The Response of Particles in Periodic Potentials to External Forces: New Perspectives

by

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Abstract

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We study the effects of an external constant and uniform force on particles in periodic potentials in the context of transport and optical phenomena. We consider two types of systems: charged carriers in a crystal subject to a constant (dc) electric field and ultracold atoms in optical lattices subject to external forces of various origins. Both systems are described by a Hamiltonian where the force is coupled to the position operator.

In the context of transport phenomena, we study the motion of a wave packet prepared in one band of a periodic potential when a uniform force is suddenly applied and left constant afterwards. The semiclassical description of wave packet dynamics in periodic potentials with applied forces, slowly varying in time and space, relies on the concepts of effective mass, group velocity, and anomalous velocity. If the force is suddenly applied, these quantities do not correctly describe the dynamics, since the wave packet cannot respond instantaneously according to the properties of the lattice. We show that dynamical generalizations of the group and anomalous velocities, and of the inverse effective mass tensor, provide an appropriate description. Our approach is based on modified Bloch states that include the interband mixing due to the force; we compare our results with full numerical calculations, showing excellent agreement when Zener tunneling is negligible. We illustrate our results with one- and two-dimensional optical lattices, where the experimental detection of these dynamics is more accessible than in typical solid-state systems.
In the context of optical phenomena, we consider the absorption of light by bulk semiconductors in the presence of a dc electric field including excitonic and interband coupling effects. The absorption coefficient is calculated from the time evolution of the interband polarization excited by an optical pulse. We illustrate the formalism with a numerical calculation for bulk GaAs using a 14-band $k \cdot p$ model, and we study the dependence of the excitonic enhancement of the absorption coefficient on the strength of the dc field and the optical polarization. We find that the polarization anisotropy described by the independent particle approximation can be modified significantly by the Coulomb interaction.
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Chapter 1

Introduction

The interaction between external electromagnetic fields and crystals is a very important and rich area of solid-state physics. External fields can be used to probe the microscopic properties of matter, since these fields induce charge and current densities, which have macroscopic effects that can be measured experimentally [1]. The periodic array of atoms in a crystal has important consequences on the behavior of charged carriers moving through such an array; these carriers are affected by the external applied fields and the internal fields from the crystal and the other carriers. From a spectral point of view, the appearance of gaps of forbidden energies completely modifies the behavior of such carriers and leads to a distinction between transport phenomena, associated with “intraband” properties, and optical phenomena, associated with “interband” properties [2]; the band structure also has topological properties, which have attracted the attention of the physics community in recent years [3–7].

In this thesis we study some examples of transport and optical phenomena in the presence of a uniform and constant (dc) electric field. Despite its apparent simplicity, the problem of a periodic crystal in a uniform electric field has been a controversial topic in the quantum theory of solids [8, 9]. Only recently, experimental evidence has confirmed phenomena predicted in the early days of solid-state physics, such as Bloch
oscillations [10–15] and Wannier-Stark ladders [16–19]. The reasons are both physical and mathematical, as we will discuss in the following sections. In the context of these controversies, “artificial” lattices, such as superlattices [20] and optical lattices [21], have played a key role from the experimental point of view, since they provide clean and highly tunable potentials that “simulate” a lot of the physics of crystalline materials with more accessible length and time scales.

We begin with a brief description of the minimal coupling Hamiltonian, which is the traditional starting point in the quantum description of the interaction between electromagnetic fields and matter (Sec. 1.1). Next, we discuss in more detail the case of a uniform electric field, which is one of the main subjects of this thesis, in the context of intra- and interband phenomena (Sec. 1.2); we review some of the main results in the literature in connection with the material that will be presented later. The final section summarizes the structure of the remaining chapters (Sec. 1.3).

1.1 The minimal coupling Hamiltonian

Classical electromagnetism can be formulated in terms of electric and magnetic fields, $\mathbf{E}(\mathbf{r}, t)$ and $\mathbf{B}(\mathbf{r}, t)$, or in terms of a vector potential $\mathbf{A}(\mathbf{r}, t)$ and a scalar potential $A_4(\mathbf{r}, t)$ [22]. The latter formulation is used to describe quantum mechanically the interaction of classical electromagnetic fields with matter through the minimal coupling Hamiltonian [1, 23],

$$\hat{H}_{\text{m.c.}}(t) \equiv \frac{1}{2m} \left( \hat{\mathbf{p}} - \frac{e}{c} \mathbf{A}(\hat{\mathbf{r}}, t) \right)^2 + V(\hat{\mathbf{r}}) + eA_4(\hat{\mathbf{r}}, t),$$  

(1.1)

where $\hat{\mathbf{r}}$ is the position operator and $\hat{\mathbf{p}}$ is the canonical momentum operator. Eq. (1.1) is in the Gaussian system, with $c$ denoting the speed of light, $m$ the bare (free) mass of the charged carrier and $e$ its charge; typically, the charged carrier is an electron, in which case $e = -|e|$. We have also included a background potential energy $V(\mathbf{r})$, which in our case is given by the rigid lattice of ions in a crystal. With this Hamiltonian, we consider
the time evolution of the state $|\Psi(t)\rangle$ of one of the charged carriers, neglecting at first the interaction between them. The time-dependent Schrödinger equation for $|\Psi(t)\rangle$,

$$i\hbar \frac{\partial}{\partial t} |\Psi(t)\rangle = \hat{H}_{\text{m.c.}}(t) |\Psi(t)\rangle$$

(1.2)

is invariant under the simultaneous gauge transformation of the potentials,

$$\mathbf{A}(\mathbf{r}, t) \rightarrow \mathbf{A}(\mathbf{r}, t) + \nabla \chi(\mathbf{r}, t), \quad A_4(\mathbf{r}, t) \rightarrow A_4(\mathbf{r}, t) - \frac{1}{c} \frac{\partial}{\partial t} \chi(\mathbf{r}, t)$$

(1.3)

and the wave function,

$$|\Psi(t)\rangle \rightarrow e^{i\frac{\hbar}{c} \chi(\mathbf{r}, t)} |\Psi(t)\rangle,$$

(1.4)

where $\chi(\mathbf{r}, t)$ is an arbitrary scalar function [24].

A common gauge choice in semiconductor optics is to describe the applied electromagnetic field through a vector potential. Furthermore, the variation of the fields is typically slow over the length scale on which the electronic properties of the solid change (of the order of a few lattice constants) allowing for a multipole expansion [1]. In the lowest order approximation, the dipole approximation, the applied fields are assumed to be uniform and therefore Eq. (1.2) can be written as

$$i\hbar \frac{\partial}{\partial t} |\Psi(t)\rangle = \left[ \frac{1}{2m} \left( \hat{\mathbf{p}} - \frac{e}{c} \mathbf{A}(t) \right)^2 + V(\mathbf{r}) \right] |\Psi(t)\rangle.$$

(1.5)

In semiconductor optics this is usually called the $\mathbf{p} \cdot \mathbf{A}$ gauge [1], or simply the velocity gauge [25]. Another possibility is to use the so-called length gauge where the Hamiltonian depends on the electric field, instead of a vector potential; this can be obtained by a phase transformation of $|\Psi(t)\rangle$ according to

$$|\Psi(t)\rangle \rightarrow e^{i\frac{\hbar}{c} \mathbf{A}(t) \cdot \hat{\mathbf{r}}} |\Psi(t)\rangle,$$

(1.6)

which results in the time-dependent Schrödinger equation [1]

$$i\hbar \frac{\partial}{\partial t} |\Psi(t)\rangle = \left[ \frac{1}{2m} \hat{\mathbf{p}}^2 + V(\mathbf{r}) - e \mathbf{E}(t) \cdot \hat{\mathbf{r}} \right] |\Psi(t)\rangle.$$

(1.7)
The length gauge has the important advantage that the dynamical equations are formulated in terms of the electric field, which is what can be measured experimentally. Furthermore, its applicability in practice is not restricted by the frequency of the applied field. This is in contrast with the velocity gauge, where it is well-known that apparent divergences occur at low driving frequencies; such divergences can be cancelled properly using sum rules, but they can be an issue in numerical calculations [25–27]. The length gauge has disadvantages too, especially when the crystal is assumed to be infinite or to satisfy periodic boundary conditions, which is the typical strategy to avoid considering surface effects. The problems arise when the position operator is calculated for extended states in real space, such as Bloch states (for definition, see Sec. 2.1) [28, 29]. In reciprocal space, it is difficult to construct a well-defined operator for translations because of the contribution of the Berry curvature (for definition, see Sec. 2.1) to the relative phase between Bloch states. Nevertheless, there are strategies to deal with these difficulties [25, 26], and many problems in semiconductor optics do not require one to take into account the effects of the Berry curvature explicitly (for example, the Franz-Keldysh effect discussed in Chapter 5).

In this thesis we will consider the Hamiltonian in Eq. (1.7), which we presented here as a result of choosing the length gauge; in the context of Green functions a similar equation can be derived from a gauge-independent formalism, but we leave this discussion to Sec. 5.2.1 and Appendix C. This choice allows us to study the effect of a uniform dc electric field in transport and in optical properties. In the first type of problems we consider the motion of wave packets in crystals and their semiclassical description in terms of the effective mass theorem and anomalous transport [30, 31]. In the second type of problems we examine the Franz-Keldysh effect, which describes the change of the absorption coefficient of bulk semiconductors in the presence of a dc electric field [32, 33], taking into account the important effects of the Coulomb interaction between electron and holes; in this case the difficulties due to the position operator are minimal if the
interband coupling between bands is properly constructed along lines parallel to the dc field, and it is not necessary to tailor the phase of the Bloch states across the Brillouin zone to account for the effects of the Berry curvature (see Sec. 5.2.3).

1.2 Effects of dc electric fields

The Hamiltonian in Eq. (1.7) generates a wide variety of interesting phenomena extensively discussed in the literature since the early days of solid-state physics, including Bloch oscillations, Zener tunneling, Wannier-Stark ladders, and the Franz-Keldysh effect. These examples have a common feature, the presence of a dc or slowly varying electric field.

This section is an attempt to summarize some of the theoretical and experimental approaches to study these phenomena. Following the common practice in solid-state physics, we distinguish between inter- and intraband phenomena; as we will see, this division is not as trivial as it might seem.

1.2.1 “Intraband” phenomena

The term $-eE(t) \cdot \hat{r}$ in Eq. (1.7) diverges as $r \to \infty$ along the direction of the field and breaks the periodicity of the crystal potential for any strength of the field; therefore, a rigorous mathematical treatment of the quantum dynamics described by Eq. (1.7) is not simple. Long before formal mathematical treatments were developed, effective Hamiltonians for electromagnetic fields that change slowly in space and time were widely used in transport calculations.

In the case of a uniform and constant electric field, this effective Hamiltonian approach provided justification for the existence of Bloch oscillations and Wannier-Stark ladders, which caused long disputes until they were confirmed experimentally [12, 17],

\footnote{See [9, 34–37] and references therein.}
and the underlying assumptions in the mathematical treatment were fully understood [9]. The term \(-e\mathbf{E}(t) \cdot \hat{\mathbf{r}}\) is a singular perturbation, which changes completely the energy spectrum of a bounded periodic potential. Strictly speaking, there are no isolated bands in the presence of a uniform electric field, and the spectrum becomes continuous [9, 38]. Nevertheless, the intuition behind the effective Hamiltonian technique is that it should be possible to identify bands when the field is weak enough compared to the internal fields from the crystal potential, which typically have a dominant effect. The first treatments by Adams [39–41], Kane [42], and Wannier [43] assumed that the original bands and their associated Bloch states can be modified perturbatively to include the effect of a weak electric field; in 1960 Wannier [43] constructed a recurrence procedure to include the modifications due to the electric field as a power series in the electric field. In this picture, Bloch oscillations are the natural result of the motion of a wave packet of Bloch states from one of these bands perturbed by the field; as we will see in Sec. 2.2, the electric field causes a drift in reciprocal space, where the band energies are periodic, and this leads to a periodic motion in real space, the Bloch oscillations. Furthermore, Wannier pointed out that if the decoupling of the bands were complete so that closed-band subspaces could be constructed, then square integrable eigenfunctions with a ladder-like spectrum would be possible, the Wannier-Stark ladder [16]. It later became clear that such closed bands and the associated Wannier-Stark states do not exist [9, 38, 44]. However, there are well-defined resonances or long-lived states that can be identified with such Wannier-Stark states. These resonances can be observed experimentally for weak fields such that the interband phenomena (with respect to the “perturbed bands”) does not wash them out. The impossibility of strictly closed bands for any intensity of the applied field means that the results from the decoupling procedure are only asymptotically correct; that is, Wannier’s recurrence procedure is not convergent but only asymptotically [9], and it relies on the weakness of the field to give a good approximation. At high applied fields, this one-band approximation breaks down due to Zener tunneling of the
carriers between bands due to the energy of the field [11, 42, 45].

In order to avoid the complications of the unbound energy term associated with the electric field in the length gauge, alternative treatments were formulated using the velocity gauge with \( \mathbf{A}(t) = -c \int_0^t \mathbf{E}(t')dt' \) in Eq. (1.5). In this picture, the periodicity of the crystal potential is not altered, making it quite suggestive, but this comes at the price of a time-dependent Hamiltonian, even for a dc field. For a constant or slowly varying field, adiabatic perturbation theory can be used if the field is weak [8, 46]; in this approach the condition of remaining in “one band” is related to how fast the state of the charged carrier moves in reciprocal space.

The effective Hamiltonian technique and the underlying idea of band decoupling provides the basis for the semiclassical description of wave packet dynamics and one of its main results, the effective mass theorem [30]. According to this theorem, an electron in a crystal behaves as a free particle with its inertial properties modified by the periodic potential [9]; for a uniform electric field, which pushes the electron with a force \( \mathbf{F} = e\mathbf{E} \), the acceleration of the particle is described by an effective mass calculated from the curvature of the zero-field energy dispersion (see Eqs. (2.26) and (2.27)). This is an important example of the connection between a spectral property associated with the lattice and the dynamical response of the particle. Not surprisingly, this description was also challenged in the early days of solid-state physics because it relies heavily on the correct interpretation of intra- and interband phenomena in the presence of a uniform force. As we will see in detail in Chapter 2, a simple application of Ehrenfest’s theorem shows that a wave packet strictly in one band responds with the bare mass, in apparent contradiction with the effective mass theorem. This was pointed out by Kretschmann [47], and led him to assert that the correct description of currents requires the bare mass instead of the effective mass. Later, Pfirsch and Spenke [48] provided the correct explanation, arguing that an electron initially in one band responds with the bare mass only at very early times when an electric field is suddenly applied; following this very early re-
The effective mass theorem suggests that the velocity of a wave packet in a crystal is governed solely by the gradient of the band energy (see Eq. (2.23)). However, a more careful analysis of the wave packet dynamics leads to including a correction term linear in the applied force, known as the anomalous velocity (see Eq. (2.24)). It was proposed for the first time by Karplus and Luttinger to explain the anomalous Hall effect observed in ferromagnetic materials [49]. In a typical Hall effect experiment with a paramagnetic material, the Hall resistance is proportional to the applied magnetic field; however, when the same experiment is performed with a ferromagnetic material, the Hall resistance has an additional and quite significant contribution, which is often proportional to the magnetization instead of the magnetic field. This contribution became known as the anomalous Hall effect and its explanation in terms of a microscopic mechanism remained controversial for a long time [50, 51]. Karplus and Luttinger suggested that the applied electric field in a Hall effect experiment is responsible for an interband mixing, which in turn can lead to a velocity perpendicular to the field, the anomalous velocity. Their key contribution was identifying the importance of the spin-orbit coupling and the fact that the time-reversal symmetry is broken due to the magnetization [50]. Later, Adams and Blount [28, 41] provided an additional insight when they traced the origin of the anomalous velocity to the non-commutativity of the Cartesian components of the intraband part of the position operator in the crystal momentum representation (see Sec. 2.1). However, only after the work of Berry and Simon [4, 5], the anomalous velocity acquired its modern formulation in terms of the Berry curvature (for definition, see Eq. (2.18)). In this context, Chang, Sundaram, and Niu [7, 31, 52, 53] provided an appropriate framework to understand the anomalous Hall effect using equations of motion.
for wave packets derived from a time-dependent variational principle in a Lagrangian formulation [54]; these equations include the contribution from the anomalous velocity. It is important to point out that the anomalous velocity is only one of the mechanisms that explain the anomalous Hall effect. In a full picture it is necessary to include the effects of scattering (extrinsic mechanisms); however, experimental results have shown that the intrinsic contribution from the anomalous velocity is dominant in many situations [7].

The formulation of semiclassical transport equations constitutes an intensive area of research, motivated in part by the realization of the importance of the Berry phase. Some authors have followed the traditional approach of finding an effective Hamiltonian or applying some approximate band decoupling scheme before deriving the equations of motion. Examples of this strategy include the systematic diagonalization method by Gosselin et al. [35], procedures that use phase space and WKB analysis [28, 36, 37, 55], and techniques that involve Weyl quantization [34]. The approach by Chang, Sundaram, and Niu, mentioned above in the context of the anomalous Hall effect, is an example of a different strategy where semiclassical equations of motion are found before an effective Hamiltonian, the latter being derived in a subsequent “requantization” procedure [7].

From the experimental point of view, the development of artificial lattices provided the first confirmation of many of the theoretical predictions discussed above. The effects of scattering due to impurities, defects, and thermal vibrations in real crystalline solids were the most significant impediments to realize effects such as Bloch oscillations and Wannier-Stark ladders; artificial lattices were developed to circumvent these problems in various ways. Superlattices are periodic arrays of semiconductor layers where the energy levels form subbands associated with delocalized electronic envelope wave functions [20]; therefore, these lattices effectively provide a one-dimensional periodic structure in the direction of layer stacking. Since the period of this structure is much larger than in naturally-occurring crystals, they allow one to observe more easily the Wannier-Stark ladder spectrum, where the energy separation between steps scales linearly with the
period of the lattice [17, 18]; Bloch oscillations, which can be thought as the counterpart in time domain of the Wannier-Stark ladder [18], were observed directly in superlattices [12] a few years after the first ladder-like spectrum was resolved. Shortly after these experiments, Bloch oscillations were observed with ultracold atoms in an optical lattice provided by a laser standing wave [13]. Following this first realization of the opportunities of simulating solid-state physics with optical lattices, experiments on this type of lattice were carried out to examine interesting and sometimes counterintuitive phenomena due to the band structure of the energy spectrum (for example, see [14, 19, 56–65]). The physical effect responsible for the formation of this type of lattice is the ac Stark shift, which causes the atoms to be attracted or repelled by regions of high laser field intensity; in principle, any lattice configuration with any dimensionality can be achieved, limited in practice only by the setup of laser beams [21, 66, 67]. Since atoms used in these experiments are typically neutral, the electromagnetic forces felt by charged carriers (such as electrons) need to be mimicked cleverly; for instance, a constant and uniform electric field has been replaced with the force of gravity [19], inertial forces due to the acceleration of the lattice [14], and forces induced by shifting the center of a magnetic field trap [68]. A great advantage of optical lattices over any type of lattice in solid state is that they can be abruptly turned off at will in order to measure the velocity of the atoms. In addition, applications are not restricted to one-particle experiments as the ones we have mentioned so far; since interactions between atoms in these lattices can also be controlled, they provide an invaluable tool to study many-body problems [66, 67].

In solid-state systems the observation of transport phenomena such as Bloch oscillations in bulk crystals was only possible with the development of sources of few-cycle terahertz (THz) pulses, which probe dynamics in the sub-100 fs time scale and allow experimentalists to observe ballistic transport [15]. This is an example of how the recent developments in broadband sources in the “terahertz gap” between infrared and microwave frequency ranges have opened the possibility of studying ultrafast phenomena
Chapter 1. Introduction

in solids. In this regard, ultrafast current control [69, 70] and high-order harmonic generation [71–73] in solids are probing time scales where interesting dynamics of carriers have not been observed before; in this regime, it becomes important to consider how fast carriers can respond to applied fields according to the properties of the lattice they are in [74, 75].

1.2.2 “Interband” phenomena

In the previous section we included the Wannier-Stark ladder as one of the examples of intraband phenomena, and pointed out the connection between this spectral feature and Bloch oscillations. The first experiments that mapped the ladder-like spectrum were actually optical measurements of absorption and photocurrent spectra [17]. This brings us to the question of how a uniform electric field modifies the optical properties of a solid; however, we move away from the regime where the discrete resonances are noticeable and focus on the well-known Franz-Keldysh effect, which in bulk semiconductors is characterized by a continuous absorption spectrum with two important features (see Fig. 5.1a): an exponential tail below the band gap [32, 33] and oscillations above it [76, 77].

The exponential tail was observed for the first time by Williams in CdS [78] and by Moss in GaAs [79]. A few years later, Frova et al. [80] reported observations that also included the above-gap oscillations. The first attempts to explain these features neglected the electron-hole interaction, and were based on the effective mass approximation; within these approximations, analytical expressions for the absorption coefficient can be expressed in terms of Airy functions [76, 77, 81]. A more sophisticated approach by Aspnes considered different types of critical points, anisotropic effective masses, and arbitrarily oriented fields [82, 83], but his work was still within the independent particle approximation. Regarding the effects of interband coupling due to the dc field, Keldysh et al. [84] proposed that the light-hole contribution to the absorption can be calculated without consideration of the coupling between the light-hole and heavy-hole bands, at
least below the band gap; later, Aspnes extended this approximation to the heavy-hole contribution and to the region far above the band gap [85]. Non-parabolicity [86] and band anisotropies [87] were also considered around the same time.

Band structure models based on the $\mathbf{k} \cdot \mathbf{p}$ method are particularly useful to take into account all the aforementioned effects. This method combines symmetry analysis and comparison with experimental data to calculate band structures starting at band extrema [88, 89]. Different variations of the $\mathbf{k} \cdot \mathbf{p}$ method have been used to study the Franz-Keldysh effect; examples include the Kohn-Luttinger six-band model [90], the eight-band model [91], and the 14-band model [92, 93]. These calculations have treated in detail the consequences of the band features near the $\Gamma$ point on the absorption spectrum; for example, in zinc-blende semiconductors the degeneracy of valence bands is responsible for the optical anisotropy in the presence of an electric field [94].

The independent particle approximation provides a qualitatively correct absorption lineshape and explains its various features; however, in many cases it cannot be compared directly with experimental results. First, experiments have several limitations, including the difficulty in applying a uniform dc field inside the sample; therefore, the ideal conditions assumed in many of the theoretical studies are rarely satisfied. Second, it is well-known that the Coulomb interaction between electrons and holes modifies significantly the optical properties of semiconductors, especially near the band gap, due to the formation of electron-hole pairs, which can be bound together forming an exciton. Hence, the Coulomb interaction must be included in a complete theoretical description. The first efforts in this direction, both numerically and using semianalytical approximations [95–102], involved the isotropic effective mass approximation. A different strategy to incorporate the electron-hole interaction was proposed by Rees [103]. His method consisted of including all the desired corrections, for example due to band anisotropy and exciton formation, in the calculation of the zero-field absorption and to convolute it with the Airy functions that provide the field-induced effects; Rees also claimed that this
method can be used to include lattice defects, lifetime broadening, and surface effects. Some experiments were analyzed using this semiempirical approach [104].

Even though the Franz-Keldysh effect has been extensively studied, detailed experimental measurements have only recently become available. Difficulties include inhomogeneities of the applied dc field and impurity induced broadening; both affect the visibility of the oscillations above the band gap [105]. In many experiments the dc field is restricted to the “longitudinal configuration,” in which the dc field (typically, built in the sample) is parallel to the optical field wave vector and therefore perpendicular to the optical electric field [106–108]. In such experiments it is not possible to explore the dependence of the Franz-Keldysh effect on the polarization relative to the dc field. The alternative is to use a geometry where the dc field is perpendicular to the optical field wave vector [109–113]. However, in this “transverse configuration” it is more difficult to avoid inhomogeneities of the electric field; for instance, if metal electrodes deposited on the surface of the sample are used to create the electric field, extremely large field enhancement can occur near the anode due to a trap-enhanced space-charge region [114]. Techniques based on rf bias and short light pulses have been developed to improve the quality of measurements in the transverse geometry [115]. Excitonic effects have also attracted the attention of the community in recent years, especially for experiments in high purity GaAs epilayers, where the Franz-Keldysh can serve as a diagnosis tool for measuring low densities of free carriers [116–118].

Although we will focus on bulk materials, it is worth mentioning that the Franz-Keldysh effect has also been studied in quantum wells [119–121] and quantum wires [122, 123]. Furthermore, the possibility of applying intense terahertz electric fields has opened a new regime, usually called the dynamical Franz-Keldysh effect [124, 125], with additional features not seen in the dc field case. Other new directions of the Franz-Keldysh effect include the study of nonlinear effects, such as two-photon absorption [126, 127] and coherent control [128].
1.3 Thesis overview

In this thesis we discuss two aspects of the effect of a uniform dc electric field on charged carriers in crystals. First, we study the intraband motion using a wave packet description at the one-particle level, neglecting interactions between carriers (see Chapter 2). Even at this level of approximation, interesting dynamics occur due to the dressing of the particle with the properties of the lattice; in this context, we focus our attention on the breakdown of the semiclassical description in terms of the effective mass theorem first discussed by Pfirsch and Spenke [48]. Our approach is based on the decoupling method of Wannier [43]. As we will discuss in Chapter 3, these dynamics are difficult to observe in typical solid-state systems; thus, we opted for using optical lattices where experimental realization is much simpler. In fact, following the theoretical studies described in Chapter 3, those dynamics were observed experimentally in one-dimensional lattices [68]. In the one-dimensional case, we find an interesting interplay between the fast dynamics induced by the sudden application of the force and the slower Bloch oscillations; the initial dynamical oscillations decay as a consequence of the spread of the wave packet in reciprocal space, but revivals of these oscillations appear as the wave packet completes a Bloch oscillation. In lattices of higher dimensionality the dynamics are much richer, especially when anomalous transport is important; we find that the anomalous velocity for a suddenly applied force also takes some time to develop, and we predict dynamical oscillations of this velocity about the usual prediction from the semiclassical theory of wave packet dynamics (see Eq. (2.25)). We illustrate this feature of the anomalous transport and the presence of revivals in a two-dimensional optical lattice [64] in Chapter 4.

