sum_{s' \neq 1} \frac{T_{s,s'}(\phi)T_{s',s'}(\phi)}{(E_{s'} - E_I + U)/\Omega}
\]

(E.5)

\[
= -\frac{\cos(\phi/2)^{4l}}{4l\tilde{u}} \left[ F(-2l, 2l\tilde{u}, 1 + 2l\tilde{u}, \tan(\phi/2)^2) - 1 \right]
\]

where \( \tilde{u} = U/(4I\Omega) \) and \( F(a, b, c, z) = {}_2F_1(a, b, c, z) \) is the hypergeometric function, which
we derive in the next section.

E.2. Derivation of Coupling Functions

In this section, we compute the coupling functions given above in Eqs. (E.4) to (E.6). To do
so, we require the matrix elements of the gauged hopping elements between eigenstates
of the \( \hat{S}_x \) operator for spin \( I \), e.g.

\[
T_{s,s'}(\phi) = \langle s_x | e^{-i\phi \hat{S}_z} | s_{s'} \rangle .
\]

(E.7)

We first define the raising and lowering operators in the \( \hat{S}_x \)-eigebasis as

\[
\hat{S}^+_x = \hat{S}_z + i\hat{S}_y = \hat{S}_z + \frac{1}{2}(\hat{S}_+ - \hat{S}_-).
\]

(E.8)
with respect to the usual $\hat{S}_z$ representation. Starting from the unique highest weight state in the $\hat{S}_x$ eigenbasis, $|I\rangle_x$, we can generate any $s_x$ eigenstate via

$$|m\rangle_x = \left(\frac{2I}{I + m}\right)^{1/2} \frac{1}{(I - m)!} \left(\hat{S}_x\right)^{I-m} |I\rangle_x.$$  

(E.9)

The problem now reduces to computing

$$T_{s,s'}(\phi) = \langle s_x | e^{-i\phi/2(\hat{S}_+^x + \hat{S}_-^x)} | s'_x \rangle.$$  

(E.10)

We make use of the decomposition

$$\exp \left[ w_+ \hat{S}_+^x + w_- \hat{S}_-^x + w_x \hat{S}_x \right] = \exp \left[ x_- \hat{S}_-^x \right] \exp \left[ \ln(x) \hat{S}_x \right] \exp \left[ x_+ \hat{S}_+^x \right]$$

(E.11)

which is an operator identity. Importantly, it is true independent of the specific representation chosen. With $w_+ = w_- = -i\phi/2$ and $w_x = 0$ we obtain $x_+ = x_- = -i \tan(\phi/2)$ and $x = \cos(\phi/2)^2$, which can be easily checked by using the spin-$1/2$ presentation of the spin-operators. Thus, we compute

$$e^{-i\phi/2(\hat{S}_+^x + \hat{S}_-^x)} |I\rangle_x = \exp \left[ x_- \hat{S}_-^x \right] \exp \left[ \ln(x) \hat{S}_x \right] \exp \left[ x_+ \hat{S}_+^x \right] |m\rangle_x$$

(E.12)

$$= \exp \left[ x_- \hat{S}_-^x \right] \exp \left[ \ln(x) \hat{S}_x \right] |I\rangle_x$$  

(E.13)

$$= x^I \sum_{k=0}^{\infty} \frac{1}{k!} x^k \left(\hat{S}_x\right)^k |I\rangle_x$$  

(E.14)

$$= x^I \sum_{m=-I}^{I} x^l l^{-m} \left(\frac{2I}{I + m}\right)^{1/2} |m\rangle_x$$  

(E.15)

from which it follows that

$$T_{m,l} = x^I x^{-m} \left(\frac{2I}{I + m}\right)^{1/2}.$$  

(E.16)

This immediately yields the first coupling function as

$$f_I^I(\phi) = T_{II}(\phi) = \cos(\phi/2)^{2I}$$

(E.17)

as given in Eq. (E.5). Applying this to compute the coupling function $f_{cor}^I(\phi, \tilde{u})$, we


Appendix E. Effective Model for Synthetic Dimensions in Strong Coupling Limit

obtain

\[- f^I_{\cos}(\phi, \tilde{U}) = \sum_{s' \neq I} \frac{T_{I,s'}(\phi) T_{I,s'}(\bar{\phi})}{(E_{s'} - E_I + U)/\Omega}(\text{E.18})\]

\[
= \frac{1}{2} x^{2I} \sum_{m=0}^{2I-1} \binom{2I}{m} \frac{x^{4I-2m}}{2s - m + U/(2\Omega)}
\]

\[
= \frac{1}{2} x^{2I} x^{-4I\tilde{u}} \sum_{m=0}^{2I-1} \binom{2I}{m} \frac{(x^2)^{2I-m+2I\tilde{u}}}{2I - m + 2I\tilde{u}}
\]

\[
= \frac{1}{2} x^{2I} x^{-4I\tilde{u}} \sum_{m=0}^{2I-1} \binom{2I}{m} \int_0^{x^2} y^{2I-m+2I\tilde{u}-1} dy
\]

\[
= \frac{1}{2} x^{2I} x^{-4I\tilde{u}} \int_0^{x^2} [(1 + y^{2I}) - 1] y^{2I\tilde{u}-1} dy
\]

\[
= \frac{\cos(\phi/2)^{4I}}{4I\tilde{u}} \left[ F(-2I, 2I\tilde{u}, 1 + 2I\tilde{u}, \tan(\phi/2)^2 - 1) \right]
\]

(E.23)

to be compared with the result in Eq. (E.5). The last coupling function $ f^I_{V} $ follows from a similar computation with the result given in Eq. (E.6).
Bibliography


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