The second aspect is the effect of a bias dc field on the optical properties of semiconductors, namely the Franz-Keldysh effect described in Sec. 1.2.2. Although this effect has been studied extensively in the literature, we found a disconnection between the detailed studies of the effects of the band structure, included through band models of increasing complexity, and the inclusion of the electron-hole interaction. In this context, our work
aims to fill this gap and study simultaneously the excitonic effects due to the Coulomb interaction and the interband coupling due to the dc field. We consider a bulk semiconductor with its valence bands fully occupied and empty conduction bands, excited by an optical pulse in the presence of an applied dc field. We neglect Zener tunneling and consider optical fields within the linear response regime. The formalism is illustrated in Chapter 5 with a numerical calculation using a 14-band $\mathbf{k} \cdot \mathbf{p}$ model for GaAs.

The thesis is organized as follows. In Chapter 2 we present a general discussion regarding the dynamics of wave packets in periodic potentials subject to a uniform force suddenly applied at $t = 0$ and left constant afterwards. This chapter provides the necessary background for the next two, Chapters 3 and 4, where we illustrate the formalism with one- and two-dimensional optical lattices, respectively; we show results from a semi-analytical approximation based on Wannier’s decoupling method [43] briefly described in Sec. 1.2.1, and we compare the predictions from this approach with full numerical solutions based on the split-step operator method [129]. Chapter 5 focusses on the formalism used in our study of the Franz-Keldysh effect, presenting our results for bulk GaAs in the 14-band $\mathbf{k} \cdot \mathbf{p}$ model; the numerical aspects of this calculation are discussed in Chapter 6.

included as one of the chapters.
Chapter 2

Wave packets subject to periodic potentials and uniform forces

In this chapter we present the general formalism to derive the dynamical behavior of the effective mass and the anomalous velocity for lattices of any dimensionality when a uniform force is suddenly applied and left constant afterwards. In the next two chapters we will consider the one- and two-dimensional cases in more detail, illustrating the formalism with calculations for optical lattices. Some of the notation introduced in this chapter will be used throughout the thesis.

We start in Sec. 2.1 with some general considerations regarding the Hamiltonian that describes the system, and introduce the crystal momentum representation. In Sec. 2.2 we briefly state the basic results of the semiclassical description of wave packet dynamics leading to the effective mass theorem and anomalous transport. In Sec. 2.3 we use Ehrenfest’s theorem to derive expressions for the expectation values of the velocity and the acceleration of a wave packet, and we consider the particular case of a wave packet strictly in one band, which initially responds as a free particle. In Secs. 2.4 and 2.5 the one-band approximation usually assumed in the semiclassical theory is revisited from the point of view of modified Bloch states, following Adams [39] and Wannier [43] treat-
ments. We conclude in Sec. 2.6 considering the dynamical corrections due to the sudden application of the force. For convenience, most of the derivations of the expressions in this chapter are left to Appendix B.

2.1 The crystal momentum representation

Consider the Hamiltonian introduced in Eq. (1.7). The electric field exerts a uniform force $F(t) = eE(t)$ and so we can write

$$\hat{H}(t) = \hat{H}_o - \mathbf{F}(t) \cdot \mathbf{r},$$

(2.1)

where $\hat{H}_o$ corresponds to the unperturbed Hamiltonian,

$$\hat{H}_o \equiv \frac{\mathbf{p}^2}{2m} + V(\mathbf{r})$$

(2.2)

for a periodic potential $V(\mathbf{r} + \mathbf{R}) = V(\mathbf{r})$, with $\mathbf{R}$ being a lattice vector. In the position representation, the canonical momentum operator $\hat{p}$ acts on a general state $|\psi\rangle$ according to

$$\langle \mathbf{r}|\hat{p}|\psi\rangle \equiv \frac{\hbar}{i} \nabla_{\mathbf{r}} \psi(\mathbf{r}),$$

(2.3)

where we introduced the wave function

$$\psi(\mathbf{r}) \equiv \langle \mathbf{r}|\psi\rangle.$$  

(2.4)

The remaining term in Eq. (2.1), $-\mathbf{F}(t) \cdot \mathbf{r}$, is associated with the potential energy due to the force. As described in Sec. 1.2.1, this term cannot be treated as a regular perturbation because it breaks the translational symmetry of the periodic potential, and it is unbound for an infinite crystal. In this chapter and the next two, we use the force $\mathbf{F}(t)$ instead of the electric field $\mathbf{E}(t)$, since we consider first the motion of wave packets associated with neutral atoms in optical lattices, where the force is of different origin (see Sec. 1.2.1); later, in our discussion of the Franz-Keldysh effect in Chapter 5, we use again the electric field $\mathbf{E}(t)$ in the Hamiltonian.
In the crystal momentum representation [28] we use as our basis the set of Bloch states $|\psi_{nk}\rangle$ that diagonalize $\hat{H}_o$,

$$\hat{H}_o |\psi_{nk}\rangle = \hbar \omega_n(k) |\psi_{nk}\rangle.$$  \hspace{1cm} (2.5)

These states are labeled by a discrete band index $n$ and a crystal wave vector $k$. The “momentum” associated with $k$, namely $\hbar k$, is typically called the crystal momentum or quasimomentum [30, 130, 131], and it can also be regarded as the eigenvalue of a crystal momentum operator $\hbar \hat{k}$ acting on a Bloch state,

$$\hbar \hat{k} |\psi_{nk}\rangle = \hbar k |\psi_{nk}\rangle.$$  \hspace{1cm} (2.6)

The energy spectrum $\hbar \omega_n(k)$ forms bands labeled by $n$, which are periodic in reciprocal space due to the periodicity of the potential. The periodicity in reciprocal space is described by a set of reciprocal lattice vectors $G$, which can be used to construct the (first) Brillouin zone; it is possible to restrict the wave vectors that label the Bloch states to this region of reciprocal space [30, 131]. In real space the Bloch states can be written as

$$\psi_{nk}(r) \equiv \langle r | \psi_{nk} \rangle = \frac{1}{\sqrt{(2\pi)^D}} u_{nk}(r) e^{ik \cdot r},$$  \hspace{1cm} (2.7)

where $D$ denotes the dimensionality of the lattice (for example, $D = 3$ for a three-dimensional lattice). The function $u_{nk}(r) \equiv \langle r | u_{nk} \rangle$ has the periodicity of the lattice, $u_{nk}(r + R) = u_{nk}(r)$, and is normalized according to

$$\langle u_{n_1 k} | u_{n_2 k} \rangle \equiv \int_{V_{\text{cell}}} \frac{dr}{V_{\text{cell}}} u^*_{n_1 k}(r) u_{n_2 k}(r) = \delta_{n_1 n_2},$$  \hspace{1cm} (2.8)

where the integration is over one unit cell, with volume $V_{\text{cell}}$. The Bloch functions $\psi_{nk}(r)$ satisfy the orthonormalization condition

$$\langle \psi_{n_1 k_1} | \psi_{n_2 k_2} \rangle \equiv \int d\mathbf{r} \psi^*_{n_1 k_1}(\mathbf{r}) \psi_{n_2 k_2}(\mathbf{r}) = \delta_{n_1 n_2} \delta(\mathbf{k}_1 - \mathbf{k}_2),$$  \hspace{1cm} (2.9)

for $\mathbf{k}_1$ and $\mathbf{k}_2$ within the (first) Brillouin zone. Note that the integration in Eq. (2.9) and in any matrix element of the form $\langle \psi_{nk_1} | \cdot | \psi_{nk_2} \rangle$ is over all space; for matrix elements of the form $\langle u_{n_1 k} | \cdot | u_{n_2 k} \rangle$ the integration is over one unit cell, as in Eq. (2.8).
We expand the state of the system, $|\Psi(t)\rangle$, in terms of Bloch states $|\psi_{nk}\rangle$ according to

$$|\Psi(t)\rangle = \sum_n \int_{\text{BZ}} dk \, c_n(k, t) |\psi_{nk}\rangle,$$

(2.10)

where BZ denotes integration over the (first) Brillouin zone. The $c_n(k, t)$ are complex amplitudes restricted to lie within the (first) Brillouin zone, according to the periodicity in reciprocal space; when these amplitudes are localized around some average wave vector, Eq. (2.10) describes a wave packet. We denote the expectation value of an operator $\hat{O}$ for the state $|\Psi(t)\rangle$ as

$$\langle \hat{O} \rangle \equiv \langle \Psi(t) | \hat{O} | \Psi(t) \rangle.$$

(2.11)

The position operator in the crystal momentum representation becomes [28]

$$\langle \psi_{n_1k_1}| \hat{r} | \psi_{n_2k_2}\rangle \equiv \int d\mathbf{r} \psi_{n_1k_1}^{*}(\mathbf{r}) \mathbf{r} \psi_{n_2k_2}(\mathbf{r}) = \delta_{n_1n_2} \left( i \nabla_{k_1} \delta(k_1 - k_2) \right) + \delta(k_1 - k_2) \xi_{n_1n_2}(k_1),$$

(2.12)

where we introduced the matrix elements [131]

$$\xi_{n_1n_2}(k) \equiv \langle u_{n_1k} | i \nabla_k | u_{n_2k} \rangle \equiv \int_{V_{\text{cell}}} \frac{d\mathbf{r}}{V_{\text{cell}}} u_{n_1k}^{*}(\mathbf{r}) i \nabla_k u_{n_2k}(\mathbf{r}).$$

(2.13)

For the momentum operator we have

$$\langle \psi_{n_1k_1}| \hat{\mathbf{p}} | \psi_{n_2k_2}\rangle \equiv \int d\mathbf{r} \psi_{n_1k_1}^{*}(\mathbf{r}) \frac{\hbar}{i} \nabla_{\mathbf{r}} \psi_{n_2k_2}(\mathbf{r}) = \delta(k_1 - k_2) \mathbf{p}_{n_1n_2}(k_1),$$

(2.14)

where [28]

$$\mathbf{p}_{n_1n_2}(k) \equiv \delta_{n_1n_2} \hbar \mathbf{k} + \langle u_{n_1k} | \hat{\mathbf{p}} | u_{n_2k} \rangle = \delta_{n_1n_2} \hbar \mathbf{k} + \int_{V_{\text{cell}}} \frac{d\mathbf{r}}{V_{\text{cell}}} u_{n_1k}^{*}(\mathbf{r}) \frac{\hbar}{i} \nabla_{\mathbf{r}} u_{n_2k}(\mathbf{r}).$$

(2.15)

For non-degenerate bands, the off-diagonal elements of Eq. (2.13) are related to the momentum matrix elements by [131]

$$\xi_{n_1n_2}(k) = -\frac{1}{im} \frac{\mathbf{p}_{n_1n_2}(k)}{\omega_{n_1n_2}(k)} \quad \text{(for } \omega_{n_1}(k) \neq \omega_{n_2}(k)\text{)},$$

(2.16)

where $\omega_{n_1n_2}(k) \equiv \omega_{n_1}(k) - \omega_{n_2}(k)$. The diagonal element $\xi_{nn}(k)$ is known as the *Berry connection*, and it depends on the choice of the phases for the Bloch states. Despite this
"gauge dependence," the curl of $\xi_{nn}(k)$, called the Berry curvature, is gauge-independent and has dynamical consequences [7, 31, 41, 49], as we will describe in the next section. We denote the local Berry curvature$^1$ by

$$\Omega_n(k) \equiv \nabla_k \times \xi_{nn}(k), \quad (2.17)$$

or in terms of Cartesian components as

$$\Omega^l_n(k) \equiv \epsilon^{lab} \frac{\partial}{\partial k^a} \xi^b_{nn}(k), \quad (2.18)$$

where $\epsilon^{lab}$ is the antisymmetric Levi-Civita symbol and repeated Cartesian components are summed over. It is important to point out that Eqs. (2.17) and (2.18) describe the Berry curvature of band $n$ when there are no degeneracies present. For degenerate or nearly degenerate bands it is necessary to treat them together and define the Berry curvature as a matrix over such bands (for a definition and physical examples see [7]). However, we will be interested exclusively in the non-degenerate case, where Eqs. (2.17) and (2.18) constitute the appropriate definitions.

In terms of the intraband part of the position operator in the crystal momentum representation, $\langle \psi_{nk_1} | \hat{r} | \psi_{nk_2} \rangle = r_{nn}(k_1) \delta(k_1 - k_2)$, where

$$r_{nn}(k) \equiv i \nabla_k + \xi_{nn}(k), \quad (2.19)$$

the Berry curvature can be written as the commutator between different Cartesian components of $r_{nn}(k)$,

$$[r^a_{nn}(k), r^b_{nn}(k)] = i \epsilon^{abc} \Omega^c_n(k). \quad (2.20)$$

This result, found by Adams and Blount [28, 41], can be interpreted geometrically as a non-commutativity between parallel transports along different axes in reciprocal space for Bloch states in one band [132]; this geometric character of the Berry curvature also

$^1$We use the term "local" throughout this thesis to denote physical quantities that are functions of the wave vector $k$; this convention allows us to distinguish them from quantities averaged over a wave packet.
has consequences on the dynamics of wave packets moving in “one band” as we will see in the next section. Furthermore, the Berry curvature has a topological character. For instance, in two-dimensions \((x, y)\) the integral over the entire Brillouin zone of the Berry curvature (which only has a \(z\)-component),

\[
\int_{BZ} d\mathbf{k} \Omega^z_n(\mathbf{k}) = 2\pi C_n, \tag{2.21}
\]

is proportional to the Chern number \(C_n\) of the band [3, 6, 133]. The Chern number is a global topological property of the band and it is zero for systems with time-reversal symmetry [133].

### 2.2 Semiclassical wave packet dynamics

The main goal of the semiclassical theory of wave packet dynamics in periodic potentials is to find equations of motion for the expectation values of the position, \(\langle \hat{\mathbf{r}} \rangle\), and quasi-momentum, \(\langle \hat{\mathbf{k}} \rangle\), of the wave packet as it evolves due to external fields slowly varying in space and time [30]; for simplicity, we consider a force uniform in space and constant in time in this section.\(^2\) The wave packet is assumed to be described by Bloch states from one band, say band \(N\), and with wave vectors sufficiently localized around \(\langle \hat{\mathbf{k}} \rangle\), which can change in time. According to this semiclassical model, an applied force \(\mathbf{F}\) causes a constant drift in reciprocal space according to

\[
\frac{d}{dt} \langle \hbar \hat{\mathbf{k}} \rangle \approx \mathbf{F}. \tag{2.22}
\]

In real space, the velocity of the wave packet can be found from the local group velocity associated with the band energy,

\[
\mathbf{v}_N^g(\mathbf{k}) \equiv \frac{1}{\hbar} \nabla_k (\hbar \omega_N(\mathbf{k})), \tag{2.23}
\]

\(^2\)The time dependence of the force (if any) simply modifies adiabatically the expressions shown here.
and the local anomalous velocity \([7, 31, 41, 49, 134]\) associated with the local Berry curvature (see Eq. (2.17)),

\[
v^\text{an}_N(k) \equiv \frac{1}{\hbar} \Omega_N(k) \times F,
\]

so that

\[
\frac{d}{dt} \langle \hat{r} \rangle \approx \mathbf{v}^g_N(\langle \hat{k} \rangle) + \mathbf{v}^\text{an}_N(\langle \hat{k} \rangle).
\]

As discussed in Sec. 1.2.1, the equations of motion (2.22) and (2.25) have been justified in various ways in the literature; we present a derivation using Bloch states modified by the force in Sec. 2.5 \([41, 50]\). The anomalous transport contribution is usually left out \([30]\) because the Berry curvature is zero unless space-inversion or time-reversal symmetry is broken \([31]\).\(^3\) Even in the absence of space-inversion symmetry, for example in GaAs, probing the local Berry curvature can be difficult in solid-state systems with time-reversal symmetry, where the bands are Chern class zero \((C_n = 0)\). The reason is that the dc response usually implies integrating over the entire Brillouin zone, for a fully occupied band, or over the volume determined by an occupation function, for a partially filled band \([136, 137]\); therefore, the effects of the local Berry curvature are usually washed out.

Using Eqs. (2.22) and (2.25) we can derive the effective mass theorem, which is crucial in the modern understanding of transport in solid-state physics \([30, 131, 138]\). We take the time derivative of Eq. (2.25) and use Eq. (2.22), keeping terms that are first order in the force; note that there is no contribution from the anomalous velocity to this order. The components of the resulting acceleration are

\[
\frac{d^2}{dt^2} \langle \hat{r}^a \rangle \approx \left[ \frac{1}{m^*_N(\langle \hat{k} \rangle)} \right]^{ab} F^b,
\]

where

\[
\left[ \frac{1}{m^*_N(k)} \right]^{ab} = \frac{1}{\hbar^2} \frac{\partial^2}{\partial k^a \partial k^b} (\hbar \omega_n(k))
\]

\(^3\)This is strictly true if there are no degeneracies. For example, the two-dimensional hexagonal lattice with six-fold symmetry, characteristic of systems such as graphene, has singular local Berry curvature at the Dirac points where the two lowest bands touch (see \([135]\)).
is the \textit{local inverse effective mass tensor}. Eq. (2.27) is a \textit{kinematic} definition of the effective mass as a \textit{spectral} property of the band structure; the semiclassical theory proves that the effective mass defined this way provides sufficient information to calculate the \textit{dynamical} response of the wave packet within the range of validity of this approximation.

The connection between the spectral and topological properties of the band structure and the wave packet dynamics described by Eqs. (2.25) and (2.26) lies at the heart of this semiclassical approach to transport in lattices. A crucial assumption is that the force changes slowly in time; therefore, the way the force is turned on becomes relevant, as Pfirsch and Spenke pointed out 60 years ago [48]. In this context, the main question we will consider in the following sections is how a wave packet prepared strictly in one band responds to a force suddenly applied. As expected, the response is not described simply by Eqs. (2.25) and (2.26). We start with a general description of the expectation values of the velocity and acceleration of a wave packet using Ehrenfest’s theorem; this description will reveal an important feature of the initial response.

\section{2.3 A surprise from Ehrenfest’s theorem}

In the Heisenberg picture, the position operator $\hat{r}^H$ and the momentum operator $\hat{p}^H$ satisfy

\begin{equation}
\frac{d}{dt} \hat{r}^H = \frac{1}{i\hbar} \left[ \hat{r}^H, \hat{H}^H(t) \right] = \frac{\hat{p}^H}{m},
\end{equation}

and

\begin{equation}
\frac{d}{dt} \hat{p}^H = \frac{1}{i\hbar} \left[ \hat{p}^H, \hat{H}^H(t) \right] = \frac{1}{i\hbar} \left[ \hat{p}^H, \hat{H}^H_0 \right] + \mathbf{F}(t),
\end{equation}

where $\hat{H}^H(t)$ and $\hat{H}^H_0$ are the Hamiltonians in Eqs. (2.1) and (2.2) rewritten in terms of Heisenberg operators. Combining Eqs. (2.28) and (2.29) we can write

\begin{equation}
\frac{d^2}{dt^2} \hat{r}^H = \frac{\mathbf{F}(t)}{m} + \frac{1}{i\hbar m} \left[ \hat{p}, \hat{H}^H_0 \right].
\end{equation}
Since the Heisenberg and Schrödinger pictures predict the same expectation values, we find the well-known results from Ehrenfest’s theorem,

\[
\frac{d}{dt} \langle \hat{\mathbf{r}} \rangle = \frac{1}{m} \langle \hat{\mathbf{p}} \rangle \tag{2.31}
\]

and

\[
\frac{d^2}{dt^2} \langle \hat{\mathbf{r}} \rangle = \frac{\mathbf{F}}{m} + \frac{1}{i\hbar m} \left\langle \left[ \hat{\mathbf{p}}, \hat{H}_o \right] \right\rangle, \tag{2.32}
\]

back in the Schrödinger picture (see Eq. (2.11)). Note that

\[
\frac{1}{i\hbar} \left\langle \left[ \hat{\mathbf{p}}, \hat{H}_o \right] \right\rangle = \frac{1}{i\hbar} \langle [\hat{\mathbf{p}}, V(\hat{\mathbf{r}})] \rangle = -\langle \nabla V(\hat{\mathbf{r}}) \rangle \tag{2.33}
\]

is nothing but the expectation value of the force due to the lattice.

The simple result Eq. (2.32) actually has a surprising consequence. Consider a wave packet formed only by Bloch states from a single band, say band \( N \),

\[
| \tilde{\psi}_N \rangle \equiv \int_{BZ} dk f_N(k) | \psi_{Nk} \rangle. \tag{2.34}
\]

For such a wave packet the expectation value of the force due to the lattice vanishes,

\[
\frac{1}{i\hbar} \left\langle \tilde{\psi}_N \left[ \hat{\mathbf{p}}, \hat{H}_o \right] \tilde{\psi}_N \right\rangle = 0, \tag{2.35}
\]

since the matrix elements of the commutator in the crystal momentum representation become

\[
\frac{1}{i\hbar} \left\langle \psi_{Nk_1} \left[ \hat{\mathbf{p}}, \hat{H}_o \right] \psi_{Nk_2} \right\rangle = i(\omega_N(k_1) - \omega_N(k_2)) \langle \psi_{Nk_1} | \hat{\mathbf{p}} | \psi_{Nk_2} \rangle \tag{2.36}
\]

and the momentum matrix elements are diagonal in \( k \) (see Eq. (2.14)). Therefore, if at a given time \( t_o \) a particle is described by Eq. (2.34) so that \( |\Psi(t_o)\rangle = |\tilde{\psi}_N\rangle \), the particle responds with the bare mass,

\[
\frac{d^2}{dt^2} \langle \hat{\mathbf{r}} \rangle \bigg|_{t_o} = \frac{\mathbf{F}(t_o)}{m}, \tag{2.37}
\]

as if the lattice were completely absent. Furthermore, if we use the state Eq. (2.34) to calculate the expectation value of the velocity, we only get the contribution from the group velocity,

\[
\frac{d}{dt} \langle \hat{\mathbf{r}} \rangle \bigg|_{t_o} = \int_{BZ} dk |f_N(k)|^2 v_{N}^g(k). \tag{2.38}
\]
The result Eq. (2.37) seems to contradict the effective mass theorem Eq. (2.26) and caused some confusion in the early days of solid-state physics as it was not clear which mass, the bare or the effective mass, is the right one to describe transport [47]. This confusion and the strict meaning of the one-band approximation was clarified by Pfirsch and Spenke [48], and later by Adams [39], who pointed out that any applied force inevitably couples the original Bloch bands, and it is through this coupling that the lattice makes itself felt. Even though the wave packet can be prepared at $t_0 = 0$ in the state Eq. (2.34), at later times the wave packet will acquire amplitudes over the neighboring bands, with $n \neq N$, under the action of the applied force. For a weak force and a band $N$ sufficiently isolated from its neighboring bands, these amplitudes are small but crucial to describe the response according to the effective mass theorem. The absence of the anomalous velocity term in Eq. (2.38) is another consequence of the missing interband coupling due to the force in the state $\bar{\psi}_N$, and it also reflects the important role of this coupling to allow the particle to feel the effects of the lattice in response to an applied force.

For a deep lattice potential (tight-binding limit), the initial free-particle response can be understood in a simple way, as explained by Chang et al. [68]. In this case, the wave packet can be approximated by the sum of small wave packets localized and centered at local minima of the periodic potential, as illustrated in Fig. 2.1 for a one-dimensional lattice. Clearly, the force due to the lattice vanishes when there is no external force because the slope of the potential averages to zero over each of the small wave packets; this was the result formally proven in Eq. (2.35). Therefore, when the lattice potential is suddenly tilted due to the external applied force, we expect the initial response of the wave packet to be as if the lattice were not present. After some time, the wave packet will feel the force due to the tilted potential, since the positions of the local potential minima were shifted; this sudden shift results in fast intrawell oscillations of the small wave packets, which are different from the slower Bloch oscillation associated with the interwell
Chapter 2. Dynamics of wave packets in periodic potentials

\[ V(x) - Fx \]

Figure 2.1: Schematic illustration of an initial wave packet in the lowest band of a deep lattice before and after the sudden application of a force. The local potential minima are marked by the dashed lines, before (black) and after (red) the application of the force; due to the shift of these minima, the small wave packets at each site perform intrawell oscillations.
coherence of the full wave packet. This simple picture suggests that for a suddenly applied force, which remains constant afterwards, there are some additional dynamics not described by the usual semiclassical results, Eqs. (2.25) and (2.26). As we will show in Sec. 2.6, these additional dynamics are not restricted to deep lattices, and explicit expressions can be derived to describe them. However, it is convenient to introduce first an appropriate set of modified Bloch states, which incorporate the interband mixing due to the force, and use them to build wave packets that behave according to the semiclassical results presented in Sec. 2.2; these states and their application to the effective mass theorem and anomalous transport are discussed in the following two sections.

2.4 Modified Bloch states

The method to decouple the original Bloch bands in the presence of a uniform and constant force was proposed by Adams [39–41] correctly to first order in the force and later generalized to any order by Wannier [43]. A more formal description, showing the limitations of Wannier’s procedure was developed by Nenciu [9].

In the crystal momentum representation we can use Eq. (2.12) to write the Hamiltonian Eq. (2.1) as

\[
\langle \psi_{n_1k_1} | \hat{H}(t) | \psi_{n_2k_2} \rangle = \mathcal{H}_{n_1n_2}(k_1,t) \delta(k_1 - k_2) - \delta_{n_1n_2} F(t) \cdot (-i \nabla_{k_2} \delta(k_1 - k_2)) ,
\]

where

\[
\mathcal{H}_{n_1n_2}(k,t) \equiv (\hbar \omega_{n_1}(k) - F(t) \cdot \xi_{n_1n_1}(k)) \delta_{n_1n_2} - F(t) \cdot \xi_{n_1n_2}(k)(1 - \delta_{n_1n_2}).
\]

The time evolution of the amplitudes \(c_n(k,t)\) in Eq. (2.10) is given by the time-dependent Schrödinger equation

\[
\frac{i\hbar}{\partial \tau} c_n(k,t) = \sum_{n'} (\mathcal{H}_{nn'}(k,t) - i\delta_{nn'} F(t) \cdot \nabla_k) c_{n'}(k,t).
\]
Now we look at the particular but important case where the force is uniform and constant, \( F(t) = F \). Consider a transformation of the Bloch states of the form

\[
|\phi_{nk}\rangle \equiv \sum_{n'} |\psi_{n'k}\rangle U_{n'n}(k),
\]

where \( U_{n'n}(k) \) are the elements of a unitary matrix \( U(k) \). In terms of these modified Bloch states, the wavepacket \( |\Psi(t)\rangle \) can be written as

\[
|\Psi(t)\rangle = \sum_n \int_{BZ} dk \, b_n(k, t) \, |\phi_{nk}\rangle,
\]

where the new amplitudes are

\[
b_n(k, t) \equiv \sum_{n'} U_{nn'}^\dagger(k) c_{n'}(k, t).
\]

From Eq. (2.41) the evolution of \( b_n(k, t) \) is given by

\[
i\hbar \frac{\partial}{\partial t} b_n(k, t) = \sum_{n'} \left[ U^\dagger(k) \mathcal{F}(k) U(k) - U^\dagger(k) i F \cdot \nabla_k U(k) \right]_{nn'} b_{n'}(k, t) - i F \cdot \nabla_k b_n(k, t),
\]

where \( \mathcal{F}(k) \) has matrix elements defined as in Eq. (2.40) for a time-independent force. If the unitary transformation according to \( U(k) \) satisfies the equation

\[
[U^\dagger(k) \mathcal{F}(k) U(k) - U^\dagger(k) i F \cdot \nabla_k U(k)]_{n_1n_2} = \delta_{n_1n_2} W_{n_1}(k),
\]

then the amplitude for band \( n \) is decoupled from the rest of the bands, and the solution to Eq. (2.45) can be found using the moving-frame coordinates \((\kappa, \tau)\), defined in terms the lab coordinates \((k, t)\) according to

\[
\kappa \equiv k - \frac{Ft}{\hbar} \quad \text{and} \quad \tau \equiv t.
\]

We introduce \( \mathcal{B}_n(\kappa, \tau) \equiv b_n(k, t) \), which satisfies the differential equation

\[
i\hbar \frac{\partial}{\partial \tau} \mathcal{B}_n(\kappa, \tau) = W_n(\kappa + F\tau/\hbar) \mathcal{B}_n(\kappa, \tau)
\]

with solutions of the form

\[
\mathcal{B}_n(\kappa, \tau) = \mathcal{B}_n(\kappa, \tau = 0) e^{-i \int_0^\tau W_n(\kappa + F\tau'/\hbar) d\tau'}.
\]
Back in the lab frame, we find

\[ b_n(k, t) = b_n(\kappa, 0)e^{-\frac{i}{\hbar}\int_0^t W_n(\kappa + F t'/\hbar)dt'}, \]

(2.50)

where \( \kappa \) is defined as in Eq. (2.47). Wannier proved that it is possible to find such a unitary transformation using an expansion of Eq. (2.46) in powers of \( F \) and described a recurrence procedure to construct it [43]. This expansion is only asymptotic; therefore, it is only accurate for weak forces such that Zener tunneling between bands is not significant [9, 43]. Note that the amplitude Eq. (2.50) corresponds to a wave packet with its center moving through the Brillouin zone accumulating a phase given by \( W_n(k) \). To first order in the force, we find

\[ W_n(k) \approx \hbar \omega_n(k) - F \cdot \xi_{nn}(k), \]

(2.51)

so that Eq. (2.50) becomes

\[ b_n(k, t) \approx b_n(\kappa, 0)e^{-i\gamma_n(\kappa, t)}, \]

(2.52)

where \( \gamma_n(k, t) \) is the usual dynamical phase corrected by a Berry-type phase [4, 5],

\[ \gamma_n(k, t) \equiv \int_0^t \left[ \omega_n(k + \frac{1}{\hbar}F t') - \frac{1}{\hbar}F \cdot \xi_{nn}(k + \frac{1}{\hbar}F t') \right] dt'. \]

(2.53)

In this first order approximation and assuming no degeneracies are present,\(^4\) \( U(k) \) has matrix elements

\[ U_{n_1n_2}(k) \approx \delta_{n_1n_2} + \Delta_{n_1n_2}(k), \]

(2.54)

where \( \Delta(k) \) is an off-diagonal matrix with elements that compare the interband position matrix element times the force with the energy difference between bands,

\[ \Delta_{n_1n_2}(k) \equiv \frac{F \cdot \xi_{n_1n_2}(k)}{\hbar \omega_{n_1n_2}(k)}(1 - \delta_{n_1n_2}). \]

(2.55)

In Appendix A we discuss in more detail Wannier’s decoupling procedure.

---

\(^4\)Wannier extended his method to deal with degeneracies, but for simplicity we assume they are absent. This assumption is valid for the type of potentials considered in Chapters 3 and 4.
The modified Bloch states constructed according to Eq. (2.42) can be used to justify the equations of motion (2.25) and (2.26) [41, 50]. As pointed out in the previous section, a wave packet strictly in one band cannot describe correctly the dynamics in the presence of an applied force because we need to include the interband mixing due to the force; the modified Bloch states provide this mixing. Thus, we consider a wave packet $|\phi_N(t)\rangle$ initially of the form

$$
|\phi_N(0)\rangle = \int_{BZ} d\kappa \tilde{b}_N(\kappa) |\phi_{N\kappa}\rangle,
$$

(2.56)

which evolves in time ($t \geq 0$) as

$$
|\phi_N(t)\rangle \approx \int_{BZ} d\kappa \tilde{b}_N(\kappa) e^{-i\gamma_{N}(\kappa, t)} |\phi_{N\kappa}\rangle
$$

(2.57)

(see Eq. (2.50)). Note that for $t > 0$ the wave packet is still formed by modified Bloch states with the same initial band index $N$. We refer to the wave packet $|\phi_N(t)\rangle$ as a MBS wave packet, where MBS stands for Modified Bloch State.

In the next section we will calculate the expectation values of the velocity and acceleration for a MBS wave packet, showing that we indeed recover the usual semiclassical
results. Before that calculation, it is instructive to point out that the phase $\gamma_N(\kappa, t)$ already anticipates the group and anomalous velocities. Eq. (2.57) for the MBS wave packet can be rewritten as

$$\left| \phi_N(t) \right\rangle \approx \int_{BZ} d\kappa \, b_N(\kappa) e^{-i\gamma_N(\kappa, t)} \left| \phi_{N\kappa} \right\rangle,$$

where $\kappa$ is now independent of time because the integral is expressed in a frame moving with the wave packet. The usual group velocity can be obtained from the time derivative of the difference between the usual dynamical phases in $\gamma_N(\kappa, t)$ accumulated by the center of the wave packet at $\kappa_o$ and another $\kappa$-component of the wave packet separated by a small wave vector $\delta\kappa$ [134],

$$\delta\phi^g \equiv \frac{d}{dt} \left[ \int_0^t \omega_N(\kappa + \frac{1}{\hbar} \mathbf{F} t') dt' - \int_0^t \omega_N(\kappa_o + \frac{1}{\hbar} \mathbf{F} t') dt' \right] = \omega_N(\kappa + \frac{1}{\hbar} \mathbf{F} t) - \omega_N(\kappa_o + \frac{1}{\hbar} \mathbf{F} t) \approx \frac{1}{\hbar} \delta\kappa \cdot \nabla_k (\hbar \omega_N(\kappa)) \big|_{k=\kappa_o + \frac{1}{\hbar} \mathbf{F} t} = \delta\kappa \cdot \mathbf{v}^g_N(\kappa_o + \frac{1}{\hbar} \mathbf{F} t)$$

(2.59)

(see Fig. 2.2). The remaining part of the phase, given by the Berry connection, is related to the anomalous velocity, as pointed out by Chong [134]. Similarly to Eq. (2.59), we can now consider the time derivative of the difference between the Berry phases in $\gamma_N(\kappa, t)$ accumulated by the center of the wave packet at $\kappa_o$ and another $\kappa$-component of the wave packet (separated by $\delta\kappa$, as before),

$$\delta\phi^{an} \equiv \frac{d}{dt} \left[ -\frac{1}{\hbar} \mathbf{F} \cdot \int_0^t \xi_{NN}(\kappa + \frac{1}{\hbar} \mathbf{F} t') dt' + \frac{1}{\hbar} \mathbf{F} \cdot \int_0^t \xi_{NN}(\kappa_o + \frac{1}{\hbar} \mathbf{F} t') dt' \right]$$

$$= -\frac{d}{dt} \left[ \int_{\kappa}^{\kappa_o + \frac{1}{\hbar} \mathbf{F} t} \xi_{NN}(\kappa') \cdot d\kappa' - \int_{\kappa_o}^{\kappa_o + \frac{1}{\hbar} \mathbf{F} t} \xi_{NN}(\kappa') \cdot d\kappa' \right].$$

(2.60)

Chong showed that $\delta\phi^{an}$ can be written in terms of the anomalous velocity. Note that in the limit of very small $\delta\kappa$, the integrals in Eq. (2.60) add up to the line integral along the closed circuit $\zeta(t)$ enclosing the red parallelogram in the clockwise direction (see Fig. 2.2); therefore, we can rewrite Eq. (2.60) as

$$\delta\phi^{an} \approx -\frac{d}{dt} \left[ \oint_{\zeta(t)} \xi_{NN}(\kappa') \cdot d\kappa' \right] = \frac{d}{dt} \left[ \int_{\delta\zeta(t)} \nabla_{\kappa'} \times \xi_{NN}(\kappa') \cdot d\kappa' \right]$$

(2.61)
where in the last expression \( S_\zeta(t) \) denotes the surface enclosed by \( \zeta(t) \), with area vector \( \mathbf{a}(t) = (\mathbf{F} t/\hbar) \times \delta \kappa \) pointing out of the page. In a small time interval \( dt \) the area of the parallelogram changes by \( d\mathbf{a}(t) = (\mathbf{F} dt/\hbar) \times \delta \kappa \), which is represented by the smaller pink parallelogram in Fig. 2.2; over this small area we can fix the value of \( \nabla_\kappa \times \xi_{NN}(\kappa') = \Omega_N(\kappa') \) to its value at \( \kappa' = \kappa_o + \mathbf{F} t/\hbar \). Thus, we can write

\[
\delta \varphi^\text{an} \approx \frac{1}{\hbar} \Omega_N(\kappa_o + \mathbf{F} t/\hbar) \cdot \mathbf{F} \times \delta \kappa = \delta \kappa \cdot \frac{1}{\hbar} \Omega_N(\kappa_o + \mathbf{F} t/\hbar) \times \mathbf{F} = \delta \kappa \cdot \mathbf{v}^\text{an}_N(\kappa_o + \frac{1}{\hbar} \mathbf{F} t),
\]

(2.62)

which proves that the anomalous velocity can be associated with the combination of the Berry phases accumulated by each component of the wave packet.

### 2.5 Recovering the effective mass theorem and anomalous transport

In this section we justify Eqs. (2.25) and (2.26) using a MBS wave packet to calculate the corresponding expectation values. It is convenient to apply the unitary transformation \( U(\mathbf{k}) \) to the matrix elements of the momentum operator and the lattice force from the crystal momentum representation. The momentum matrix elements in this representation, \( p_{n_1n_2}(\mathbf{k}) \), were defined in Eqs. (2.14) and (2.15); for the lattice force, consider the generalization of Eq. (2.36) to possibly different bands,

\[
\frac{1}{i\hbar} \left\langle \psi_{n_1\mathbf{k}_1} \left| \left[ \mathbf{p}, \hat{H}_o \right] \right| \psi_{n_2\mathbf{k}_2} \right\rangle = i \delta(\mathbf{k}_1 - \mathbf{k}_2) \omega_{n_1n_2}(\mathbf{k}) p_{n_1n_2}(\mathbf{k}).
\]

(2.63)

Therefore, we define

\[
\mathcal{P}^a_{n_1n_2}(\mathbf{k}) \equiv \sum_{n_1'n_2'} U^\dagger_{n_1'n_1}(\mathbf{k}) p^a_{n_1'n_2'}(\mathbf{k}) U_{n_2'n_2}(\mathbf{k})
\]

(2.64)

and

\[
\mathcal{F}^a_{n_1n_2}(\mathbf{k}) \equiv i \sum_{n_1'n_2'} U^\dagger_{n_1'n_1}(\mathbf{k}) \omega_{n_1'n_2'}(\mathbf{k}) p^a_{n_1'n_2'}(\mathbf{k}) U_{n_2'n_2}(\mathbf{k})
\]

(2.65)
as the corresponding matrix elements in the modified Bloch basis. In the particular case of a MBS wave packet, we can rewrite Eqs. (2.31) and (2.32) as

\[
\frac{d}{dt} \langle \bar{\phi}_N(t) | \hat{\tau}^a | \bar{\phi}_N(t) \rangle = \frac{1}{m} \int_{BZ} dk |\bar{b}_N(\kappa)|^2 \mathcal{P}^a_{NN}(k)
\]

and

\[
\frac{d^2}{dt^2} \langle \bar{\phi}_N(t) | \hat{\tau}^a | \bar{\phi}_N(t) \rangle = \frac{F^a}{m} + \frac{1}{m} \int_{BZ} dk |\bar{b}_N(\kappa)|^2 \mathcal{S}^a_{NN}(k).
\]

The diagonal matrix elements \( \mathcal{P}^a_{NN}(k) \) and \( \mathcal{S}^a_{NN}(k) \) can be written in terms of the local group velocity Eq. (2.23), the local anomalous velocity Eq. (2.24), and the local inverse effective mass tensor Eq. (2.27). This is a consequence of the well-known sum rules [131]

\[
\varepsilon_{ab}^{\Omega^l_N}(k) = \sum_{n \neq N} 2 \text{Im} \left[ \xi^a_{NN}(k) \xi^b_{nnN}(k) \right]
\]

and

\[
m \left[ \frac{1}{m^*_N(k)} \right]^{ab} - \delta^{ab} = \frac{1}{m} \sum_{n \neq N} 2 \text{Re} \left[ p^a_{NN}(k)p^b_{nnN}(k) \right] \frac{\hbar}{\omega_{NN}(k)},
\]

as shown in Sec. B.1 (Appendix B). Hence, we recover the semiclassical results Eqs. (2.25) and (2.26) in the form

\[
\frac{d}{dt} \langle \bar{\phi}_N(t) | \hat{\tau}^a | \bar{\phi}_N(t) \rangle = \int_{BZ} dk |\bar{b}_N(\kappa)|^2 \left( v^{g,a}_N(k) + v^{an,a}_N(k) \right)
\]

and

\[
\frac{d^2}{dt^2} \langle \bar{\phi}_N(t) | \hat{\tau}^a | \bar{\phi}_N(t) \rangle = \int_{BZ} dk |\bar{b}_N(\kappa)|^2 \left[ \frac{1}{m^*_N(k)} \right]^{ab} F^b.
\]

We can check the consistency of Eqs. (2.70) and (2.71) by taking the time derivative of the former to obtain the latter. As in Sec. 2.2, only the group velocity in Eq. (2.70) contributes to the time derivative to first order in the force,

\[
\frac{d}{dt} \int_{BZ} dk |\bar{b}_N(\kappa)|^2 v^{g,a}_N(k) = \int_{BZ} dk |\bar{b}_N(\kappa)|^2 \left[ \frac{1}{m^*_N(k)} \right]^{ab} F^b,
\]

and we recover Eq. (2.71) (see Sec. B.4 in Appendix B).
2.6 Dynamical corrections for suddenly applied forces

If the initial wave packet is different from Eq. (2.56), the equations of motion (2.70) and (2.71) do not hold anymore. Nevertheless, the modified Bloch states still provide an appropriate basis for calculating the evolution of a wave packet with a different initial condition if the uniform force stays constant after the initial time, $t = 0$. In Sec. 2.3 we found that a wave packet strictly in one band initially responds with the bare mass of the particle, while in Sec. 2.5 we showed that a MBS wave packet responds according to the inverse effective mass tensor. These observations motivate considering the initial condition Eq. (2.34) in order to study the transition between the bare mass and the effective mass, conciliating the two limits described by Eqs. (2.37) and (2.71). This transition is accompanied by the emergence of anomalous transport predicted by Eq. (2.70) but absent in Eq. (2.38).

More precisely, the problem at hand is the following. Consider a force that turns on instantaneously at $t = 0$ so that $F(t) = 0$ for $t < 0$ and $F(t) = F$ for $t \geq 0$. If the wave packet is prepared at $t = 0$ in the state Eq. (2.34),

$$|\Psi(0)\rangle = |\tilde{\psi}_N\rangle \equiv \int_{BZ} d\mathbf{k} f_N(\mathbf{k}) |\psi_N\rangle,$$

what are the dynamical corrections to the usual semiclassical picture described in Secs. 2.2 and 2.5? It is clear that if we write $|\Psi(t)\rangle$ as Eq. (2.43), the amplitudes $b_n(\mathbf{k}, t)$ will evolve according to Eq. (2.50) for $t \geq 0$; the question then is to find the right initial amplitudes compatible with the initial condition Eq. (2.73). To linear order in the force, which is the order to which we have constructed $|\phi_{nk}\rangle$, we find

$$b_N(\mathbf{k}, 0) \approx f_N(\mathbf{k}) \text{ and } b_n(\mathbf{k}, 0) \approx -f_N(\mathbf{k})\Delta_n(\mathbf{k}), \text{ for } n \neq N.$$  

(2.74)

Thus, for later times we have

$$b_N(\mathbf{k}, t) \approx f_N(\mathbf{k}) e^{-i\gamma_N(\mathbf{k}, t)} \text{ and } b_n(\mathbf{k}, t) \approx -f_N(\mathbf{k})\Delta_n(\mathbf{k}) e^{-i\gamma_n(\mathbf{k}, t)}, \text{ for } n \neq N.$$  

(2.75)
Note that the amplitudes for the modified Bloch states labeled by $N$ are of zeroth order, while the amplitudes for the remaining modified Bloch states are of first order. Back in the crystal momentum representation with the usual Bloch states, Eq. (2.10), the amplitudes satisfy the same property, since

$$c_N(k, t) \approx f_N(\kappa)e^{-i\gamma_N(\kappa,t)}$$

(2.76)

and

$$c_n(k, t) \approx f_N(\kappa)(\Delta_{nN}(k)e^{-i\gamma_N(\kappa,t)} - \Delta_{nN}(\kappa)e^{-i\gamma_n(\kappa,t)}), \text{ for } n \neq N,$$

(2.77)

to first order in the force.

Using the amplitudes $b_n(k, t)$ we can write the components of the expectation values for $|\Psi(t)\rangle$ of the velocity, $\langle \hat{\mathbf{v}}(t) \rangle \equiv d \langle \mathbf{r} \rangle / dt$, and the acceleration, $\langle \hat{\mathbf{a}}(t) \rangle \equiv d^2 \langle \mathbf{r} \rangle / dt^2$, as

$$\langle \hat{v}^a(t) \rangle = \frac{1}{m} \sum_{n_1, n_2} \int_{BZ} dk \, b^*_n(k, t)b_{n_2}(k, t) \Phi^{a}_{n_1n_2}(k)$$

(2.78)

and

$$\langle \hat{a}^a(t) \rangle = \frac{F^a}{m} + \frac{1}{m} \sum_{n_1, n_2} \int_{BZ} dk \, b^*_n(k, t)b_{n_2}(k, t) \Phi^{a}_{n_1n_2}(k),$$

(2.79)

respectively. Therefore, we need the matrix elements Eqs. (2.64) and (2.65) to first order in the force, and the amplitudes from Eq. (2.75). In Sec. B.2 (Appendix B) we show that Eqs. (2.78) and (2.79) reduce to

$$\langle \hat{v}^a(t) \rangle \approx \int_{BZ} dk \, |f_N(\kappa)|^2 \left( v^a_N(k) + v^{an,a}_N(k) + \mathbf{V}^{a}_N(k, t) \right),$$

(2.80)

and

$$\langle \hat{a}^a(t) \rangle \approx \int_{BZ} dk \, |f_N(\kappa)|^2 \left( \left[ \frac{1}{m_N^*(k)} \right]^{ab} F^b + A^a_N(k, t) \right).$$

(2.81)

The first two contributions on the right-hand-side of Eq. (2.80) involve the usual group velocity from Eq. (2.23) and the anomalous velocity from Eq. (2.24). With respect to the acceleration, the first contribution on the right-hand-side of Eq. (2.81) involves the
usual inverse effective mass tensor from Eq. (2.27). The additional terms in Eqs. (2.80) and (2.81), namely $V^a_N(k, t)$ and $A^a_N(k, t)$, can be written as

$$V^a_N(k, t) \equiv -\frac{1}{\hbar} J_{ab}^N(k, t) F^b \quad \text{and} \quad A^a_N(k, t) \equiv -\frac{1}{m} K_{ab}^N(k, t) F^b,$$

(2.82)

in terms of the tensors

$$J_{ab}^N(k, t) = \sum_{n \neq N} \frac{\omega_{nN}(k)}{2\hbar} \text{Im} \left[ \xi^a_{nN}(k) \xi^b_{nN}(\kappa) e^{-i\gamma_{nN}(\kappa, t)} \right]$$

(2.83)

and

$$K_{ab}^N(k, t) = -\frac{m}{\hbar} \sum_{n \neq N} \frac{(\omega_{nN}(k))^2}{\omega_{nN}(\kappa)} \text{Re} \left[ \xi^a_{nN}(k) \xi^b_{nN}(\kappa) e^{-i\gamma_{nN}(\kappa, t)} \right],$$

(2.84)

where $\gamma_{n_1n_2}(k, t) \equiv \gamma_{n_1}(k, t) - \gamma_{n_2}(k, t)$. In Chapters 3 and 4, we will see that $V^a_N(k, t)$ and $A^a_N(k, t)$ are responsible for oscillations of $\langle \hat{v}^a(t) \rangle$ and $\langle \hat{a}^a(t) \rangle$ about the usual semiclassical results Eqs. (2.70) and (2.71). Note that these tensors only have a definite symmetry with respect to the order of the Cartesian indices for $t = 0$, when they become

$$J_{ab}^N(0) = \epsilon^{ab} \Omega^N(k) \quad \text{and} \quad K_{ab}^N(0) = m \left[ \frac{1}{m^*_N(k)} \right]^{ab} - \delta^{ab},$$

(2.85)

which are antisymmetric and symmetric, respectively (see Eqs. (2.68) and (2.69)). At the initial time, $V^a_N(k, 0)$ cancels out the anomalous velocity contribution in Eq. (2.80), and $A^a_N(k, 0)$ replaces the inverse effective mass tensor by the inverse bare mass in Eq. (2.81); hence, we recover the bare mass response and the absence of anomalous transport for the initial time, described by Eqs. (2.37) and (2.38) (with $t_o = 0$).

For $t > 0$ we can decompose $J_{ab}^N(k, t)$ and $K_{ab}^N(k, t)$ uniquely in symmetric and antisymmetric parts,

$$J_{ab}^N(k, t) = J_{ab}^N(k, t) + \tilde{J}_{ab}^N(k, t) \quad \text{and} \quad K_{ab}^N(k, t) = K_{ab}^N(k, t) + \tilde{K}_{ab}^N(k, t),$$

(2.86)

where the bar and the tilde denote the symmetric and antisymmetric parts, respectively.

In order to write explicit expressions for them we define

$$X_{Nn}^{a,ab}(k, t) \equiv \xi^a_{nN}(k) \xi^b_{nN}(\kappa) e^{-i\gamma_{nN}(\kappa, t)} \pm \xi^a_{nN}(\kappa) e^{-i\gamma_{nN}(\kappa, t)} \xi^b_{nN}(k).$$

(2.87)
In Sec. B.3 (Appendix B) we show that the two types of contributions can be written compactly as

\[ \tilde{J}^{ab}_N(k, t) = \sum_{n \neq N} \text{Im} \left[ X^{\mp,ab}_{Nn}(k, t) \right] \frac{\omega_{nN}(k)}{\omega_{nN}(\kappa)} \]  

(2.88)

and

\[ \tilde{K}^{ab}_N(k, t) = -\frac{m}{\hbar} \sum_{n \neq N} \text{Re} \left[ X^{\pm,ab}_{Nn}(k, t) \right] \left( \frac{\omega_{nN}(k)}{\omega_{nN}(\kappa)} \right)^2, \]  

(2.89)

where the upper bar and lower tilde label the symmetric and antisymmetric terms, respectively, each one with its corresponding upper or lower signs on the right-hand-side. The antisymmetric tensors in Eqs. (2.88) and (2.89) can also be expressed in terms of axial-vectors \( \Lambda^l_N(k, t) \) and \( \Xi^l_N(k, t) \) with components

\[ \Lambda^l_N(k, t) \equiv -\frac{1}{2} \epsilon^{lab} \tilde{J}^{ab}_N(k, t) \]  

and

\[ \Xi^l_N(k, t) \equiv -\frac{1}{2} \epsilon^{lab} \tilde{K}^{ab}_N(k, t), \]  

(2.90)

so that

\[ \tilde{J}^{ab}_N(k, t) = \epsilon^{ab} \Lambda^l_N(k, t) \]  

and \( \tilde{K}^{ab}_N(k, t) = \epsilon^{ab} \Xi^l_N(k, t). \)  

(2.91)

This formal decomposition allows us to link some of the dynamical oscillations described by \( V^a_N(k, t) \) with the group velocity and some with the anomalous velocity. We can write the expectation value of the velocity \( \langle \dot{v}^a(t) \rangle \) as

\[ \langle \dot{v}^a(t) \rangle \approx V^{g,a}(t) + V^{an,a}(t), \]  

(2.92)

where we identify the dynamical group velocity \( V^{g}(t) \) of the wave packet, with components

\[ V^{g,a}(t) \equiv \int_{\text{BZ}} d\kappa \left| f_N(\kappa) \right|^2 \left( v_{N}^{g,a}(k) - \frac{1}{\hbar} \tilde{J}^{ab}_N(k, t) F^{b} \right), \]  

(2.93)

and the dynamical anomalous velocity \( V^{an}(t) \) of the wave packet, with components

\[ V^{an,a}(t) \equiv \int_{\text{BZ}} d\kappa \left| f_N(\kappa) \right|^2 \left( v_{N}^{an,a}(k) - \frac{1}{\hbar} \tilde{J}^{ab}_N(k, t) F^{b} \right). \]  

(2.94)

The leading term in parentheses in the integrands from Eqs. (2.93) and (2.94) are the contributions that would be expected from a MBS wave packet associated with band \( N \).
Chapter 2. Dynamics of wave packets in periodic potentials

(see Eq. (2.70)); the other terms in parentheses give oscillatory corrections. Note that Eq. (2.94) can be written as

\[ V^{an,a}(t) = \frac{1}{\hbar} \epsilon_{\alpha \beta}^l \Omega_N^l(t) F^b, \]  

(2.95)

where

\[ \Omega_N(t) \equiv \int_{BZ} d\mathbf{k} |f_N(\boldsymbol{\kappa})|^2 (\Omega_N(\mathbf{k}) - \Lambda_N(\mathbf{k}, t)) \]  

(2.96)

can be interpreted as the dynamical Berry curvature “seen” by the wave packet as it moves through the Brillouin zone.

The identification of the term involving \( J_N^{ab}(\mathbf{k}, t) \) with the group velocity of the wave packet is justified by the fact that the time derivative (to first order in the force) of \( V^g(t) \),

\[ \mathbf{A}^g(t) \equiv \frac{d}{dt} V^g(t), \]  

(2.97)

is found to have components

\[ A^{g,a}(t) = \left[ \frac{1}{M^*(t)} \right]^{ab} F^b, \]  

(2.98)

where we have introduced a dynamical inverse effective mass tensor,

\[ \left[ \frac{1}{M^*(t)} \right]^{ab} \equiv \int_{BZ} d\mathbf{k} |f_N(\boldsymbol{\kappa})|^2 \left( \left[ \frac{1}{m_N^*(\mathbf{k})} \right]^{ab} - \frac{1}{m} K_N^{ab}(\mathbf{k}, t) \right) \]  

(2.99)

(see Sec. B.4 in Appendix B). Since both the local inverse effective mass tensor \([1/m_N^*(\mathbf{k})]^{ab}\) and the additional tensor \( K_N^{ab}(\mathbf{k}, t) \) in Eq. (2.99) are symmetric with respect to their Cartesian components, they lead to a dynamical inverse effective mass tensor that is symmetric as well. The first contribution in parentheses in the integrand of Eq. (2.99) gives the result that would be expected for a MBS wave packet (see Eq. (2.71)); the term involving \( K_N^{ab}(\mathbf{k}, t) \) describes oscillatory corrections.

The time derivative (to first order in the force) of the dynamical anomalous velocity defined in Eq. (2.95),

\[ \mathbf{A}^{an}(t) \equiv \frac{d}{dt} V^{an}(t), \]  

(2.100)
can be regarded as a \textit{dynamical anomalous acceleration}, and it completes the total acceleration of the wave packet

\[ \langle \hat{a}(t) \rangle = \frac{d}{dt} \langle \hat{v}(t) \rangle \approx A^g(t) + A^{an}(t), \]  

(2.101)

since the elements of \( A^{an}(t) \),

\[ A^{an,a}(t) = \int_{BZ} d\mathbf{k} |f_N(\mathbf{k})|^2 \left( -\frac{1}{m} \tilde{K}^{ab}_N(\mathbf{k}, t) \right) F^b, \]

(2.102)
can be written in terms of the antisymmetric tensor defined in Eq. (2.89) (see Sec. B.4 in Appendix B). Note that from Eq. (2.91) we conclude that this anomalous acceleration is perpendicular to the force. Unlike the dynamical inverse effective mass tensor and the acceleration it describes, to first order in the force the dynamical anomalous acceleration contains only oscillatory terms (see the discussion after Eq. (2.71)).

At the initial time, Eq. (2.85) implies that

\[ \tilde{J}^{ab}_N(\mathbf{k}, 0) = 0 \quad \text{and} \quad \tilde{\Lambda}^l_N(\mathbf{k}, 0) = \Omega^l_N(\mathbf{k}), \]

(2.103)

and so

\[ V^{g,a}(0) = \int_{BZ} d\mathbf{k} |f_N(\mathbf{k})|^2 \nu^g_N(\mathbf{k}) \quad \text{and} \quad V^{an,a}(0) = 0, \]

(2.104)

consistently with the initial behavior found in Eq. (2.38) (with \( t_o = 0 \)) using Ehrenfest’s theorem; initially the Berry curvature “seen” by the wave packet vanishes, and there is no anomalous velocity. For \( t > 0 \) the wave packet’s velocity acquires dynamical oscillations about the usual group velocity. Since at the initial time

\[ \tilde{K}^{ab}_N(\mathbf{k}, 0) = m \left[ \frac{1}{m^*_N(\mathbf{k})} \right]^{ab} - \delta^{ab} \quad \text{and} \quad \tilde{K}^{ab}_N(\mathbf{k}, 0) = 0 \]

(2.105)

(see Eq. (2.85)), the dynamical inverse effective mass tensor is initially given by the inverse bare mass,

\[ \left[ \frac{1}{M^*(0)} \right]^{ab} = \frac{\delta^{ab}}{m} \quad \text{and} \quad A^{an,a}(0) = 0. \]

(2.106)

Hence, the particle initially responds with the bare mass \([48, 139]\); afterwards, the dynamical inverse effective mass tensor acquires oscillations about the usual inverse effective
mass tensor. In addition, the anomalous transport described by \( V^{an}(t) \) has its own dynamics; rather than just the Berry curvature, it is governed by the dynamical Berry curvature \( \Omega_N^l(t) \), which contains its own oscillatory terms.
Chapter 3

Dynamics of the effective mass in one-dimensional lattices

The experimental detection of the dynamical behavior of the effective mass and the anomalous velocity can be challenging in typical solid-state systems. In these systems, the time scale of the dynamical oscillations is of the order of femtoseconds [48]; therefore, it is necessary to probe the carrier response in the sub-femtosecond regime, which is becoming accessible only in recent years through new experimental techniques [75]. As discussed in Chapter 1, artificial lattices are an excellent alternative to explore phenomena that are difficult to probe in naturally occurring crystals. In this chapter and the next, we illustrate the dynamics of the effective mass and the anomalous velocity with simulations appropriate for experiments with ultracold atoms in optical lattices. We start here with the simplest example: a one-dimensional lattice. In this case, only the dynamics of the group velocity and the effective mass can be explored, since anomalous transport requires at least a two-dimensional lattice.\(^1\)

The chapter is organized as follows. In Sec. 3.1 we present a brief review of the

\(^1\)Under certain circumstances it is possible to observe anomalous transport in one-dimensional lattices, but this requires a lattice potential that changes in time [63].
semianalytical approximation described in more detail in Chapter 2, summarizing the expressions required for the one-dimensional case. Next, in Sec. 3.2, we introduce the main features of the one-dimensional optical lattice of interest (Sec. 3.2.1), illustrating the semianalytical results for parameters adjusted to resemble a one-dimensional semiconductor (Sec. 3.2.2); we also describe a method to solve the problem fully numerically (Sec. 3.2.3), which is used later to verify the validity of the semianalytical approximation.

In Sec. 3.3 we present simulations for one-dimensional optical lattices, modifying various parameters and comparing the results from the approximate and full numerical solutions. Finally, in Sec. 3.4 we summarize the main results and possible future directions for experiments based on the simulations presented here.

3.1 Semianalytical approximation for the dynamics

In this chapter we consider the particular one-dimensional case of the results presented in Chapter 2. The Hamiltonian Eq. (2.1) reduces to

$$\hat{H}(t) = \hat{H}_o - F(t) \hat{r}^x,$$

(3.1)

with $F(t) = 0$ for $t < 0$ and $F(t) = F$ for $t \geq 0$. The Bloch states that diagonalize the unperturbed Hamiltonian

$$\hat{H}_o \equiv \frac{(\hat{p}^x)^2}{2m} + V(\hat{r}^x)$$

(3.2)

are given by Eq. (2.7) with $D = 1$. We assume that the lattice and the force are oriented along the $\hat{x}$ direction and use $x \equiv r^x$; we denote the period of the lattice by $a$, and so $V(x + a) = V(x)$. The usual semiclassical results for the wave packet dynamics, Eqs. (2.70) and (2.71), become

$$\frac{d}{dt} \langle \bar{\phi}_N(t) | \hat{r}^x | \bar{\phi}_N(t) \rangle = \int_{\text{BZ}} dk |\tilde{b}_N(\kappa)|^2 v_N^g(k)$$

(3.3)

and

$$\frac{d^2}{dt^2} \langle \bar{\phi}_N(t) | \hat{r}^x | \bar{\phi}_N(t) \rangle = \int_{\text{BZ}} dk |\tilde{b}_N(\kappa)|^2 \frac{1}{m_N(k)} F;$$

(3.4)
where $\kappa \equiv k - Ft/\hbar$. Note that in this case there is no anomalous contribution to the velocity, and the local inverse effective mass tensor Eq. (2.27) simply becomes a scalar,

$$
\frac{1}{m^*_N(k)} = \frac{1}{\hbar^2} \frac{d^2}{dk^2} (\hbar \omega_N(k)).
$$

(3.5)

In order to find the dynamical behavior of the expectation values in Eq. (3.3) and (3.4) due to the instantaneous application of the force, we consider the diagonal elements $J_{xx}^N(k,t)$ and $K_{xx}^N(k,t)$ of the tensors Eqs. (2.83) and (2.84). First, note that in the one-dimensional case there is no antisymmetric contribution, and so we find

$$
J_{xx}^N(k,t) = \bar{J}_{xx}^N(k,t) = \sum_{n \neq N} \frac{\omega_{nN}(k)}{\omega_{nN}(\kappa)} 2 \text{Im} \left[ \xi_{nN}^x(k) \xi_{nN}^x(\kappa) e^{-i\gamma_{nN}(\kappa,t)} \right]
$$

(3.6)

and

$$
K_{xx}^N(k,t) = \bar{K}_{xx}^N(k,t) = -\frac{m}{\hbar} \sum_{n \neq N} \frac{(\omega_{nN}(k))^2}{\omega_{nN}(\kappa)} 2 \text{Re} \left[ \xi_{nN}^x(k) \xi_{nN}^x(\kappa) e^{-i\gamma_{nN}(\kappa,t)} \right].
$$

(3.7)

Thus, we can write Eqs. (2.80) and (2.81) as

$$
\langle \hat{v}(t) \rangle \approx \int_{\text{BZ}} dk |f_{N}(\kappa)|^2 \left( v_N^g(k) - \frac{1}{\hbar} \sum_{n \neq N} \frac{\omega_{nN}(k)}{\omega_{nN}(\kappa)} 2 \text{Im} \left[ \xi_{nN}(k) \xi_{nN}(\kappa) e^{-i\gamma_{nN}(\kappa,t)} \right] \right) F
$$

(3.8)

and

$$
\langle \hat{a}(t) \rangle \approx \int_{\text{BZ}} dk |f_{N}(\kappa)|^2 \left( \frac{1}{m^*_N(k)} + \frac{1}{\hbar} \sum_{n \neq N} \frac{(\omega_{nN}(k))^2}{\omega_{nN}(\kappa)} 2 \text{Re} \left[ \xi_{nN}(k) \xi_{nN}(\kappa) e^{-i\gamma_{nN}(\kappa,t)} \right] \right) F,
$$

(3.9)

where we have dropped the superscript ‘$x$’ for convenience.

### 3.2 Model and numerical calculation

#### 3.2.1 One-dimensional optical lattice

We consider a one-dimensional optical lattice formed by the standing wave pattern of two interfering laser fields of wavelength $\lambda$. A cloud of atoms cooled down to nanokelvin
temperatures can be loaded in this lattice ramping up the laser fields adiabatically. The atoms interact with the light through the ac Stark shift and feel a sinusoidal potential associated with the standing wave. For a specific implementation using a Bose-Einstein condensate of $^{87}\text{Rb}$ atoms we refer the reader to [68], where an experiment to detect the dynamics presented here was implemented.

We assume that the periodic potential has the form

$$V(x) = V_o \sin^2(k_R x),$$

(3.10)

where $V_o$ is a constant that determines the strength of the potential and $k_R$ is the photon wave vector $k_R = 2\pi/\lambda$. The period of the lattice is $a = \lambda/2 = \pi/k_R$ in real space and $K = 2k_R$ in reciprocal space. Since the momentum carried by a photon of the laser field is $\hbar k_R$, the energy gained (lost) by an atom of mass $m$ when it absorbs (emits) a photon is

$$E_R = \frac{(\hbar k_R)^2}{2m},$$

(3.11)

which is usually called the recoil energy and sets the characteristic energy scale. The eigenvalue problem for the Hamiltonian Eq. (3.2) can be written as Mathieu’s differential equation. The two linearly independent solutions can be combined appropriately to construct Bloch-type solutions analytical and periodic in reciprocal space over the Bril-
louin zone for each band index [140–143]. An example of the band structure calculated for \( V_0 = 10E_R \) is shown in Fig. 3.1, where the bands are labeled in order of increasing energy, starting with \( n = 1 \).

Because of the space-inversion symmetry of the potential \( V(x) \) and the procedure used to find the Bloch functions, the diagonal matrix elements \( \xi_{nn}(k) \) are set to zero [141], and the off-diagonal elements \( \xi_{n_1n_2}(k) (n_1 \neq n_2) \) are purely imaginary. From Eq. (2.16) we conclude that the momentum matrix elements are purely real so it is convenient to rewrite Eqs. (3.8) and (3.9) in terms of these,

\[
\langle \hat{v}(t) \rangle \approx \int_{\text{BZ}} dk |f_N(\kappa)|^2 \left( v_N^k(k) + \frac{2}{\hbar m^2} \sum_{n \neq N} \frac{1}{(\omega_{nN}(\kappa))^2} p_{nN}(k)p_{nN}(\kappa) \sin(\gamma_{nN}(\kappa,t))F \right)
\]

and

\[
\langle \hat{a}(t) \rangle \approx \int_{\text{BZ}} dk |f_N(\kappa)|^2 \left( \frac{1}{m_N^2(k)} + \frac{2}{\hbar m^2} \sum_{n \neq N} \frac{\omega_{nN}(k)}{(\omega_{nN}(\kappa))^2} p_{nN}(k)p_{nN}(\kappa) \cos(\gamma_{nN}(\kappa,t)) \right) F.
\]

These simplifications are particular to this one-dimensional case, as we will see in the next chapter where we consider a two-dimensional lattice. For the envelope function \( f_N(k) \), we choose a Gaussian of the form

\[
f_N(k) = \sqrt{\frac{1}{\sigma\sqrt{\pi}}} \exp \left( -\frac{(k - k_o)^2}{2\sigma^2} \right),
\]

where \( k_o \) is the mean of the envelope function.

For times short enough after the force is applied, the variations of the momentum matrix elements \( p_{nN}(\kappa) \) and the frequencies \( \omega_{nN}(\kappa) \) as \( \kappa \) changes in time can be neglected, and we recover the expression found by Iafrate and Krieger [139, 144, 145] for an electron in a dc field electric field using the velocity gauge (see Sec. 1.2.1 in Chapter 1). However, as we will show in Sec. 3.3, Eqs. (3.12) and (3.13) give a good approximation to the behavior for longer times, over which the variations of \( p_{nN}(\kappa) \) and \( \omega_{nN}(\kappa) \) cannot be neglected, as long as the wave packet remains mainly in one band. This feature of
Eqs. (3.12) and (3.13) is useful to study the interplay between the dynamics of the effective mass and the Bloch oscillations, which occur over a period of time

$$\tau_B = \frac{\hbar K}{F} = \frac{2\hbar k_R}{F} = \frac{2\pi \hbar}{aF},$$

(3.15)
typically longer than the period of oscillations associated with the phase $\gamma_{nN}(\kappa, t)$; we will discuss this interplay in Sec. 3.3. Since the observation of Bloch oscillations in optical lattices for the first time by Ben Dahan et al. [13], experiments in this type of lattice are performed routinely in order to observe phenomena on the time scale of the Bloch period; therefore, it is plausible to study simultaneously the dynamical oscillations due to the sudden application of the force and the usual Bloch oscillations. In practice, there are technical limitations due to the time resolution required to resolve the first type of oscillations as discussed in [68].

3.2.2 Example: Toy model for a semiconductor

We now illustrate some of the features contained in the result Eq. (3.13) for an electron in the potential described by Eq. (3.10) with parameters adjusted to resemble the energy and length scales of a typical semiconductor; specifically, we choose $V_o = 10E_R$ and $a = 0.5$ nm. For this example the wave packet is centered at $k = 0$ in the band $N = 3$, which resembles the first conduction band of a semiconductor (see Fig. 3.1). We use a force that corresponds to a strong dc field of $1.7 \times 10^2$ kV/cm, and the band gap $\hbar \omega_{32}(k = 0)$ is of the order of 1 eV (here $E_R = 1.5$ eV). Using these parameters in Eq. (3.13), we plot the dynamical effective mass (see Eq. (2.99)), defined as

$$M^*(t) \equiv \frac{F}{\langle \hat{a}(t) \rangle},$$

(3.16)
in Fig. 3.2.

Note that the system behaves initially with the bare mass, and so $M^*(0) = m$; afterwards, the dynamical effective mass oscillates about the value predicted by the local
Figure 3.2: Dynamical effective mass for an electron wave packet \( (\sigma \approx 0.3k_R = 0.15K) \) initially centered at \( k = 0 \) in the band \( N = 3 \) of the one-dimensional potential Eq. (3.10) with \( V_o = 10E_R \) and \( a = 0.5 \text{ nm} \), calculated from the semianalytical approximation (red solid line); the blue dotted line corresponds to the usual effective mass associated with the wave packet. The inset shows a comparison with the full numerical calculation (green crosses) over a smaller time range (see Sec. 3.2.3).

The effective mass Eq. (3.5) averaged over the extension of the wave packet. Thus, at very early times, the local effective mass \( m^*_N(k) \) defined \textit{kinematically} in terms of the band energy does not describe correctly the dynamical response of the wave packet to the suddenly applied force; at later times, \( m^*_N(k) \) provides an appropriate description on average. Although there is a superposition of various oscillations in the second term of Eq. (3.13),

\[
\langle a^{\text{osc}}(t) \rangle \equiv \int_{\text{BZ}} dk \, |f_N(k)|^2 \frac{2F}{\hbar m^2} \sum_{n \neq N} \frac{\omega_{Nn}(k)}{(\omega_{Nn}(k))^2} p_{Nn}(k)p_{nN}(k) \cos(\gamma_{nN}(k,t)), \quad (3.17)
\]

associated with the different neighboring bands, Fig. 3.2 shows a distinctive oscillation with period

\[
\tau_{\text{osc}} = \frac{2\pi}{|\omega_{N\bar{n}}(0)|}, \quad (3.18)
\]

given by the energy difference between the main band, \( N = 3 \), and its next neighbor band, \( \bar{n} = 2 \), in the region near the center of the Brillouin zone. In Fig. 3.2 this period is
Figure 3.3: Expectation value of the acceleration for the same wave packet described in Fig. 3.2 but starting in the band \( N = 1 \), calculated from the semianalytical approximation (red solid line) and the usual inverse effective mass (blue dotted line). The light blue slash-dotted line corresponds to the envelope function in Eq. (3.21), adjusted to give the correct initial value of the acceleration. The inset shows a comparison with the full numerical calculation (green crosses) over a smaller time range (see Sec. 3.2.3).

\( \tau_{\text{osc}} \approx 1.30 \text{ fs} \). The remaining oscillating terms have small contributions because of the much larger energy difference with respect to the main band.

In Fig. 3.3 we show another example for the same system but starting in the lowest band \( (N = 1) \). Compared with the previous example, the local inverse effective mass of the main band \( N = 1 \) in this case is smaller because this band is flatter than the band \( N = 3 \) discussed before. Due to the smaller local inverse effective mass, the average value of the acceleration is smaller and the expectation value of the acceleration, \( \langle \hat{a}(t) \rangle \), goes to zero several times. Therefore, it is more convenient to plot \( \langle \hat{a}(t) \rangle \) instead of the dynamical effective mass \( M^*(t) \).

Note that the oscillations decay as a consequence of the spread of the wave packet in reciprocal space, as pointed out by Pfirsch and Spenke [48]. We can derive an approximate expression for the envelope of the decaying oscillations of the acceleration while the wave packet is moving close to the center of the Brillouin zone. If we consider only the
contribution from the next neighbor band,\textsuperscript{2} which we denote by $\bar{n}$, and neglect the change of $p_{\bar{n}N}(\kappa)$ and $\omega_{\bar{n}N}(\kappa)$ in Eq. (3.17) we can write the approximate expression \[ \langle a^{\text{osc}}(t) \rangle \approx \frac{2F(p_{\bar{n}N}(0))^2}{m^2 \hbar \omega_{\bar{n}N}(0)} \int_{\text{BZ}} dk |f_N(k)|^2 \cos(\omega_{N\bar{n}}(k)t). \] (3.19)

The energy difference associated with the frequency of the oscillations can be approximated by a parabolic dispersion near $k = 0$,

\[ \hbar \omega_{N\bar{n}}(k) \approx \frac{\hbar^2 k^2}{2} \left( \frac{1}{m^*_N(0)} - \frac{1}{m^*_\bar{n}(0)} \right) + \hbar \omega_{N\bar{n}}(0) = \frac{\hbar^2 k^2}{2m_{\bar{n}N}^\text{red}(0)} + \hbar \omega_{N\bar{n}}(0), \] (3.20)

where we introduced the reduced effective mass $m_{\bar{n}N}^\text{red}(0)$ associated with the pair of bands $N$ and $\bar{n}$. Using this approximation and the Gaussian envelope function from Eq. (3.14), we can evaluate Eq. (3.19) analytically and obtain

\[ \langle a^{\text{osc}}(t) \rangle \approx \frac{2F(p_{\bar{n}N}(0))^2}{m^2 \hbar \omega_{\bar{n}N}(0)} \left[ 1 + \left( \frac{\hbar \sigma}{2m_{\bar{n}N}^\text{red}(0)}t \right)^2 \right]^{-1/4} \cos \left[ \frac{\hbar \omega_{N\bar{n}}(0)t}{2} + \frac{1}{2} \tan^{-1} \left( \frac{\hbar \sigma^2}{2m_{\bar{n}N}^\text{red}(0)}t \right) \right], \] (3.21)

which is essentially an oscillating cosine function with angular frequency $|\omega_{N\bar{n}}(0)|$ multiplied by an envelope function that controls the decay. There is an additional contribution to the phase of the cosine function, but it is small in the time range where the approximation is valid. In Fig. 3.3 we show that the approximation Eq. (3.21) describes appropriately the form of the decay. We can also define the decay time,

\[ \tau_{\text{decay}} \equiv \frac{2\sqrt{15} |m_{\bar{n}N}^\text{red}(0)|}{\hbar \sigma^2}, \] (3.22)

as the time it takes the oscillations in Eq. (3.21) to reduce by half; we will use $\tau_{\text{decay}}$ as an estimate for the decay of the oscillations of the acceleration about the value predicted by the usual inverse effective mass. For the examples shown in Figs. 3.2 and 3.3 the estimated decay times are 1.89 fs and 4.78 fs, respectively; these values correspond to a small fraction of the Bloch period, $\tau_B \approx 485$ fs, for this system.

\textsuperscript{2}The contributions from each band decrease roughly as the inverse of the energy difference with respect to the main band.
3.2.3 Full numerical calculation

The usual inverse effective mass can be understood as the result of a “dressing” process of the wave packet in one band with amplitudes over neighboring bands, as we discussed in Secs. 2.4 and 2.5; the initial response of the wave packet, according to the bare mass, induces the oscillatory behavior in Eq. (3.13). However, this simple picture is valid only if the wave packet remains mainly in one band. The approximate solution Eq. (2.77) for the amplitudes associated with the neighboring bands predicts a small second-order correction for the probability of finding the wave packet in those bands. Hence, situations where the population of the neighboring bands becomes important due to Zener tunneling cannot be described within this scheme. In order to verify that effects of the population of neighboring bands beyond our semianalytical approximation can be neglected in our examples, we compare the results from Eqs. (3.12) and (3.13) with a full numerical calculation that solves the time-dependent Schrödinger equation for the Hamiltonian Eq. (3.1) with the initial condition Eq. (2.73).

For the full numerical calculation we use the split-step operator method [129]. As usual, the kinetic energy term of the Hamiltonian is treated in Fourier space and the potential energy term (including the applied force) is treated in real space, switching back and forth between the two spaces with a Fast Fourier Transform implementation [146]. The force term in Eq. (3.1) must be treated carefully because no periodic boundary conditions can be assumed in the direction of the force. In practice, this complication implies that the computational window must be large enough so that the wave packet never approaches the boundaries during the time of the calculation. An alternative is to apply a unitary transformation $\hat{S}(t)$ to the time-independent Hamiltonian

$$\hat{H} \equiv \hat{H}_o - F \hat{\tau}^x, \quad (3.23)$$

given by Eq. (3.1) for $t \geq 0$, in order to remove the force term; the new Hamiltonian
after the transformation can be written as

\[
\hat{H}'(t) = \hat{S}^\dagger(t) \hat{H} \hat{S}(t) - i\hbar \frac{d}{dt} \hat{S}(t).
\]

(3.24)

If we define \( \hat{S}(t) \) according to

\[
\hat{S}(t) \equiv e^{i\alpha(t) \hat{p}_x/\hbar} e^{-i\beta(t) \hat{r}_x/\hbar} e^{i\gamma(t)/\hbar},
\]

(3.25)

where \( \alpha(t) \equiv a_L t^2/2, \beta(t) \equiv ma_L t, \gamma(t) \equiv ma_L^2 t^3/3 \) and \( F = -ma_L \), Eq. (3.24) becomes

\[
\hat{H}'(t) = \frac{\hat{p}_x^2}{2m} + V (\hat{r} - a_L t^2/2).
\]

(3.26)

The new Hamiltonian is time dependent for \( t \geq 0 \), but it has the original periodicity of the unperturbed Hamiltonian Eq. (3.2).\(^3\) Note that Eq. (3.26) is the Hamiltonian for a lattice with acceleration \( a_L \), which in the lattice frame translates into a uniform force \( F \). This is a common approach in experiments with ultracold atoms because it simply requires increasing the frequency difference between the lattice beams linearly in time \([13, 14]\); the transformation \( \hat{S}(t) \) provides a rigorous proof that the accelerating lattice provides an inertial force (see Appendix in \([14]\)). From the point of view of our numerical calculation, the Hamiltonian Eq. (3.26) has the advantage that periodic boundary conditions can be imposed on the calculation window. We use both Hamiltonians \( \hat{H} \) and \( \hat{H}'(t) \) to calculate the wave packet dynamics; our results agree for sufficiently large computational windows.

In Figs. 3.2 and 3.3 we already showed a comparison between the semianalytical approximation and the full numerical solution, showing almost perfect agreement. This observation confirms that Eq. (3.13) is appropriate for short times after the force is suddenly applied. In the next section we show that the semianalytical approximation also provides a useful estimate for longer times, of the order of a Bloch period \( \tau_B \).

\(^3\)In the case of a charged particle in a dc electric field, the transformation used here becomes the gauge transformation required to move back from the length gauge to the velocity gauge (see Sec. 1.1 in Chapter 1).
3.3 Results and discussion

As illustrated in Sec. 3.2.2, the oscillations displayed in Figs. 3.2 and 3.3 decay in a few femtoseconds for electron motion in a semiconductor, a time scale that is difficult to resolve experimentally. The corresponding time scales in optical lattices are of the order of microseconds, as we discuss in this section. Considering the additional advantages of tunability and low decoherence that experiments in optical lattices offer, this type of lattice provides an ideal scenario for exploring the dynamical behavior associated with the application of the force. In fact, Chang et al. [68] were able to resolve and study the dynamical oscillations of the group velocity at early times after the application of the force in a one-dimensional optical lattice, showing the expected behavior for different lattice depths and forces; the turn-on times of the force were small enough compared to the period of the dynamical oscillations so that the initial response was correctly described by the bare mass of the atoms. In their experiment, a Bose-Einstein condensate of $^{87}$Rb atoms inside a hybrid optical and magnetic trap is loaded adiabatically in the lowest band of an optical lattice; the force required to observe the dynamics is applied by shifting the center of the magnetic trap, and the velocity of the atoms is measured by abruptly turning off all the potentials and imaging the cloud after time-of-flight expansion. Due to the low atomic densities used in these experiments (less than $3 \times 10^{13}$ atoms/cm$^3$), the effect of interparticle interactions was minimal and effectively reduced to a small correction to the lattice depth in the independent particle calculations.

For optical lattices the physical scales change drastically compared to the electron case described before, but the behavior is qualitatively the same. In order to compare the two cases, it is appropriate to consider the ratio of the initial oscillation period Eq. (3.18) to the Bloch period,

$$\frac{\tau_{osc}}{\tau_B} = \frac{a F}{|\hbar \omega_{N\hbar}(0)|} = \frac{\pi \hat{F}}{|E_{N\hbar}(0)|},$$  \hspace{1cm} (3.27)
and the ratio of the decay time Eq. (3.22) to the Bloch period,

\[
\frac{\tau_{\text{decay}}}{\tau_B} = \sqrt{\frac{15aF|\hat{m}_{N_H}^\text{red}(0)|}{\pi\hbar^2\sigma^2}} = \frac{\sqrt{15}}{2} \frac{\hat{F}|\hat{m}_{N_H}^\text{red}(0)|}{\sigma^2}.
\]  

(3.28)

In Eqs. (3.27) and (3.28) we included the ratios in terms of the scaled wave vector, energy and mass:

\[
\hat{k} \equiv \frac{k}{k_R}, \quad \hat{E}_{n_1n_2}(\hat{k}) \equiv \frac{\hbar\omega_{n_1n_2}(k)}{E_R}, \quad \text{and} \quad \hat{m}_{n_1n_2}^\text{red}(\hat{k}) \equiv \frac{m_{n_1n_2}^\text{red}(k)}{m}.
\]  

(3.29)

Note that since \( \sigma \) is the spread of the wave packet in reciprocal space, the corresponding scaled variable is \( \hat{\sigma} \equiv \sigma/k_R \). We also introduced the scaled force

\[
\hat{F} \equiv \frac{F}{k_Re_R} = \frac{aF}{\pi E_R},
\]  

(3.30)

which compares the energy drop over a unit cell, \( aF \), with the characteristic energy of the system, \( E_R \). These scaled variables are useful to compare systems with different physical scales. For the example shown in Fig. 3.2 the ratios are \( \tau_{\text{osc}}/\tau_B \approx 0.003 \) and \( \tau_{\text{decay}}/\tau_B \approx 0.004 \), while for the example shown in Fig. 3.3 they are \( \tau_{\text{osc}}/\tau_B \approx 0.001 \) and \( \tau_{\text{decay}}/\tau_B \approx 0.010 \). In both electron cases the ratios are small because \( \hat{F} \approx 0.002 \) is also small, even though we employed a high electric field to provide the force. In contrast, for ultracold atoms in optical lattices it is easy to make these ratios bigger while maintaining coherence over times of the order of a Bloch period.

Consider, for example, the expectation value of the acceleration calculated for rubidium atoms prepared at the center of the lowest band (\( N = 1 \)) of an optical lattice with \( a = 390 \) nm, \( V_o = 7E_R \), and \( F/m = 24.2 \) m/s\(^2\). The ratios in Eqs. (3.27) and (3.28) are now larger than in the electron case due to the increase in the force parameter to \( \hat{F} \approx 0.173 \). In the present example \( \tau_{\text{osc}}/\tau_B \approx 0.105 \) and \( \tau_{\text{decay}}/\tau_B \approx 0.425 \), which correspond to \( \tau_{\text{osc}} \approx 51.1 \) \( \mu \)s and \( \tau_{\text{decay}} \approx 207 \) \( \mu \)s. Fig. 3.4 shows how the atom’s acceleration oscillates about the behavior expected for a response with the usual inverse effective mass.

\(^4\)A similar definition is used in [61]. Our definition has an additional factor of \( 1/\pi \).
Figure 3.4: Expectation value of the acceleration of a wave packet ($\sigma \approx 0.3k_R = 0.15K$) initially centered at $k = 0$ in the band $N = 1$ for a rubidium atom in an optical lattice with $V_o = 7E_R$ and $a = 390$ nm, calculated from the semianalytical approximation (red solid line), the full numerical solution (green dashed line), and the usual inverse effective mass (blue dotted line). The applied force is such that $F/m = 24.2 \, \text{m/s}^2$, which corresponds to $\tilde{F} \approx 0.173$ at all times. Strictly speaking Eq. (3.21) does not apply here because in this case the decay occurs as the center of the wave packet has moved through a considerable portion of the Brillouin zone; nevertheless, Eq. (3.22) still gives a rough estimate of the initial decay time (see Fig. 3.4).

One of the most striking features of Fig. 3.4 is the revival of the oscillations as the wave packet returns to $k = 0$ completing a Bloch oscillation. This is not surprising given the periodicity of $p_{Nn}(k)$ and $\omega_{nN}(k)$ over the Brillouin zone. Consider the integral from Eq. (3.17) in a frame moving with the wave packet in reciprocal space so that $\kappa$ is independent of time,

$$\langle a^{osc}(t) \rangle = \int_{BZ} d\kappa |f_N(\kappa)|^2 \frac{2F}{\hbar m^2} \sum_{n \neq N} \frac{\omega_{nN}(\kappa + Ft/\hbar)}{(\omega_{nN}(\kappa))^2} p_{Nn}(\kappa + Ft/\hbar)p_{nN}(\kappa) \cos(\gamma_{nN}(\kappa, t)).$$  \hspace{1cm} (3.31)

After a Bloch period, each cosine function in Eq. (3.31) accumulates a phase $\gamma_{nN}(k, \tau_B) = \int_0^{\tau_B} \omega_{nN}(\kappa + Ft/\hbar) dt' = \varphi_{nN}$, which only depends on the bands $n$ and $N$; furthermore,
the factors that multiply these cosine functions are also periodic in time with period $\tau_B$. Thus, the contributions from each neighboring band $n \neq N$ to Eq. (3.31) are separately periodic, but when they are combined, the resulting oscillations are not strictly periodic because each contribution accumulates a different phase. However, usually the nearest neighboring band has the most significant contribution (see Sec. 3.2.2), and so $\langle a_{osc}(t) \rangle$ is almost periodic and displays a revival after a Bloch period.

The revival is also present in the example in Fig. 3.3 for the electron wave packet when the acceleration is plotted for a full Bloch period. In the situation shown in Fig. 3.2, however, we cannot use Eq. (3.13) to describe the behavior of the electron wave packet for an entire Bloch oscillation because the gap with respect to the band $n = 4$ (the closest to band $N = 3$ in the region near the edge of the Brillouin zone, see Fig. 3.1) becomes increasingly small as the wave packet moves closer to the band edge, and significant Zener tunneling occurs.

In many experiments that study the motion of ultracold atoms in optical lattices, the
measured variable is the velocity of the wave packet rather than the acceleration (for example in [13]). In Fig. 3.5 we show a plot of the velocity for the same parameters as Fig. 3.4. As before, we include a plot of the prediction based on the usual effective mass, which corresponds to the group velocity (see Eq. (3.3)); this prediction clearly shows a full Bloch oscillation. Note also the good agreement between the prediction based on the semianalytical approximation Eq. (3.12) and the full numerical solution, even for long times after the force was suddenly applied.

In the rest of this section we discuss the behavior of the velocity in various situations realizable in experiments with ultracold atoms, where the natural scale for the velocity is given by the recoil velocity,

\[ v_R = \frac{\hbar k_R}{m} = \frac{\hbar \pi}{ma}. \]  

(3.32)

Accordingly, we use the scaled velocity \( \langle \dot{\hat{v}}(\hat{t}) \rangle \equiv \langle \dot{\hat{v}}(t) \rangle / v_R \), which can be written entirely in terms of dimensionless variables as

\[ \langle \dot{\hat{v}}(\hat{t}) \rangle \approx \int_{BZ} d\hat{k} |\hat{f}_N(\hat{k})|^2 \left( \hat{\bar{v}}^g_N(\hat{k}) + 4 \sum_{n \neq N} \frac{1}{(\hat{E}_{nN}(\hat{k}))^2} \hat{p}_{nN}(\hat{k}) \hat{p}_{nN}(\hat{k}) \sin(\hat{\gamma}_{nN}(\hat{k}, \hat{t})) \right) \hat{F}. \]  

(3.33)

In this expression we introduced the additional scaled variables

\[ \hat{t} \equiv \frac{E_R}{\hbar} t \quad \text{and} \quad \hat{k} \equiv \hat{k} - \hat{F} \hat{t}, \]  

(3.34)

and the scaled functions

\[ \hat{f}_N(\hat{k}) \equiv \sqrt{k_R} f_N(k) \quad \text{and} \quad \hat{p}_{n_1n_2}(\hat{k}) \equiv \frac{p_{n_1n_2}(k)}{\hbar k_R} \quad \text{and} \quad \hat{\gamma}_{n_1n_2}(\hat{k}, \hat{t}) \equiv \gamma_{n_1n_2}(k, t). \]  

(3.35)

According to Eq. (3.33), \( \langle \dot{\hat{v}}(\hat{t}) \rangle \) for a given band \( N \) depends only on the width of the wave packet in reciprocal space; the strength of the potential, characterized by \( \hat{V}_o \equiv V_o / E_R \); and the scaled force, \( \hat{F} \). For fixed values of these three parameters, the oscillations preserve their shape, and are only rescaled when the recoil velocity is modified due to a different bare mass or lattice constant. For the first example with ultracold atoms in optical lattices, shown in Figs. 3.4 and 3.5, the recoil velocity is \( v_R \approx 5.89 \text{ mm/s} \). In
Figure 3.6: Expectation value of the velocity for the same wave packet described in Fig. 3.5 but with a stronger applied force, $F/m = 72.6 \text{ m/s}^2$ or $\hat{F} \approx 0.520$, calculated from the semianalytical approximation (red solid line), the full numerical solution (green dashed line), and the usual group velocity (blue dotted line). The inset shows the difference between the semianalytical approximation and the usual group velocity prediction with the same units as the main plot.

The width of the wave packet in reciprocal space and the reduced effective mass control how fast the oscillations decay according to Eq. (3.28). However, as pointed out before, the estimate in Eq. (3.28) does not take into account the motion of the wave packet through the Brillouin zone during one Bloch period because it was derived from Eq. (3.21), which misses completely the revival of the dynamical oscillations of the inverse effective mass. The initial decay can be minimized or even removed if the oscillations about the usual group velocity do not have enough time to decay before the periodicity of the terms in Eq. (3.33) (over one Bloch period) produces the revivals.

From Eq. (3.28) we expect the decay time to become comparable to the Bloch period when increasing the scaled force $\hat{F}$ and the reduced effective mass $\hat{m}_{\text{red}}^{\text{red}}(0)$. The first case is illustrated in Fig. 3.6, where we show how an increase in $\hat{F}$, keeping the other parameters fixed, eliminates the decay over the first half of the Bloch period shown in
Figure 3.7: Expectation value of the velocity for the same wave packet described in Fig. 3.5 with the same applied force but for a deeper lattice with $V_o = 13E_R$, calculated from the semianalytical approximation (red solid line), the full numerical solution (green crosses), and the usual group velocity (blue dotted line). The inset shows the difference between the semianalytical approximation and the usual group velocity prediction with the same units as the main plot; this difference oscillates with a period approximately given by $\tau_{osc} \approx 0.0859\tau_B \approx 41.8 \mu s$.

Fig. 3.5. The second case is shown in Fig. 3.7 where, instead of changing $\hat{F}$, we increase $\hat{V}_o$ in the parameters used for Figs. 3.4 and 3.5 so that the bands $N = 1$ and $\bar{n} = 2$ become flatter and the reduced effective mass increases. In all the cases considered so far the width of the wave packet in reciprocal space is set to $\hat{\sigma} \approx 0.3$. We can also control the decay by changing the spread of the wave packet as shown in Fig. 3.8, where we plot our results for the same original parameters used in Figs. 3.4 and 3.5 except for a much smaller width of the wave packet, $\hat{\sigma} \approx 0.006$. Note that in this case, instead of a decay of the oscillations after half a Bloch period, there is a slight increase of the amplitude of the oscillations due to the higher sensitivity of the wave packet to the changes of the momentum matrix elements and the energy differences at the center of the wave packet as it moves through the Brillouin zone. Such a small width in reciprocal space can be achieved experimentally in Bose-Einstein condensates of sodium atoms [147].

The parameters $\hat{F}$ and $\hat{V}_o$ also control the amplitude of the dynamical oscillations of
Figure 3.8: Expectation value of the velocity for the same wave packet described in Fig. 3.5 with the same applied force but with a smaller width in reciprocal space, $\sigma \approx 0.006k_R = 0.003K$, calculated from the semianalytical approximation (red solid line), the full numerical solution (green crosses), and the usual group velocity (blue dotted line). The inset shows the difference between the semianalytical approximation and the usual group velocity prediction with the same units as the main plot.

From expression Eq. (3.33) it is clear that the amplitude of the oscillations scales linearly with $\hat{F}$ (compare Figs. 3.5 and 3.6). In the range of $\hat{V}_o$ values explored here (from $\hat{V}_o = 7$ to $\hat{V}_o = 14$), the effect of modifying $\hat{V}_o$ on the amplitude of the oscillations is much smaller than the effect of $\hat{F}$ (compare Figs. 3.5-3.7). Thus, in an experimental setting, the oscillations can be made more visible by increasing the force within the limits where Zener tunneling is not significant.

The velocity deviations tend to be larger for lighter atoms and smaller lattice constants, since the recoil velocity is larger. For instance, the expectation value of the velocity calculated for sodium atoms in an optical lattice with $a = 295$ nm for the same $\hat{V}_o$, $\hat{\sigma}$, and $\hat{F}$ as in Fig. 3.5 is a simple rescaled version of the results in that figure according to the new recoil velocity of the system ($v_R \approx 29.4$ mm/s). Some other examples of calculations for sodium atoms are shown in Figs. 3.9 and 3.10 with parameters previously used in experiments that investigate the acceleration of Bose Einstein condensates.
Figure 3.9: Expectation value of the velocity of a wave packet ($\sigma \approx 0.01k_R = 0.005K$) initially centered at $k = 0$ in the band $N = 2$ for a sodium atom in an optical lattice with $V_0 = 13E_R$ and $a = 295$ nm, calculated from the semianalytical approximation (red solid line), the full numerical solution (green dashed line), and the usual group velocity (blue dotted line). The applied force is such that $F/m = 800$ m/s$^2$, which corresponds to $\tilde{F} \approx 0.173$. Parameters are as in [60]. The inset shows the difference between the semianalytical approximation and the usual group velocity prediction with the same units as the main plot. The oscillations shown in the inset start with a period approximately given by $\tau_{osc} \approx 0.176\tau_B \approx 12.9\ \mu s$; then they squeeze as the wave packet moves through the edge of the Brillouin zone (where the gap between bands $N = 2$ and $n = 3$ increases); and finally they return to the starting period.

[58, 60]. The detection of the oscillations shown here implies resolving deviations from the usual Bloch oscillation that are small compared to the recoil velocity and probably within the uncertainty in the measurements in those references.\textsuperscript{5}

Fig. 3.9 illustrates the case where the initial band is $N = 2$ instead of the ground-state band used in all the other examples for ultracold atoms. An important difference with respect to the case with $N = 1$ is the increase of the amplitude of the oscillations. Compare, for instance, the insets of Figs. 3.7 and 3.9 in terms of the scaled velocity

\textsuperscript{5}The predicted oscillations are even smaller for other experiments with rubidium atoms such as the ones in [13, 14].
Figure 3.10: Expectation value of the velocity of a wave packet \( \langle \hat{v}(t) \rangle \) initially centered at \( k = 0 \) in the band \( N = 1 \) for a sodium atom in an optical lattice with \( V_o = 14E_R \) and \( a = 295 \) nm, calculated from the semianalytical approximation (red solid line), the full numerical solution (green crosses), and the usual group velocity (blue dotted line). The applied force is such that \( F/m = 1700 \) m/s\(^2\), which corresponds to \( F \approx 0.369 \). Parameters are as in [58]. The inset shows the difference between the semianalytical approximation and the usual group velocity prediction with the same units as the main plot.

\( \langle \hat{v}(t) \rangle \). Although Fig. 3.7 corresponds to rubidium atoms, in scaled units it is equivalent to a plot for sodium atoms with the same \( \tilde{V}_o = 13 \) and \( \tilde{F} \approx 0.173 \) as in Fig. 3.9 but with \( N = 1 \) and \( \tilde{\sigma} \approx 0.3 \). One of the reasons for this increase is the smaller energy gap \( \tilde{E}_{32}(0) \) compared to \( \tilde{E}_{21}(0) \). Both figures predict almost no decay, but the reasons are different. For the situation in Fig. 3.7 the cause is the small curvature of the band \( N = 1 \), which increases the reduced effective mass associated with \( N = 1 \) and \( \bar{n} = 2 \), compared, for example, with the case shown in Fig. 3.5. In Fig. 3.9, on the other hand, the cause is the small spread in reciprocal space and not the curvature of the bands; in fact, the larger magnitudes of the curvatures of \( N = 2 \) and \( \bar{n} = 3 \) make the absolute value of the reduced effective mass associated with them smaller, and therefore the decay would be faster if the spread \( \tilde{\sigma} \) were the same as for Fig. 3.7.

The last example, shown in Fig. 3.10, corresponds to a situation where the wave packet
is again in the lowest band \((N = 1)\) but under a force \(\hat{F} \approx 0.369\), which is approximately two times larger than the one used in Fig. 3.9; the strength of the potential is \(\hat{V}_o = 14\). Accordingly, the amplitude of the dynamical oscillations of \(\langle \hat{v}(t) \rangle\) is approximately doubled compared to the case shown in Figs. 3.7 and 3.8. The first order approximation still works very well due to the large gap between the bands \(N = 1\) and \(\bar{n} = 2\) for \(\hat{V}_o = 14\), as can be seen from the comparison with the full numerical solution. In Fig. 3.9 using \(\hat{V}_o = 13\) is not enough to prevent deviations with respect to the full numerical solution because the gap between the bands \(N = 2\) and \(\bar{n} = 3\) at \(k = 0\) is smaller than the energy difference between bands \(N = 1\) and \(\bar{n} = 2\).

The validity of the first order approximations in Eqs. (3.8) and (3.9) relies on the population

\[
\mathcal{N}_n \equiv \int_{\text{BZ}} dk |c_n(k, t)|^2
\]  

(3.36)

in the bands \(n \neq N\) being small because there is no population of these bands to first order in \(\Delta_{nN}(k)\) according to Eq. (2.77). In all the examples shown here, the probabilities in the bands \(n \neq N\) do not exceed 2\%, justifying the good agreement in most of the cases. In Figs. 3.11 and 3.12 we show the population of various bands as they change in time for the cases presented in Figs. 3.6 and 3.9, where the largest deviations of the semianalytical approximation with respect to the full numerical solution occur. Note that in Fig. 3.11 the population of the band \(\bar{n} = 2\) is distinctively larger than the other neighboring bands, \(n \geq 3\); therefore, the incorrect prediction of the amplitude of the oscillations from the semianalytical approximation in Fig. 3.6 is essentially due to the population of band \(\bar{n} = 2\), which is also the band that contributes more significantly to the dynamical oscillations in Eq. (3.33). A different situation is shown in Fig. 3.9, where the full numerical solution clearly shows a superposition of faster oscillations near the end of the Bloch period not predicted by the semianalytical approximation. Such faster oscillations suggest that the population of the neighboring bands \(n = 1\) and \(n \geq 4\) have a significant contribution in addition to the effect of the population of \(\bar{n} = 3\), which is the
Figure 3.11: Probability of the rubidium atoms in the optical lattice described in Fig. 3.6 to be in (a) the main band $N = 1$ (red solid line) and (b) the next two neighboring bands: $\bar{n} = 2$ (green dashed line) and $n = 3$ (blue dotted line). All the populations were calculated using the full numerical solution. The probabilities for $n > 3$ are significantly smaller than the populations shown here.

nearest neighbor to the main band $N = 2$ for most of the Brillouin zone. Accordingly, the probability in Fig. 3.12 for the band $n = 4$ ($\lesssim 0.30\%$) is larger than the probability in Fig. 3.11 for the band $n = 3$ ($\lesssim 0.07\%$).

### 3.4 Conclusion

In this chapter we have shown a first set of examples that illustrate the dynamical corrections to the effective mass theorem discussed in Chapter 2. When a uniform force is suddenly applied, the expectation value of the acceleration for a wave packet prepared initially in one band follows the response according to the bare mass at very early times; later on, the acceleration oscillates about the value predicted by the effective mass theorem. In general, the oscillatory behavior due to the sudden turn-on also implies corrections to the anomalous transport, but in this chapter we only considered the one-dimensional case where no contribution from anomalous transport arises, and so all the
Figure 3.12: Probability of the sodium atoms in the optical lattice described in Fig. 3.9 to be in
(a) the main band $N = 2$ (dashed green line) and (b) the next three neighboring bands: $n = 1$
(red solid line) and $n = 3$ (blue dotted line), and $n = 4$ (light blue slash-dotted line). All the
populations were calculated using the full numerical solution. The probabilities for $n > 4$ are
significantly smaller than the populations shown here.

dynamical corrections can be associated with the group velocity and the inverse effective
mass.

We used the semianalytical expressions for the velocity and acceleration derived in
Chapter 2 based on Wannier’s decoupling procedure [39, 43]. The results from this
approximation were compared with full numerical calculations, showing excellent agreement
over times of the order of a Bloch period, provided that Zener tunneling is not significant.
In the semianalytical approach, the wave packet responds with the usual inverse effective
mass when it has acquired certain small components of Bloch functions from bands
close to the main band where most of the wave packet is. Due to the initial condition,
which requires the wave packet to be strictly in one band at the initial time and respond
with the bare mass (see Sec. 2.3), the expectation value of the acceleration (3.13) has
various terms oscillating about the usual inverse effective mass prediction with different
frequencies. For the cases considered in this chapter, the most important contribution in
the sum over the different bands in Eq. (3.13) comes from the closest band to the main
one; accordingly, the frequency of the oscillations is governed by the energy difference between these two bands as the wave packet moves through the Brillouin zone. The oscillations can decay because of the width of the wave packet in reciprocal space, but the periodicity of the matrix elements and angular frequencies in Eq. (3.17) produces revivals of the oscillations as the wave packet completes a full Bloch oscillation.

We analyzed the one-dimensional case in the context of experiments with ultracold atoms in optical lattices, comparing it with a toy model for a one-dimensional semiconductor. In the semiconductor case we found the initial decay to occur in a few femtoseconds; during this time the wave packet moves over a small portion of the Brillouin zone, allowing us to write a simple expression for the envelope function that controls the decay of the oscillations in agreement with the features first described by Pfirsch and Spenke [48]. In the examples with ultracold atoms, where the time scales of the oscillations and the decay are much longer (of the order of microseconds) and comparable to a Bloch period, we analyzed the effects of tuning the different parameters such as the force, the strength of the potential, the width of the wave packet in reciprocal space, the bare mass of the atom, and the lattice constant. Since it is relatively simple to measure the velocity of the atoms in experiments of this type, we plotted the expectation value of the velocity, showing that the deviations from the usual group velocity prediction can be comparable to the Bloch oscillations calculated from the group velocity alone. Experiments in optical lattices have confirmed our predictions for the initial behavior of the expectation value of the velocity [68], but they have left open the study of the dynamical oscillations of the effective mass for a full Bloch period. Since decoherence in optical lattices is much smaller than in typical solid-state systems, it would be possible, in principle, to observe not only the initial oscillations but also their decay and revivals during a Bloch period. As shown in some of the simulations in Sec. 3.3, the decay can be minimized or even suppressed when the revival of the dynamical oscillations of the effective mass is faster than the decay due to the width of the wave packet in reciprocal space. This feature could be
exploited to determine how much decoherence occurs during a full Bloch oscillation.
Chapter 4

Dynamics of the effective mass and the anomalous velocity in two-dimensional lattices

In this chapter we continue illustrating the formalism presented in Chapter 2 with examples from optical lattices. Since the topological properties of the lattice only become important in lattices with dimensionality $\mathcal{D} \geq 2$, we consider the two-dimensional case, which fully displays the dynamics described in Chapter 2. These dynamics include the corrections to anomalous transport predicted for a wave packet from one of the original bands in the presence of a uniform force suddenly applied.

In Sec. 4.1 we describe a two-dimensional optical lattice studied earlier by Tarruell et al. [64], which will be used in our examples; we describe the properties of the potential relevant to our description of the dynamical inverse effective mass tensor and the anomalous velocity. The results from our numerical calculations are presented in Sec. 4.2. We discuss the semianalytical approximation, described in Chapter 2, and consider the dependence of the dynamics on the path followed by the wave packet in the Brillouin zone (Sec. 4.2.1); we also confirm the validity of the semianalytical results with a full nu-
Figure 4.1: Honeycomb lattice given by Eq. (4.1) for $V_X = 0.25E'_R$, $V_Y = 1.0E'_R$, $V_{\bar{X}} = 3.5E'_R$, and $\theta = 1.02\pi$. The x- and y-axes give the position, in units of the lattice constant. The color plot shows the value of the potential in units of the recoil energy $E'_R$. Two lattice vectors are also shown with black arrows.

numerical calculation and show an example where the semianalytical approximation starts to break down (Sec. 4.2.2). Finally, in Sec. 4.3 we present some conclusions.

### 4.1 Two-dimensional optical lattice

We consider the optical lattice described by Tarruell et al. [64], created by the interference of three retro-reflected laser beams, which leads to a potential

\[
V(x, y) = -\frac{V_X}{2} \cos (k'_R (x + y) + \theta) - \frac{V_X}{2} \cos (k'_R (x + y)) - \frac{V_Y}{2} \cos (k'_R (x - y)) \\
- \sqrt{V_XV_Y} \left( \cos(k'_R x) + \cos(k'_R y) \right) - \frac{1}{2} (V_{\bar{X}} + V_X + V_Y), \tag{4.1}
\]

where $V_X$, $V_Y$, and $V_{\bar{X}}$ are proportional to the intensities of each of the laser beams, and $\theta$ is controlled by a small detuning between the beams $X$ and $\bar{X}$.\(^1\) The lattice vectors in

\(^1\)The expression for the potential used here is the same as Eq. (1) in [64] after a $\pi/4$ rotation in the counterclockwise direction.
Figure 4.2: Energy spectrum of the first two bands. When $\theta = 1.02\pi$, a band gap of size $E_G = 0.042E'_R$ is opened at the two Dirac points, where the two bands meet when $\theta = \pi$.

real space are in the $\hat{x}$ and $\hat{y}$ directions and have magnitude $a = \lambda/\sqrt{2}$, where $\lambda$ is the wavelength of all three lasers (see Sec. 3.2.1 in Chapter 3); in their experiments, Tarruell et al. used $\lambda = 1064$ nm [64]. The potential resembles a “squeezed” honeycomb lattice and is shown in Fig. 4.1.

As in Sec. 3.2.1, the photon wave vector of each laser field is $k_R = 2\pi/\lambda$, but for convenience we use the wave vector $k'_R \equiv \sqrt{2}k_R$, which is the magnitude of the sum of the wave vectors associated with the laser beams X and Y, since $|k_R\hat{x} + k_R\hat{y}| = \sqrt{2}k_R$. The wave vector $k'_R$ is also the magnitude of the reciprocal lattice vectors, $K = k'_R$, which are oriented in the $\hat{x}$ and $\hat{y}$ directions. We can use $k'_R$ to define a new recoil energy,

$$E'_R \equiv \frac{(\hbar k'_R)^2}{2m} = \frac{(\hbar K)^2}{2m}, \quad (4.2)$$

and a new recoil velocity,

$$v'_R \equiv \frac{\hbar k'_R}{m} = \frac{\hbar K}{m}. \quad (4.3)$$

These definitions replace the usual recoil energy, $E_R \equiv (\hbar k_R)^2/(2m)$, and the usual recoil velocity, $v_R \equiv \hbar k_R/m$, associated with each laser field (see Eqs. (3.11) and (3.32)). In Eq. (4.1), we use values of $V_X = 0.25E'_R$, $V_Y = 1.0E'_R$, and $V_{\bar{X}} = 3.5E'_R$. 
When $\theta$ is set to $\pi$, the lattice satisfies space-inversion symmetry, and the two lowest energy bands intersect each other at two Dirac points. In this case, the local Berry curvature is zero everywhere except at the two Dirac points, where it is singular [135]. However, tuning $\theta$ to values slightly different from $\pi$ breaks space-inversion symmetry, opens up a band gap (see Fig. 4.2), and results in a more well-behaved local Berry curvature, (see Fig. 4.3). It is for this reason that we take $\theta = 1.02\pi$. Although the local Berry curvature is no longer singular, the region of significant local Berry curvature is still very localized. This allows for a great degree of control of the amount of Berry curvature “seen” by the wave packet.

For the envelope function in Eq. (2.73) we will use a Gaussian of spread $\sigma = 0.05K$,

$$f_N(k) = \frac{1}{\sigma \sqrt{\pi}} \exp \left( -\frac{(k-k_0)^2}{2\sigma^2} \right),$$

(4.4)

where $k_0$ is the mean of the envelope function (compare with Eq. (3.14) for the one-dimensional case). Initially, the wave packet is entirely in the first band, that is $N = 1$. To study the evolution of the wave packet, a force of magnitude $F = \tilde{F} k'_R E'_R$ will be applied, where $\tilde{F} = 1/2000$ is a dimensionless parameter analogous to the one introduced
Figure 4.4: Two paths $\alpha$ and $\beta$ in the first energy band ($n = 1$). The direction of the energy gradient, proportional to the local group velocity, is shown with the vector field. Both paths pass through at least one of the Dirac points, shown with black dots. For the diagonal path $\alpha$, which is highly symmetric, the group velocity is always aligned with the path; for the horizontal path $\beta$ this is not so. Three trajectories with different starting points (indicated by black diamonds) are discussed here. In the first one, the wave packet is prepared at point $P$ and travels along $\alpha$ in the direction indicated by the arrow. In the second one, the wave packet is prepared at $Q$ and takes the same path. In the last trajectory, the wave packet starts at $R$ and travels along $\beta$. The inset magnifies the region near $P$ and $R$ to clarify the difference between the two.

in Eq. (3.30). With the application of a constant force, the wave packet travels in a straight line through the Brillouin zone. As described in Fig. 4.4, we will consider three trajectories that pass through at least one of the Dirac points, where the band gap is the smallest and local Berry curvature the strongest. This allows the wave packet to exhibit more noticeable oscillations associated with the dynamical inverse effective mass tensor and the dynamical anomalous velocity.

The results shown in Figs. 4.2-4.4 are found by numerical diagonalization of the unperturbed Hamiltonian. We combine this method with the approach described by Lax
Figure 4.5: Expectation value of the velocity from the semianalytical approximation, Eq. (4.5), without the oscillating term \( \langle v_{\text{osc}}(t) \rangle \) (dashed lines) and including it (solid lines). In this example the force points in the \((\hat{x} - \hat{y})/\sqrt{2}\) direction with \(\hat{F} = 1/2000\); the wave packet moves through the Brillouin zone starting at point \(\mathbf{P}\) and following path \(\alpha\) (see Fig. 4.4). The red curves correspond to \(\langle v_{\parallel}(t) \rangle\), the component of the velocity parallel to the force, while the green curves correspond to \(\langle v_{\perp}(t) \rangle\), the component of the velocity perpendicular to the force \(((\hat{x} + \hat{y})/\sqrt{2}\) direction). Note that \(\langle v_{\parallel}(t) \rangle\) and \(\langle v_{\perp}(t) \rangle\) only contribute to the parallel and perpendicular directions, respectively. [(a) and (b)] Results over one Bloch period, \(\tau_B = hK/F\). [(c) and (d)] Initial behavior of the velocity, showing the oscillations due to \(\langle v_{\text{osc}}(t) \rangle\).
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[131] to construct Berry connections and Bloch functions periodic in $k$, which are used for the semianalytical approximation discussed in the next section.

4.2 Results and discussion

Following the same approach as in Chapter 3, we calculate the expectation value of the velocity for the wave packet described in the previous section using the semianalytical approximation from Chapter 2, and we confirm our results with full numerical calculations similar to the ones described in Sec. 3.2.3. For convenience, we present first the semianalytical results in Sec. 4.2.1, without the corresponding results from the full numerical calculation; the purpose is to show more clearly the contributions associated with the group velocity and the anomalous velocity. We leave the comparison with the full numerical calculations to Sec. 4.2.2.

4.2.1 Semianalytical approximation

It is natural to decompose the full expression for the expectation value of the velocity of the wave packet in the same manner as Eq. (2.80),

$$\langle \hat{v}(t) \rangle \approx \langle v^g(t) \rangle + \langle v^{an}(t) \rangle + \langle v^{osc}(t) \rangle,$$

(4.5)

where each of the three terms is an integration of $v^g_N(k)$, $v^{an}_N(k)$, and $v^{osc}_N(k,t)$ over the wave packet, respectively. In our first example, we start with a wave packet at point P and a force in the direction of path $\alpha$ (see Fig. 4.4). The decomposition above is shown in Fig. 4.5. The dashed line corresponds to $\langle v^g(t) \rangle + \langle v^{an}(t) \rangle$, where both the group velocity and the anomalous velocity are taken into account. The solid line gives the full expression for $\langle v(t) \rangle$, with the oscillation term included. As expected from the discussion in Sec. 2.6, at $t = 0$ the full expression for the velocity coincides with the prediction by just the group velocity. For $t > 0$, the velocity oscillates about the sum of the group and
anomalous velocities. These oscillations decay within a tenth of the Bloch period, but they reappear near the end of the Bloch oscillation.

Because of the high symmetry of path $\alpha$, the group velocity in this example is directed entirely along the direction of the force. This offers the closest analogy to a one-dimensional lattice (see Chapter 3). To further explore this analogy, we decompose the dynamical oscillation term $\langle v_{osc}^\alpha(t) \rangle$ in components parallel and orthogonal to the applied force ($\langle v_{||}^\alpha(t) \rangle$ and $\langle v_{\perp}^\alpha(t) \rangle$, respectively), and we identify the contributions from the dynamical group velocity, $V_N^{g}(t)$, and the dynamical anomalous velocity, $V_N^{an}(t)$ (see Eqs. (2.93) and (2.94)); this decomposition is shown in Fig. 4.6.

The local anomalous velocity is derived from the cross product of the local Berry curvature with the force, and therefore it is orthogonal to the force; similarly, the oscillating term associated with the anomalous velocity is also perpendicular to the force.
Figure 4.7: Expectation value of the velocity from the semianalytical approximation for the same parameters used in Fig. 4.5, but using $\mathbf{Q}$ as the starting point for the wave packet (see Fig. 4.4); the red (green) curves correspond the parallel (perpendicular) components of the velocity.

Thus, all of the contribution to the parallel component of the dynamical oscillation of the velocity comes from oscillations of the group velocity. Interestingly, the converse is not true. Even though for this trajectory the group velocity is strictly parallel to the force, and so the acceleration predicted simply by the inverse effective mass tensor would be in that direction, the dynamical oscillation associated with the group velocity is not confined to this direction for $t > 0$. In fact, the dynamical oscillations in both $\mathbf{V}^g(t)$ and $\mathbf{V}^{an}(t)$ contribute in the direction orthogonal to the force (see Fig. 4.6b). Hence, even for highly symmetric paths there can be oscillations of the velocity perpendicular to the force that are associated with the group velocity, and so the strict analogy to motion in a one-dimensional lattice breaks down.

Both the group velocity and the anomalous velocity are periodic because they depend only on properties of the band structure, which is periodic. However, the last term of Eq. (4.5), associated with $\mathbf{V}^{an}_N(\mathbf{k}, t)$, is also dependent on the dynamics of the wave packet itself. As such, the full expression for velocity does not exhibit periodicity. This dependence on the dynamics of the wave packet is even more evident when we change the starting point of the trajectory; for example, in Fig. 4.7 we choose $\mathbf{Q}$ as the starting point but we keep the force in the same direction so that the wave packet moves along the path $\alpha$ (see Fig. 4.4). In this case the wave packet “experiences” the least amount of
Figure 4.8: Expectation value of the velocity from the semianalytical approximation, Eq. (4.5), without the oscillating term $\langle v_{\text{osc}}(t) \rangle$ (dashed lines) and including it (solid lines). In this example the force points in the $\hat{x}$ direction with $F = 1/2000$; the wave packet moves through the Brillouin zone starting at point $R$ and following path $\beta$ (see Fig. 4.4). The red curves correspond to $\langle v_{\parallel}(t) \rangle$, the component of the velocity parallel to the force, while the green curves correspond to $\langle v_{\perp}(t) \rangle$, the component of the velocity perpendicular to the force ($\hat{y}$ direction). For reference, the component of the group velocity perpendicular to the force is plotted with dotted green lines. (a) Results over one Bloch period, $\tau_B = \sqrt{2}\hbar K/F$. [(b) and (c)] Initial behavior of the velocity, showing the oscillations due to $\langle v_{\text{osc}}(t) \rangle$.

Berry curvature at the beginning (see Figs. 4.3 and 4.7). As expected, we see that the group and anomalous velocities are shifted due to the new starting point; the dynamical oscillations in $V^g(t)$ and $V^{an}(t)$, on the other hand, have virtually vanished. From this observation, we conclude that the dynamical oscillations depend on the starting point of the wave packet, even when following the same path.

For the last example of this subsection, shown in Figs. 4.8 and 4.9, we present a more general path without the symmetries of path $\alpha$. Starting at the point $R$, we direct the force parallel to path $\beta$ (see Fig. 4.4). Unlike in path $\alpha$, here the group velocity does not
point exclusively along the direction of the force. The initial behavior shown in Fig. 4.8 is similar to what was seen in the first example. The velocity starts at the group velocity (dashed line for $\langle v_\parallel(t) \rangle$ and dotted line for $\langle v_\perp(t) \rangle$) and oscillates about the combination of the group and anomalous velocities (dashed lines). Despite not being strictly periodic, the dynamical oscillations of the velocity of the wave packet in path $\alpha$ were repetitive, at least qualitatively; we observed dynamical oscillations of similar amplitude and frequency at the start and the end of the Bloch oscillation. This is no longer true in the present example. After the initial dynamical oscillations of the velocity, no more revivals are seen near the end of the first Bloch oscillation; even during the second Bloch period, the dynamical oscillations are completely absent (see Fig. 4.11). This lack of revivals can be described as a form of dephasing. The tensor $J_{abN}(k, t)$, responsible for the oscillations, contains a phase $\gamma_{nN}(k, t)$ (see Eq. (2.83)). This tensor is integrated over the wave packet as it moves through the Brillouin zone. In general, the phase in $J_{abN}(k, t)$ accumulated by each $k$-component of the wave packet can be different even after a full Bloch period and we expect to observe dephasing. For the central path $\alpha$, however, the $k$-components of the wave packet trace pairs of parallel paths that are reflections of each other along the diagonal and acquire the same phase; therefore, with respect to the dephasing, the motion for path $\alpha$ is essentially as in the one-dimensional case, where revivals are observed (see discussion about Eq. (3.31) in Chapter 3). This kind of symmetry is not seen for a wave packet moving along a central path $\beta$, which explains why the oscillations decay in this case.

### 4.2.2 Comparison with full numerical solution

In order to verify the validity of the semianalytical results presented in Sec. 4.2.1, we compare them with full numerical solutions of the time-dependent Schrödinger equation for the Hamiltonian Eq. (2.1) in the two-dimensional case, with a force suddenly applied at $t = 0$ and left constant afterwards. The approximate expression for the wave packet
Figure 4.9: Decomposition of the oscillating term \( \langle \mathbf{v}^{\text{osc}}(t) \rangle \) (solid lines) in its group velocity and anomalous velocity contributions, for the example shown in Fig. 4.8; the red (green) curves correspond the parallel (perpendicular) components of the velocity. In the direction parallel to the force (panel (a)), only the dynamical oscillations from \( \mathbf{V}^g_N(t) \) contribute. However, in the perpendicular direction (panel (b)), both the dynamical oscillations from \( \mathbf{V}^g_N(t) \) (dotted line) and the dynamical oscillations from \( \mathbf{V}^\text{an}_N(t) \) (dashed line) contribute; in contrast to the behavior in Fig. 4.6, the two types of oscillations have similar contributions to \( \langle \mathbf{v}^{\text{osc}}(t) \rangle \).

velocity, Eq. (2.80), is expected to be accurate for forces such that \( \Delta_{nN}(k) \), defined in Eq. (2.55), is small [39, 43]; roughly, this requirement means that the energy drop over one unit cell associated with the force should be small compared with the energy gap between the starting band \( N \) and its closest neighboring band (see Appendix A). As in Chapter 3, we use the split-step operator method for the full numerical calculation [129].

For the required Fast Fourier Transform, we used the library FFTW3,\(^2\) which provides an efficient implementation that can run in parallel [148].

In Figs. 4.10 and 4.11 we compare the expectation value of the velocity for paths \( \alpha \) and \( \beta \) in the Brillouin zone presented in Figs. 4.5 and 4.8 with full numerical calculations over

\(^2\)For documentation see: http://www.fftw.org/.
Figure 4.10: Comparison between the expectation value of the velocity shown in Fig. 4.5 for path $\alpha$ in the Brillouin zone (solid lines) and a full numerical calculation (dots and crosses). The red lines and black dots correspond to the components of the velocity parallel to the force; the green lines and black crosses correspond to the components of the velocity perpendicular to the force. [(a) and (b)] Results over two Bloch periods. [(c) and (d)] Initial behavior of the velocity, showing the oscillations due to $\langle v_{\text{osc}}(t) \rangle$ (see Eq. (4.5)).
Figure 4.11: Comparison between the expectation value of the velocity shown in Fig. 4.8 for path $\beta$ in the Brillouin zone (solid lines) and a full numerical calculation (dots and crosses). The red lines and black dots correspond to the components of the velocity parallel to the force; the green lines and black crosses correspond to the components of the velocity perpendicular to the force. (a) Results over two Bloch periods. [(b) and (c)] Initial behavior of the velocity, showing the oscillations due to $\langle v_{\text{osc}}(t) \rangle$ (see Eq. (4.5)).

two Bloch periods. Note the excellent agreement between the two approaches, over short and long time scales. The force used in these examples is small enough to guarantee that the semianalytical expression Eq. (2.80) predicts correctly the oscillations associated with the dynamics of the effective mass and anomalous transport. Furthermore, the presence of revivals for path $\alpha$ (see Fig. 4.10) and their absence for path $\beta$ (see Fig. 4.11) are confirmed by the full numerical calculation.

We can also illustrate the evolution of the wave packet in real space using the results from the time propagation with the split-step operator method. In Fig. 4.12 we show snapshots of the wave packet in the two situations considered in Figs. 4.10 and 4.11, for different times within one Bloch period. In both cases the initial wave packets are the same, but in time the trajectory (dashed line in Fig. 4.12) and dispersion of the
wave packets evolve differently. Due to the symmetry of path $\alpha$ (see Fig. 4.4), the group velocity is always parallel or antiparallel to the force, resulting in an oscillation along that direction (see Figs. 4.12a-e). On the other hand, for path $\beta$, the wave packet traces a more complicated trajectory in real space, and it does not return to its starting point (see Figs. 4.12f-j). The anomalous velocity and the dynamical corrections modify the real space trajectories described by the group velocity alone, but this change is small compared with the scale of the trajectories shown in Fig. 4.12 over one Bloch period. With respect to the dispersion of the wave packet, the spread is more pronounced for path $\beta$ than path $\alpha$ (compare Figs. 4.12c and Fig. 4.12h), and the shape of the wave packet remains more symmetric around its center for path $\alpha$ (compare Figs. 4.12c-e and Figs. 4.12h-j).

The ultimate breakdown of the semianalytical expression Eq. (2.80) is associated with Zener tunneling, the probability of which increases for larger forces. Wannier’s method of decoupling the bands in the presence of an applied force [43] cannot describe Zener tunneling even if higher orders of his power expansion are considered [9]. Accordingly, the picture presented in Chapter 2 is only valid for wave packets mainly in one band with small amplitudes over neighboring bands, which is the typical requirement in the semiclassical description of transport. The start of the breakdown of the semianalytical approximation is shown in Fig. 4.13 for path $\alpha$ (see Fig. 4.4) and a force twice as large as the one used so far. In this case the most significant difference between the semianalytical approximation and the full numerical calculation appears in the component of the velocity parallel to the force, as the semianalytical result overestimates the amplitude of the Bloch oscillation of the usual group velocity. This deviation occurs early in the evolution of the expectation value of the velocity, since the starting point of the trajectory in the Brillouin zone is near one of the Dirac points, where the first two bands are close and Zener tunneling is more probable. Nevertheless, note that Eq. (2.80) is still a good approximation, as it agrees at least qualitatively with the full numerical calculation.
Figure 4.12: Time evolution of the absolute value of the wave packet in real space calculated using the split-step operator method for [(a)-(e)] path \( \alpha \) and [(f)-(j)] path \( \beta \) in the Brillouin zone. The parameters are the same as the ones used in Figs. 4.10 and 4.11. The black dots mark the expectation value of the position for the snapshot time, and the dashed line shows the trajectory starting at \( t = 0 \). The horizontal and vertical axes show position in units of the lattice constant; the color scale, from blue to red, indicates increasing absolute value of the amplitude of the wave function.
Figure 4.13: Comparison between the semianalytical approximation (solid lines) and the full numerical calculation (dots and crosses) for the same parameters as in Fig. 4.5 but doubling the force ($\vec{F} = 1/1000$). The red lines and black dots correspond to the components of the velocity parallel to the force; the green lines and black crosses correspond to the components of the velocity perpendicular to the force. [(a) and (b)] Results over two Bloch periods. [(c) and (d)] Initial behavior of the velocity, showing the oscillations due to $\langle v^{\text{osc}}(t) \rangle$ (see Eq. (4.5)).
In the semianalytical approximation the wave packet $|\Psi(t)\rangle$ is a superposition of a main MBS wave packet associated with band $N$ and MBS wave packets with smaller amplitudes associated with neighboring bands, $n \neq N$ (see Eq. (2.75)). This suggests that the initial wave packet in real space will split into a main wave packet associated with band $N$ and small ones associated with $n \neq N$; these wave packets will move differently according to the properties of the band to which they correspond. The presence of this splitting is confirmed by the full numerical calculation, as illustrated in Fig. 4.14 for the parameters used in Fig. 4.13. The snapshots in Fig. 4.14 show a main wave packet associated with band $N = 1$ and a small wave packet associated with the next band, $n = 2$, which moves in the opposite direction to the main wave packet.

Even though the semianalytical approximation predicts the splitting of the initial wave packet, it cannot describe correctly the amplitude and shape of the small wave packet for strong forces, such as the one used in Fig. 4.14. The failure of the semianalytical approach in this example is shown in Fig. 4.15, where we compare the wave packets calculated using this approximation and the results from the full numerical calculation. Note that the main wave packet is essentially the same in the two approaches (compare Figs. 4.15a and b), but the semianalytical result predicts a small wave packet with a different shape and underestimates its amplitude (compare Figs. 4.15c and d). Consequently, the expectation value of the position differs in the two calculations as can be seen in Figs. 4.14 and 4.15, where the expectation value of the position calculated with the semianalytical approximation (red dots) is shifted in the direction of the small wave packet for the full numerical calculation (black dots). The incorrect description of the small wave packet by the semianalytical approximation is responsible for the overestimation of the group velocity calculated with this method in Fig. 4.13. As the applied force is increased, Zener tunneling becomes more important and the amplitudes of the wave packets associated with the neighboring bands, $n \neq N$, increase; consequently, the weight of these amplitudes modifies more significantly the expectation values of position.
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Figure 4.14: Snapshots of the absolute value of the wave packet for the parameters used in Fig. 4.13 calculated from the time evolution using the split-step operator method. At $t = 0.1\tau_B$ a wavelet starts to form, and afterwards it moves towards the lower right corner of the real space window. The black and red dots mark the expectation value of the position for the snapshot time, calculated from the full numerical and semianalytical calculations, respectively. In (b-d) the smaller frames show the absolute value of the wave packet amplified ten times. The horizontal and vertical axes show position in units of the lattice constant; the color scale, from blue to red, indicates increasing absolute value of the amplitude of the wave function.
Figure 4.15: Detailed view of the wave packet shown in Fig. 4.14c. The black and red dots (and the dashed lines) mark the expectation value of the position calculated from the full numerical and semianalytical calculations, respectively. The horizontal and vertical axes show position in units of the lattice constant; the color scale, from blue to red, indicates increasing absolute value of the amplitude of the wave function. [(a) and (b)] Main wave packet from the full numerical and semianalytical calculations, respectively. [(c) and (d)] Small wave packet from the full numerical and semianalytical calculations, respectively.

and velocity predicted by the main wave packet alone. Since the semianalytical approximation cannot predict correctly the contribution of these wave packets, the dynamics calculated with this approach become less accurate.

4.3 Conclusion

In this chapter we have shown a second set of examples that illustrate the dynamics of a wave packet in a periodic potential prepared in one band and subject to the sudden application of a uniform force, which remains constant afterwards. We considered a two-
dimensional optical lattice [64] where the full dynamics described in Chapter 2 could be potentially observed.

In the two-dimensional case discussed in this chapter, we replace the scalar inverse effective mass used in Chapter 3 by a tensor, and it is necessary to include the anomalous velocity. These quantities fully describe the dynamics if the force is applied slowly so that the wave packet has time to respond according to the properties of the lattice. In contrast, when the force is suddenly applied, the proper description of the motion of the wave packet requires dynamical quantities associated with the inverse effective mass tensor (see Eq. (2.99)) and the anomalous velocity (see Eq. (2.95)). These quantities initially take the values that would characterize a free particle; at later times, they oscillate about the usual expressions for these quantities as the wave packet moves through the Brillouin zone. In this chapter we considered the total velocity of the wave packet (see Eq. (2.92)), which includes a dynamical group velocity, associated with the dynamical inverse effective mass tensor, and the aforementioned dynamical anomalous velocity. Even for cases when the usual inverse effective mass tensor predicts an acceleration parallel to the applied force (for example, in the path \( \alpha \) shown in Fig. 4.4), the dynamical inverse effective mass tensor allows for oscillations of the velocity parallel and perpendicular to the force (see Fig. 4.6). In addition to the acceleration described by the dynamical inverse effective mass tensor, there is a dynamical anomalous acceleration associated with the dynamical anomalous velocity (see Eq. (2.101)); both dynamical anomalous quantities are always perpendicular to the applied force.

Besides exhibiting aspects of wave packet motion involving the topology of the bands, which do not arise in one-dimensional lattices, the wave packet motion in the two-dimensional lattice shows interesting features in the interplay between the Bloch oscillations and the dynamics of the group and anomalous velocities. In Chapter 3 we showed that the initial dynamical oscillations have revivals after a Bloch period as a result of the cyclic path of the wave packet in the Brillouin zone. In the two-dimensional
lattice considered here, we showed that not every cyclic path in the Brillouin zone leads to revivals after one Bloch period (see Fig. 4.11); these revivals only occur for paths where the symmetry of the band structure allows each $k$-component of the wave packet to accumulate similar phases over a Bloch period (see Fig. 4.10). This behavior shows that while the group velocity and the Berry curvature “seen” by the wave packet have a periodicity given by the Bloch period, the dynamical oscillations discussed here do not display such periodicity. Revivals are still possible in the two-dimensional lattice for some paths, but the dynamical oscillations are still not periodic over one Bloch period. Furthermore, these oscillations depend on the starting location on the chosen path in the Brillouin zone (compare Figs. 4.5 and 4.7).

Following the same approach as in Chapter 3, the results from the semianalytical approximation were confirmed by a full numerical solution of the dynamics of the wave packet. The agreement breaks down for strong forces, due to the limitations of the modified Bloch states to decouple completely the bands in the presence of an applied force [9]. In real space the wave packet splits into a main wave packet, associated with the original initial band, and a small wave packet, associated with the next neighboring band (see Fig. 4.14); the semianalytical approximation fails to capture correctly the amplitude and shape of the small wave packet, affecting the expectation values of position and velocity calculated with this method (see Fig. 4.15). However, since the main wave packet is well described by the semianalytical approximation, we find that even for a strong force the prediction of the dynamical oscillations given by this approximation is at least qualitatively correct (see Fig. 4.13).

Two-dimensional optical lattices are readily available, suggesting that the dynamics described here can be observed experimentally in this type of system, similarly to the one-dimensional case presented in [68]. For the application of a force to be “sudden” requires in practice that the time scale for its appearance is short compared to the time associated with the energy difference between the band where the wave packet is
prepared and the nearest neighboring band. In solid-state systems the time scales and the difficulties in controlling the properties of the lattice have prohibited the observation of the dynamical inverse effective mass tensor, even though some deviations from the usual effective mass behavior have been attributed to its dynamical oscillations [74]; nonetheless, attosecond science is pushing the time scales on which carrier dynamics in solids can be observed to the sub-femtosecond regime [71, 73, 75]. We believe that these developments, combined with the growing interest in topological properties of periodic potentials and their dynamical consequences [7, 137, 149, 150], make the oscillations discussed here an interesting phenomenon to be studied experimentally both in optical lattices and in solid-state systems.
Chapter 5

The excitonic Franz-Keldysh effect

A complete description of the Franz-Keldysh effect requires considering both interband coupling and electron-hole interaction. Earlier independent particle calculations show the importance of the interband coupling due to the applied dc field in the context of $\mathbf{k} \cdot \mathbf{p}$ models used to describe the Franz-Keldysh effect [93]. In addition, simple calculations with a parabolic two-band model predict that the excitonic effects due to the electron-hole interaction enhance considerably the absorption spectrum with and without an applied electric field [2]. Motivated by developments in experiments for studying the Franz-Keldysh effect in levels of detail that were not possible before [115, 117, 118], we present a framework that combines interband coupling and excitonic effects, and can be applied to realistic band models.

We illustrate our approach with a 14-band $\mathbf{k} \cdot \mathbf{p}$ model for bulk GaAs, which describes realistically many important features of this material such as spin-splitting and band-warping. We also test our approach with a simpler parabolic two-band model in the effective mass approximation. For the excitonic effects we include the Coulomb interaction through the exchange contribution of the Hartree-Fock self-energy [2]. The calculation is divided in two steps. First, we consider the time evolution of the interband polarization of the crystal excited by an optical pulse in the presence of an applied dc
field; the interband coupling induced by the dc field is treated non-perturbatively, but
Zener tunneling is neglected. In the next step we find the frequency response of the sys-
tem from the interband polarization in the time domain, and we calculate the absorption
coefficient in the linear response regime.

We observe that the expected enhancement of the optical absorption due to the
Coulomb interaction is qualitatively the same in the two-band and 14-band models. The
various features of the absorption coefficient captured by the 14-band model at the in-
dependent particle level are preserved and enhanced in the presence of the Coulomb
interaction. Some of these features can be used to explore the dependence of the ab-
sorption coefficient on the optical polarization [91, 93, 113]. We find that the Coulomb
interaction modifies significantly the polarization anisotropy predicted by calculations at
the independent particle level, especially for energies near the split-off valence band to
conduction band transition.

In Sec. 5.1 we explain the main features of the Franz-Keldysh effect with a simple
qualitative discussion using the electron and hole wave functions for the “tilted bands” in
the presence of a dc electric field. For the actual calculations of the Franz-Keldysh effect,
it is necessary to go beyond that simple picture and consider the time evolution of the
interband polarization between conduction and valence bands driven by an optical pulse;
the dynamical equation that describes this evolution is presented in Sec. 5.2 starting from
the lesser Green function of the system and considering carefully the interband coupling
due to the dc field. In Sec. 5.3 we show how the interband polarization can be used
to calculate the absorption coefficient, which is a common quantity measured in Franz-
Keldysih effect experiments. In Sec. 5.4 we discuss the diverse matrix elements required
as input for the calculation in the two models mentioned before; the methods, however,
can be applied to any other type of $\mathbf{k} \cdot \mathbf{p}$ calculation. We also analyze the time evolution
of the interband polarization for pulsed optical excitation, which provides a useful insight
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into the system and the process of optical injection in the conduction bands. In Sec. 5.5 we present the results for the absorption coefficient in various cases, with and without Coulomb interaction and for different dc fields. Finally, we present some conclusions in Sec. 5.6.

5.1 A simple picture for the Franz-Keldysh effect

In the presence of a dc electric field, the absorption spectrum of bulk semiconductors develops an exponential tail below the band gap and oscillations above it. As mentioned in Sec. 1.2.2 of Chapter 1, these are the distinctive features of the Franz-Keldysh effect; we show them in Fig. 5.1a for the simplest possible calculation, using a parabolic two-band model and neglecting any electron-hole interaction.

In the absence of the dc field, the electron and hole are described by Bloch functions, which extend over the entire crystal. However, when the dc field is applied, these Bloch functions become coupled in the direction of the field, resulting in wave functions with a tail that extends into the classically-forbidden region associated with the band gap, as shown in Fig. 5.1b [91]. Away from this region and as the distance to the classical turning points becomes larger, the wave functions oscillate with an increasing frequency and decreasing amplitude; this behavior, also shown in Fig. 5.1b, is consistent with charged particles that accelerate due to the dc electric field. The shape of the electron and hole wave functions determine the behavior of the absorption coefficient, since the latter is proportional to the square of the overlap between the wave functions (for example, see [138]). The absorption below the band gap can be understood as a photon-assisted process where an electron in the valence band with energy $E_v$ tunnels into the forbidden energy gap, absorbs a photon with energy below the band gap, $h\omega < E_G$, and tunnels.

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1 A similar approach has already been used in semiconductor quantum wires; for example see [122].

2 More detailed examples using this model are discussed in Sec. 5.5; for instance, see Figs. 5.6 and 5.12.
Figure 5.1: Simple model for the Franz-Keldysh effect. (a) Absorption spectra as a function of photon energy, calculated in the independent particle approximation for a parabolic two-band model with applied dc field (solid blue line) and without (purple dashed line). (b) Schematic illustration of the electron (red) and hole (blue) wave functions; the tilted solid lines represent the conduction and valence band edges in the presence of a dc electric field. The vertical and horizontal axes represent energy and position along the direction of the dc field, respectively.
out of the forbidden energy gap into the conduction band with energy $E_c^{\text{below}}$ \cite{151}; the overlap between the tails of the electron and hole wave functions leads to absorption for photon energies below the band gap. The oscillations of the absorption coefficient for energies above the band gap, $\hbar \omega > E_G$, are a consequence of the overlap of the oscillating parts of the electron and hole wave functions with energies $E_c^{\text{above}}$ and $E_v$, respectively.

This simple picture of the Franz-Keldysh effect can be formalized by considering the wave function for the electron-hole pair in the parabolic two-band model. The slowly varying envelope of this wave function satisfies a time-independent Schrödinger equation identical to that of a charged particle in the presence of a dc field, with the reduced effective mass of the electron-hole pair (for example, see \cite{138}). The solutions to this type of equation can be expressed in terms of Airy functions \cite{140}, which have an exponentially decaying tail and oscillations of increasing frequency and decreasing amplitude. Such features are reflected in the absorption coefficient calculated from the electron-hole envelope function. Even though this approach is quite suggestive, it is restricted to the effective mass approximation; one possibility to go beyond this model for the band structure is to formulate the problem in reciprocal space, where the energy dispersion can be included in a simple way, and the tilt of the potential in real space becomes a gradient. Furthermore, such a gradient can be removed by considering the problem in the time domain, since the only the effect of the gradient is to cause a constant drift in reciprocal space, which can be easily captured in a moving frame. We will follow this approach in the next section to derive the dynamical equation satisfied by the interband polarization (essentially the electron-hole pair wave function) driven by an optical pulse.

## 5.2 Dynamical equation for the interband polarization

The goal of this section is to derive a dynamical equation for the interband polarization of a system of charges excited by an optical pulse in the presence of a crystal potential $V(\mathbf{r})$. 
and an applied dc electric field. Within the dipole approximation described in Sec. 1.1, we can use a uniform electric field, which we decompose as $E(t) = E^{dc}(t) + E^{opt}(t)$. The optical pulse, $E^{opt}(t)$, is centered at $t = 0$, and its amplitude is effectively zero outside the finite time range $[t_1, t_2]$. The dc field, $E(t)$, is turned on at some initial time $t_{init} \ll t_1$ and left constant afterwards (see Fig. 5.2).

We begin in Sec. 5.2.1 considering the lesser Green function for the system, which contains the interband polarization. Treating the optical field perturbatively in Sec. 5.2.2, we derive an equation for the interband polarization to first order in this field. The effects of the dc field are discussed in Sec. 5.2.3.

### 5.2.1 Lesser Green function

The populations and correlations necessary for studying the Franz-Keldysh effect are contained in the lesser Green function

$$\mathcal{G}^<(r_1, t_1; r_2, t_2) \equiv -\frac{1}{i\hbar} \langle \hat{\Psi}^\dagger(r_2, t_2) \hat{\Psi}(r_1, t_1) \rangle,$$  

(5.1)

where $\hat{\Psi}^\dagger(r, t)$ ($\hat{\Psi}(r, t)$) is the creation (annihilation) operator for the electron field, evolving due to the full Hamiltonian of the system in the Heisenberg picture. The angular brackets indicate the expectation value with respect to the thermal equilibrium density.
matrix that describes the system before the time-dependent perturbations are turned on [152]. For simplicity, in our calculations we assume that the system in equilibrium is described by the semiconductor vacuum with valence bands fully occupied and empty conduction bands; this is a good approximation for experiments performed at low temperatures.

The simplest approximation to include excitonic effects due to the electron-hole interaction is through the exchange contribution of the Hartree-Fock self-energy,

$$
\Sigma^{ex}(r_1, t_1; r_2, t_2) \equiv i\hbar U(r_1 - r_2)\delta(t_1 - t_2)G^<(r_1, t_1; r_2, t_2)
$$

(5.2)

where $U(r)$ is the Coulomb potential,

$$
U(r) = \frac{e^2}{\epsilon_b r}.
$$

(5.3)

This approximation, described for instance by Haug and Koch [2], leads to the predictions of bound states below the band gap and the enhancement of the absorption coefficient above the band gap in the absence of an applied dc field. We consider the screening effects at the level of the polarizability of the valence electrons and of the lattice, captured in a background dielectric constant $\epsilon_b$ (we use the value $\epsilon_b = 12.9$ for GaAs) [1, 2]; a static screening is also discussed briefly in Sec. 5.5. Within this simple treatment, it is enough to consider the density matrix of the system for calculating the interband polarization and the density of excited carriers. The density matrix is essentially Eq. (5.1) in the equal-time limit, $G^<(r_1, t; r_2, t)$, where the average time $(t_1 + t_2)/2 \to t$ and the time difference $t_1 - t_2 \to 0$.

We are interested in a situation where the only applied field is a uniform electric field $E(t)$. As discussed in Chapter 1 (Sec. 1.1), this field can be introduced in the Hamiltonian through a uniform vector potential $A(t)$ in the velocity gauge, and we can

---

3This is the usual choice for the calculation of the expectation value in non-equilibrium problems. The main assumption is that the thermodynamic degrees of freedom do not follow instantaneously the variations of the time-dependent perturbations in the Hamiltonian. Other choices are possible; for instance, see Refs. [23, 152]
use the phase transformation in Eq. (1.6) to obtain the Hamiltonian in the length gauge. Therefore, we expand $\hat{\Psi}(r, t)$ in terms of field operators $\hat{a}'_n(k, t)$ for the usual Bloch functions $\psi_{nk}(r) \equiv \langle r|\psi_{nk} \rangle$ (Eq. (2.7) from Chapter 2 with $D = 3$) modified by the appropriate phase,

$$\psi'_{nk}(r, t) \equiv \psi_{nk}(r)e^{i\frac{\mathbf{A}(t)}{\hbar}\cdot \mathbf{r}}. \quad (5.4)$$

Recall that the Bloch states $|\psi_{nk}\rangle$ are solutions of the eigenvalue problem Eq. (2.5) for the unperturbed Hamiltonian $\hat{H}_o$. In practice we use band structures that include spin-orbit coupling and in principle other relativistic corrections. For situations where only points and lines of degeneracy are present, the Bloch functions can be constructed to be periodic in reciprocal space and therefore well-defined for all $\mathbf{k}$, except for degeneracy points [26, 131]. Note that the Bloch functions $\psi'_{nk}(r, t)$ form a complete set of orthonormal states; in this representation, $G^<(r_1, t_1; r_2, t_2)$ becomes

$$G^<_{n_1n_2}(k_1, t; k_2, t) \equiv \frac{-1}{i\hbar} \langle \hat{a}'_{n_2}(k_2, t)\hat{a}'_{n_1}(k_1, t) \rangle. \quad (5.5)$$

Within our approximations, only the relative position between the electron and hole is relevant (see Appendix C); thus, we look for solutions of the form

$$G'_{n_1n_2}(k_1, t; k_2, t) = \delta(k_1 - k_2)G^<_{n_1n_2}(k_1, t). \quad (5.6)$$

The Green function $G^<_{n_1n_2}(k, t)$ can be used to calculate the density of carriers injected in the conduction bands by the optical pulse,

$$n_{\text{exc}}(t) \equiv -i\hbar \sum_c \int_{\text{BZ}} \frac{d\mathbf{k}}{(2\pi)^3} G^<_{cc}(k, t), \quad (5.7)$$

where the band index $c$ denotes only conduction bands. We now consider the time evolution of the matrix $G^<(k, t)$ labeled by the crystal wave vector $\mathbf{k}$, which is associated with the relative position of the electron-hole pair. The dynamical equation for $G^<(k, t)$ is

$$i\hbar \frac{\partial}{\partial t} G^<(k, t) + e\mathbf{E}(t) \cdot i\nabla_k G^<(k, t) - [\beta(k, t) + \Sigma(k, t), G^<(k, t)] = 0, \quad (5.8)$$
where $e = -|e|$ is the electron charge. Note that this equation is formulated in terms of the electric field $E(t)$ instead of the vector potential $A(t)$, and it is the equivalent of Eq. (1.7) for $G_{n_{1}n_{2}}^{<}(k, t)$. In Appendix C we show an alternative derivation of Eq. (5.8) from a gauge-independent formalism using a basis of Wannier functions modified by the Peierls phase [23]. The two energy terms in the commutator of Eq. (5.8) correspond to the single-particle energy, $\beta(k, t)$, and the self-energy, $\Sigma(k, t)$; at each $k$ they are matrices labeled by band indices. The former is given by

$$
\beta_{n_{1}n_{2}}(k, t) \equiv \delta_{n_{1}n_{2}} \hbar \omega_{n_{1}}(k) - eE(t) \cdot \xi_{n_{1}n_{2}}(k),
$$

with the matrix elements $\xi_{n_{1}n_{2}}(k)$ defined in Eq. (2.13). The matrix representing the exchange self-energy, Eq. (5.2), is

$$
\Sigma(k, t) = i\hbar \int \frac{dq}{(2\pi)^3} U(q) \Delta(k, k - q) G^{<}(k - q, t) \Delta^{\dagger}(k, k - q),
$$

where $U(q)$ is the Fourier transform of the Coulomb potential,

$$
U(q) = \int U(r) e^{-iqr} dr = \frac{4\pi e^2}{\epsilon_b q^2},
$$

and the overlap matrix $\Delta(k_{1}, k_{2})$ has elements [89]

$$
\Delta_{n_{1}n_{2}}(k_{1}, k_{2}) \equiv \langle u_{n_{1}k_{1}} | u_{n_{2}k_{2}} \rangle = \int_{V_{cell}} \frac{dr}{V_{cell}} u_{n_{1}k_{1}}^{*}(r) u_{n_{2}k_{2}}(r)
$$

(compare with Eq. (2.13)).

### 5.2.2 Perturbative solution in the optical field

In order to solve Eq. (5.8) for $E(t) = E^{dc}(t) + E^{opt}(t)$, we use an expansion of the lesser Green function in powers of the optical field,

$$
G^{<}(k, t) = G^{<}(0)(k, t) + G^{<}(1)(k, t) + ...
$$

Accordingly, the single-particle energy can be decomposed as $\beta(k, t) = \beta^{(0)}(k, t) + \beta^{(1)}(k, t)$, with

$$
\beta^{(0)}_{n_{1}n_{2}}(k, t) \equiv \delta_{n_{1}n_{2}} \hbar \omega_{n_{1}}(k) - eE^{dc}(t) \cdot \xi_{n_{1}n_{2}}(k)
$$
and

$$\beta_{n_1n_2}^{(1)}(k, t) \equiv -eE_{\text{opt}}(t) \cdot \xi_{n_1n_2}(k), \quad (5.15)$$

where we associate $E_{\text{opt}}(t)$ with the Maxwell field in the medium. The exchange self-energy is also expanded in powers of the optical field according to which term of Eq. (5.13) is used in Eq. (5.10). The zeroth order self-energy, $\Sigma^{(0)}(k, t)$, essentially renormalizes the band energies and matrix elements [2]. This effect can be absorbed in the band structure model, such as the $k \cdot p$ model that will be used in Sec. 5.4.2; hence, we will not include $\Sigma^{(0)}(k, t)$ explicitly.

We keep the dc field to all orders, but we neglect the coupling between conduction and valence bands due to the dc field; this is equivalent to neglecting Zener tunneling [93].

This approximation is reasonable in many cases, such as the ones discussed in Sec. 5.5 for GaAs in 44 kV/cm and 66 kV/cm dc fields, because Zener tunneling is only significant for extremely high dc fields applied to materials with small band gap [93]. Hence, we do not include the contribution of $-eE_{dc}(t) \cdot \xi_{n_1n_2}(k)$ to Eq. (5.14) when $(n_1, n_2)$ are not both conduction or both valence bands. Within this approximation, the matrix $\beta_{n_1n_2}^{(0)}(k, t)$ takes a block diagonal form with zero matrix elements between conduction and valence bands. Matrices of this form are denoted by a tilde on top; therefore, instead of the full $\beta_{n_1n_2}^{(0)}(k, t)$ we use $\tilde{\beta}_{n_1n_2}^{(0)}(k, t)$. A consequence of this approximation is that $G^{<(0)}(k, t)$ does not change in time for an initial state with valence bands fully occupied and empty.

\footnote{According to the discussion in Chapters 2-4, not all the interband coupling is associated with Zener tunneling; therefore, a more accurate calculation in this context should include part of the interband coupling between the conduction and valence bands due to the dc field. A possible strategy is to use the basis of modified Bloch states defined in Sec. 2.4. However, in the present chapter we follow the approach of Wahlstrand and Sipe [93], which is considerably simpler; in cases such as the one for GaAs presented here, the valence bands are closer in energy to each other than to the conduction bands and so it is justified to consider conduction and valence bands in separate blocks (see also [25]).}

\footnote{A simple estimate of Zener tunneling can be found in [45]. A more detailed estimate using a two-band model was derived by Kane [42]. Kane illustrated his formula for Zener tunneling with InSb in a 50 kV/cm dc field, finding a value of $1.4 \times 10^{25} \text{cm}^{-3} \text{s}^{-1}$ for the density of carriers per unit time in the conduction band due to Zener tunneling. Since GaAs has a band gap about six times larger, the tunneling probability is many orders of magnitude smaller than for InSb.}

\footnote{In this chapter we will use the bar and tilde notation in a way different from that of Chapters 2-4, where it is used to distinguish symmetric and antisymmetric tensors (see for example Eq. (2.86)).}
conduction bands. Thus, only when \( n_1 \) and \( n_2 \) are valence bands, \( G^{<\!(0)}_{n_1n_2}(k, t) \) is different from zero and it is given by

\[
G^{<\!(0)}_{n_1n_2}(k, t) = -\frac{\delta_{n_1n_2}}{i\hbar},
\]

(5.16)
even after the dc field is applied. Additionally, the first order contribution, \( G^{<\!(1)}_{n_1n_2}(k, t) \), is different from zero only after the pulse starts at \( t_1 \) and if \( n_1 \) and \( n_2 \) are not both conduction or both valence bands. Matrices of this off-diagonal block form are denoted by a bar on top; thus, we can replace \( G^{<\!(1)}(k, t) \) by \( \bar{G}^{<\!(1)}(k, t) \). Note that \( \bar{G}^{<\!(1)}(k, t) \) is essentially the interband polarization between conduction and valence bands, so we define the matrix

\[
\bar{\Pi}(k, t) = -i\hbar\bar{G}^{<\!(1)}(k, t).
\]

(5.17)

Using Eq. (5.8) we find that the time evolution of \( \bar{\Pi}_{cv}(k, t) \), the matrix element of \( \bar{\Pi}(k, t) \) associated with a conduction band \( c \) and a valence band \( v \), is governed by

\[
\begin{align*}
    i\hbar \frac{\partial}{\partial t} \bar{\Pi}_{cv}(k, t) + ieE^{dc}(t) & \frac{\partial}{\partial k_{\parallel}} \bar{\Pi}_{cv}(k, t) - \bar{\beta}^{(0)}(k, t) \bar{\Pi}(k, t) - \Sigma^{(1)}_{cv}(k, t) = \bar{\beta}^{(1)}_{cv}(k, t),
\end{align*}
\]

(5.18)

which has the same form as the usual semiconductor Bloch equations [2]. Since we only need the matrix elements of \( \beta^{(1)}(k, t) \) that couple conduction and valence bands, we use \( \bar{\beta}^{(1)}(k, t) \). In Eq. (5.18) we denote the component of \( k \) parallel to the dc field by \( k_{\parallel} \); later, we will use \( k_{\perp} \) for the perpendicular component.

5.2.3 Interband coupling due to the dc field

The matrix elements \( \xi_{n_1n_2}(k) \) for \( n_1 \neq n_2 \) are responsible for the interband coupling induced by the electric field \( E(t) \). We reformulate Eq. (5.18) so that the interband coupling due to the dc field is calculated separately from the dynamical equation for the interband polarization. In our approach we apply a unitary matrix transformation accompanied by appropriate phase factors; both are discussed in this subsection.

For the matrix transformation, recall that the off-diagonal terms of Eq. (2.13) for
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Non-degenerate bands are related to the momentum matrix elements through Eq. (2.16), which can be written as

$$\xi_{n_1n_2}(k) = \frac{v_{n_1n_2}(k)}{i\omega_{n_1n_2}(k)} \quad \text{(for } \omega_{n_1}(k) \neq \omega_{n_2}(k)),$$

(5.19)

where we introduced the velocity matrix $v(k)$ with elements $v_{n_1n_2}(k) \equiv p_{n_1n_2}(k)/m$. It is convenient to transform the $v_{n_1n_2}(k)$ according to

$$V(k) \equiv e^{i\Xi(k)}v(k)e^{-i\Xi(k)},$$

(5.20)

where

$$\Xi_{n_1n_2}(k) \equiv -\delta_{n_1n_2}\int_0^{k_{||}} \xi_{n_1n_2}(k_{\perp} + k'_{||}\hat{e}^{dc})dk'_{||}$$

(5.21)

is the phase associated with the Berry connection along the dc field direction, $\xi_{n_1n_2}(k)$. Here $\hat{e}^{dc}$ is a unit vector pointing in the same direction as the dc field. The advantage of this phase transformation will be evident when we apply it to $\Pi(k, t)$ in order to remove the explicit dependence of the interband polarization on the phase of the Bloch functions fixed by $\xi_{n_1n_2}(k)$. Now we can introduce the dipole moment matrix with elements

$$\mu_{n_1n_2}(k) \equiv \frac{eV_{n_1n_2}(k)}{i\omega_{n_1n_2}(k)} \quad \text{if } \omega_{n_1n_2}(k) \neq 0,$$

$$\equiv 0 \quad \text{otherwise.}$$

(5.22)

As usual, the block diagonal version of this matrix, without coupling between conduction and valence bands, is denoted by $\tilde{\mu}(k)$. The remaining matrix elements, which connect conduction and valence bands, are kept in the off-diagonal block matrix $\tilde{\mu}(k)$. In order to neglect Zener tunneling, we only keep the coupling due to $\tilde{\mu}(k)$ and define a block diagonal matrix $\tilde{M}(k)$ that satisfies the differential equation

$$ieE^{dc}\frac{\partial}{\partial k_{||}}\tilde{M}_{n_1n_2}(k) - \hbar\omega_{n_1n_2}(k)\tilde{M}_{n_1n_2}(k) + \sum_{n'_1} E^{dc}\tilde{\mu}_{n_1n_1'}^{dc}(k)\tilde{M}_{n'_1n_2}(k) = 0,$$

(5.23)

subject to the condition $\tilde{M}_{n_1n_2}(k_{\perp}) = \delta_{n_1n_2}$ on the plane with $k_{||} = 0$. Here $E^{dc}$ is the magnitude of the dc field once it is left constant, and $\tilde{\mu}_{n_1n_2}^{dc}(k)$ is the component of $\tilde{\mu}_{n_1n_2}(k)$ parallel to $\hat{e}^{dc}$. 
We define our transformed interband polarization according to

\[ \tilde{P}(k, t) \equiv \tilde{M}^\dagger(k) e^{i \Xi(k)} \tilde{\Pi}(k, t) e^{-i \Xi(k)} \tilde{M}(k), \]  

which combines the phase factors used previously in Eq. (5.20) and the matrix \( \tilde{M}(k) \).

Note that the time evolution of \( \tilde{P}_{cv}(k, t) \),

\[ i \hbar \frac{\partial}{\partial t} \tilde{P}_{cv}(k, t) - \hbar \omega_{cv}(k) \tilde{P}_{cv}(k, t) + i e E_{dc} \frac{\partial}{\partial k} \| \tilde{P}_{cv}(k, t) - \Sigma_{cv}^0(k, t) = -E_{opt}^\text{dc}(t) \cdot \tilde{\Theta}_{cv}(k), \]  

is independent of the Berry connection, and the interband coupling due to the dc field is implicit in the transformed dipole moment matrix

\[ \tilde{\Theta}(k) \equiv \tilde{M}^\dagger(k) \mu(k) \tilde{M}(k). \]

The Coulomb term in Eq. (5.25),

\[ \Sigma_{cv}^0(k, t) = - \int \frac{dq}{(2\pi)^3} U(q) K(k, k - q) \tilde{P}(k - q, t) K^\dagger(k, k - q), \]

has the same structure as Eq. (5.10) but involves the overlap matrix \( \Delta(k_1, k_2) \) transformed to

\[ K(k_1, k_2) \equiv \tilde{M}^\dagger(k_1) e^{i \Xi(k_1)} \Delta(k_1, k_2) e^{-i \Xi(k_2)} \tilde{M}(k_2), \]

in a generalization of the transformation indicated in Eq. (5.24).

For calculating the matrices \( V(k) \) and \( K(k_1, k_2) \) it is actually not necessary to find the Berry connections. Wahlstrand and Sipe [93] presented a procedure to construct such matrices dealing properly with lines and points of degeneracy [26]; we will apply this approach in Sec. 5.4.2.

### 5.3 Absorption coefficient

In the perturbation expansion Eq. (5.13), the diagonal elements of the second order term contain the lowest order contributions to the density of carriers excited to the conduction bands. The dynamical equation for \( G^{<2}(k, t) \) is derived in the usual way, substituting
Eq. (5.13) in Eq. (5.8) and keeping only second order terms. Then the total density of excited carriers after the pulse has excited the system, \( n_{\text{exc}} \equiv n_{\text{exc}}(t \to \infty) \), can be written as

\[
n_{\text{exc}} = \frac{1}{\hbar} \sum_{c,v} \int_{BZ} d{k} \frac{2}{(2\pi)^3} \text{Im} \left[ \int_{-\infty}^{\infty} \tilde{P}_{cv}(k, \omega) (E_{\text{opt}}(\omega) \cdot \tilde{\Theta}_{cv}(k))^* \frac{d\omega}{2\pi} \right], \tag{5.29}
\]

where

\[
\tilde{P}_{cv}(k, \omega) \equiv \int_{-\infty}^{\infty} \tilde{P}_{cv}(k, t) e^{i\omega t} \, dt \tag{5.30}
\]

is the Fourier transform of the interband polarization and BZ denotes integration over the (first) Brillouin zone. The Fourier transform of the optical pulse, \( E_{\text{opt}}(\omega) \), is defined similarly to Eq. (5.30). Since the interband polarization is linear in the optical field, we can write

\[
\tilde{P}_{cv}(k, \omega) = \tilde{X}_{cv}^{(a)}(k, \omega) E_{\text{opt},a}(\omega), \tag{5.31}
\]

where \( \tilde{X}_{cv}^{(a)}(k, \omega) \) characterizes the response of \( \tilde{P}_{cv}(k, \omega) \) to an optical field in the \( a \)th Cartesian direction, and as usual we sum over repeated Cartesian components. After using Eq. (5.31) and taking the limit to a long pulse of frequency \( \omega_o \), \( E_{\text{opt}}(t) \to E_o e^{-i\omega_o t} + \text{c.c.} \), we rewrite Eq. (5.29) in the form of Fermi’s Golden Rule

\[
\frac{dn_{\text{exc}}}{dt} = \eta^{ab}(\omega_o) E_o^a (E_o^b)^*, \tag{5.32}
\]

where the tensor

\[
\eta^{ab}(\omega) = \frac{1}{i\hbar} \sum_{c,v} \int_{BZ} d{k} \frac{1}{(2\pi)^3} \left[ \tilde{X}_{cv}^{(a)}(k, \omega) (\tilde{\Theta}_{cv}^{(b)}(k))^* - (\tilde{X}_{cv}^{(b)}(k, \omega))^* \tilde{\Theta}_{cv}^{(a)}(k) \right] \tag{5.33}
\]

describes the rate of injection of carriers into the conduction bands. Here \( \tilde{\Theta}^{a}(k) \) denotes the \( a \)th Cartesian component of the transformed dipole moment matrix. If both the optical and the dc field are aligned with principal axes of the dielectric tensor, the absorption coefficient becomes [93, 138]

\[
\alpha(\omega) = \frac{2\pi\hbar \eta^{aa}(\omega)}{n(\omega)c}, \tag{5.34}
\]
for an optical field linearly polarized along the \(a\)th Cartesian direction (no summation over repeated indices in this case) and associated refractive index \(n(\omega)\). For the results presented in Sec. 5.5, we neglect the frequency dependence of the refractive index and use \(n(\omega) = 3.7\) for GaAs.

While the injection rate \(\eta^{ab}(\omega)\) and the absorption coefficient \(\alpha(\omega)\) for CW excitation at frequency \(\omega\) are the quantities in which we are primarily interested, it is useful to consider the response of the crystal to pulsed excitation in the time domain to illustrate the physics of the injection process; furthermore, a numerical evaluation of the response to a pulse is one strategy for determining \(\eta^{ab}(\omega)\). Therefore, we consider an optical pulse of finite duration with its polarization oriented in the \(a\)th Cartesian direction and calculate the interband polarization in time domain, \(\bar{P}^{cv}_{a}(k,t)\), from Eq. (5.25). The linear response function, \(\bar{X}^{cv}_{a}(k,\omega)\), is then found from the Fourier components according to Eq. (5.31).

We assume a pulse of the form

\[
E^{\text{opt},a}(t) = \mathcal{E}^{\text{opt},a}(t)e^{-i\omega_o t} + (\mathcal{E}^{\text{opt},a}(t))^*e^{i\omega_o t},
\]

where \(\omega_o\) is the carrier frequency and \(\mathcal{E}^{\text{opt},a}(t)\) is a slowly varying envelope. Since we are interested in frequencies \(\omega_o\) near the band gap, it is convenient to write the solution of Eq. (5.25) as \(\bar{P}^{cv}_{a}(k,t) = \mathcal{P}^{cv}_{a}(k,t)e^{-i\omega_o t}\). In the rotating wave approximation, the function \(\bar{P}^{cv}_{a}(k,t)\) satisfies

\[
i\hbar \frac{\partial}{\partial t} \bar{P}^{cv}_{a}(k,t) - \hbar(\omega_{cv}(k) - \omega_o)\bar{P}^{cv}_{a}(k,t) + ieE^{dc}_{cv} \frac{\partial}{\partial k||} \bar{P}^{cv}_{a}(k,t) - \Sigma^{\bar{P}^{cv}_{a}}(k,t) = -\mathcal{E}^{\text{opt},a}(t)\Theta^{a}_{cv}(k),
\]

with no summation over repeated indices on the right-hand-side. The self-energy (5.27) is written in terms of \(\bar{P}^{(a)}(k,t)\),

\[
\Sigma^{\bar{P}^{(a)}}(k,t) = -\int \frac{dq}{(2\pi)^3} U(q)K(k,k-q)\bar{P}^{(a)}(k-q,t)K^\dagger(k,k-q).
\]

We solve Eq. (5.36) numerically for a convenient Gaussian envelope function

\[
\mathcal{E}^{\text{opt},a}(t) = \frac{1}{2}\mathcal{E}^{ a}_o e^{-(t/\tau)^2},
\]
where $\tau$ is the duration of the pulse, and extract the linear response from the Fourier transform with

$$
\tilde{X}^{(a)}_{cv}(k, \omega) = \frac{\tilde{P}^{(a)}_{cv}(k, \omega - \omega_o)}{E_{\text{opt},a}(\omega - \omega_o)},
$$

(5.39)

for frequencies near $\omega_o$. The linear response function calculated this way can then be inserted in Eq. (5.33) to find the tensor $\eta^{ab}(\omega)$.

## 5.4 Calculation

We illustrate the type of calculations presented in Secs. 5.2 and 5.3 for bulk GaAs in a simple parabolic two-band model [2, 100] and a 14-band $k \cdot p$ model [92, 153]. We start by calculating the various matrices that capture the interband coupling in the system. The first is the velocity matrix $V(k)$ that couples to the dc field in Eq. (5.23) through the usual dipole moment matrix elements and allows us to calculate the transformation matrix $\tilde{M}(k)$. With these matrix elements we can calculate the modified dipole moment matrix $\tilde{\Theta}(k)$, which couples to the optical field and drives the interband polarization in Eq. (5.36). Additionally, the Coulomb term requires calculating the transformed overlap matrix $K(k_1, k_2)$. In the two-band model, discussed in Sec. 5.4.1, these matrix elements are trivial. But in the 14-band model, described in Sec. 5.4.2, we need to combine the standard $k \cdot p$ method with the equations described in Sec. 5.2.3. The resulting matrices are required in the dynamical equation for the interband polarization, Eq. (5.36).

We use an additional transformation of the interband polarization in order to optimize the numerical calculation; we describe that transformation and illustrate the time evolution of the calculated interband polarization in Sec. 5.4.3. The details of the numerical calculation are left to Chapter 6.
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5.4.1 The parabolic two-band model

In the parabolic two-band model the energy difference between the conduction and the valence bands around the Γ point (k = 0) is simply given by

\[ \hbar \omega_{cv}(k) = \frac{\hbar^2 k^2}{2m_{cv}^{\text{red}}(0)} + E_G, \]  

where \( m_{cv}^{\text{red}}(0) \) is the reduced effective mass of the electron-hole pair at the Γ point (see Eq. (3.20) in Chapter 3), and \( E_G \equiv \hbar \omega_{cv}(0) \) is the energy gap. The \( u_{nk}(r) \) and the \( v_{cv}(k) \) are fixed to the value at the Γ point. Therefore, we have

\[ V_{cv}(k) = v_{cv}(0). \]  

Similarly, the interband coupling due to the dc field, Eq. (5.23), and the transformed overlap matrices, Eq. (5.28), are uniform in \( k \),

\[ \tilde{M}_{n_1n_2}(k) = K_{n_1n_2}(k_1, k_2) = \delta_{n_1n_2}, \]  

where \( n_1 \) and \( n_2 \) can only be either \( c \) or \( v \). This model has been used to describe experimental data by fitting appropriately the effective mass and the velocity matrix element \( v_{cv}(0) \) [117]. For the examples shown here we use the values

\[ m_{cv}^{\text{red}} = 0.0553m_e \text{ and } \hbar v_{cv}^x(0) = 10.3 \text{ eV Å}, \]  

which correspond to the pair formed by one of the lowest conduction bands and one of the heavy hole bands; \( m_e \) is the electron mass.

5.4.2 The 14-band \( k \cdot p \) model

The 14-band model considered here consists of six p-like valence bands, two s-like conduction bands, and six p-like conduction bands; these are shown in Fig. 5.3. Effects beyond this set of bands are included using Löwdin perturbation theory [154]. The relevant aspects of the model were summarized by Wahlstrand and Sipe [93]; for further
Figure 5.3: Band structure calculated with the 14-band model for GaAs (solid lines). For reference, the parabolic bands used for the two-band model are also shown (dashed blue lines); these correspond to the lowest conduction and the heavy hole bands. Note the significant nonparabolicity of the bands, for example the band warping of the heavy and light holes. Spin splitting of the bands ($\lesssim 1$ meV) is not shown.
details we refer the reader to the work of Bhat and Sipe [153], whose numerical values for the relevant parameters are the ones used here.

For the $k \cdot p$ model calculation we use the basis of the $\Gamma$ point [89] to write

$$u_{nk}(r) = \sum_{n'} u_{n'0}(r) C_{n'n}(k), \quad (5.44)$$

where the coefficients $C_{n'n}(k)$ can be arranged in a unitary matrix $C(k)$. Once these coefficients are found, we can calculate all the required matrix elements. The elements of $C(k)$ satisfy

$$\sum_{n'_1} (\hat{H}_k)_{n1'n'_1} C_{n'_1n}(k) = \hbar \omega_{n2}(k) C_{n1}(k), \quad (5.45)$$

where

$$\hat{H}_k \equiv e^{-i\hat{r}} \hat{H}_0 e^{i\hat{r}} \quad (5.46)$$

is the $k \cdot p$ Hamiltonian [93], with matrix elements

$$(\hat{H}_k)_{n1n2} \equiv \langle u_{n10}|\hat{H}_k|u_{n20}\rangle \quad (5.47)$$

(see discussion after Eq. (2.13) in Chapter 2). Hence, the $C_{n1n2}(k)$ can be found by simple diagonalization of the matrix with elements $(\hat{H}_k)_{n1n2}$ at each $k$.

The dc field couples Bloch states along lines parallel to it. Consequently, the phase of the Bloch states along these lines needs to be smooth in order to calculate the matrix elements in Eq. (2.13). In Sec. 5.2 we implicitly assumed that it was possible to find Bloch states conforming to such a requirement. Numerical diagonalization of the $k \cdot p$ Hamiltonian introduces a random phase, which is incompatible with this assumption; however, there can still be a random phase between different lines parallel to the dc field. Therefore, we diagonalize only on a plane perpendicular to the dc field that crosses the $\Gamma$ point ($k_\parallel = 0$) to determine $C(k_\perp)$ (see Sec. 6.2 in Chapter 6).

In order to proceed along lines parallel to the dc field we follow the method used by Sipe and Ghahramani, which can deal with points and lines of degeneracy [26]. This
method also allows us to calculate the velocity matrix elements $V_{n_1 n_2}(k)$ without finding first the Berry-type phases in Eq. (5.21). We define

$$C(k) \equiv C(k)e^{-i\Xi(k)},$$

which satisfies $C(k_\perp) = C(k_\perp)$. We can write the velocity matrix elements Eq. (5.20) in terms of these matrices as [93, 153]

$$V_{n_1 n_2}(k) = \frac{1}{\hbar} \sum_{n_1', n_2'} C_{n_1 n_1'}(k)(\nabla_k \hat{H}_k)n_1' n_2' C_{n_2 n_2'}^\dagger(k).$$

(5.49)

For $k_\parallel \neq 0$ we require [26, 93]

$$ie \frac{\partial}{\partial k_\parallel} C_{n_1 n_2}(k) - \sum_{n_2'} C_{n_1 n_2'}(k) \mu_{n_2 n_2'}^{dc}(k) = 0,$$

(5.50)

using Eq. (5.22) and Eq. (5.49). Recall that $\mu^{dc}(k)$ denotes the full matrix, which includes the coupling between conduction and valence bands.

Once the matrix $V(k)$ has been calculated over the region of interest in the Brillouin zone, we can solve numerically Eq. (5.23) to find the interband coupling matrix $\tilde{M}(k)$ and the transformed dipole moment matrix $\tilde{\Theta}(k)$ defined in Eq. (5.26). Note that the matrix elements $\tilde{M}_{n_1 n_2}(k)$ defined here are equal to the matrix elements $\tilde{m}_{n_1 n_2}(k_\perp; k_\parallel/\epsilon)$ used by Wahlstrand and Sipe [93] except for a phase,

$$\tilde{M}_{n_1 n_2}(k) = \tilde{m}_{n_1 n_2}(k_\perp; k_\parallel/\epsilon)e^{-i\int_{k_\parallel}^k \omega_{n_1 n_2}(k_\perp+k'_\parallel) e^{dc}dk'_\parallel}/\epsilon,$$

(5.51)

where we introduce the reduced electric field

$$\epsilon \equiv \frac{eE^{dc}}{\hbar}.$$

(5.52)

Finally, we need to find the transformed overlap matrix $K(k_1, k_2)$ defined in Eq. (5.28). We write

$$e^{i\Xi(k_1)}\Delta(k_1, k_2)e^{-i\Xi(k_2)} = C^\dagger(k_1)C(k_2)$$

(5.53)

in terms of $C(k)$. In this form, $K(k_1, k_2)$ can be found from

$$K(k_1, k_2) = \tilde{M}^\dagger(k_1)C^\dagger(k_1)C(k_2)\tilde{M}(k_2).$$

(5.54)
Figure 5.4: Snapshots of $|\mathcal{R}^{(x)}(\kappa, t)|$ in the independent particle approximation for the two-band (left column) and 14-band (right column) models in arbitrary units (the plots for $t = -\tau$ are amplified 10 times). The dc field is oriented along the [001] direction and its reduced value is $\epsilon = 1/(\text{ps } \text{Å})$, which corresponds to 66 kV/cm. The horizontal and vertical axes represent $\kappa^x = k^x$ and $\kappa^z$, respectively. The optical pulse has a duration of $\tau = 16$ fs and it is polarized along the [100] direction; for simplicity, we tune its frequency to the band gap of GaAs, $\hbar\omega_o = 1.519$ eV.
5.4.3 Time evolution of the interband polarization

The interband polarization $\bar{P}_{cv}^{(a)}(k, t)$ in Eq. (5.36) oscillates due to the term with the energy difference $\hbar \omega_{cv}(k)$ and moves in $k$-space due to the gradient term. For these reasons we introduce a slowly varying interband polarization, $\bar{P}_{cv}^{(a)}(\kappa, t)$, in the moving frame, so that

$$\bar{P}_{cv}^{(a)}(k, t) = \bar{P}_{cv}^{(a)}(\kappa, t)e^{-i\int_0^t(\omega_{cv}(\kappa + \epsilon t' \hat{e}^{dc}) - \omega_0)dt'},$$

(5.55)

where $\kappa \equiv k - \epsilon t \hat{e}^{dc}$ is a moving coordinate in reciprocal space (see Eq. (2.47)), and $\epsilon$ is the reduced electric field, Eq. (5.52). The new interband polarization satisfies the dynamical equation

$$i\hbar \frac{\partial}{\partial t} \bar{P}_{cv}^{(a)}(\kappa, t) - \mathcal{S}^{(a)}_{cv}(\kappa, t) = -E_{opt,a}(t)\bar{T}_{cv}(\kappa, t),$$

(5.56)

where, similarly to Eq. (5.55), we define

$$\mathcal{S}^{(a)}_{cv}(\kappa, t) \equiv \sum_{cv} (\kappa + \epsilon t' \hat{e}^{dc}, t)e^{i\int_0^t(\omega_{cv}(\kappa + \epsilon t' \hat{e}^{dc}) - \omega_0)dt'}$$

(5.57)
and
\[ \tilde{\Sigma}^a_{cv}(\kappa, t) \equiv \tilde{\Theta}^a_{cv}(\kappa + \epsilon t \hat{e}_{dc}) e^{i \int_0^t (\omega_{cv}(\kappa + \epsilon t' \hat{e}_{dc}) - \omega_o) dt'}. \]  

(5.58)

We illustrate the time evolution of the interband polarization with the function
\[ N^{(a)}(\kappa, t) = \sum_{cv} \tilde{P}^{(a)}_{cv}(\kappa, t) \tilde{\Theta}^a_{cv}(\kappa + \epsilon t \hat{e}_{dc}) \]  

(5.59)

(no summation over repeated Cartesian indices). The imaginary part of this function is proportional to the density of excited carriers after multiplication by the optical field envelope and integration over \( \kappa \) and time. In the moving frame Eq. (5.59) becomes
\[ \mathcal{N}^{(a)}(\kappa, t) = \sum_{cv} \tilde{P}^{(a)}_{cv}(\kappa, t) e^{-i \int_0^t (\omega_{cv}(\kappa + \epsilon t' \hat{e}_{dc}) - \omega_o) dt'} \tilde{\Theta}^a_{cv}(\kappa + \epsilon t \hat{e}_{dc}) \]  

(5.60)

(no summation over repeated Cartesian indices), where \( \mathcal{N}^{(a)}(\kappa, t) \equiv N^{(a)}(\kappa, t) \). The color maps in Figs. 5.4 and 5.5 show the absolute value and imaginary part of \( \mathcal{N}^{(a)}(\kappa, t) \) for the two models considered here. We choose the [001] direction for the dc field, \( \hat{e}_{dc} = \hat{z} \), and a positive reduced electric field, \( \epsilon > 0 \); therefore, the region of non-zero \( \mathcal{N}^{(a)}(\kappa, t) \) moves in the positive \( k_z \) direction in the lab frame. For simplicity, we first calculate \( \mathcal{N}^{(a)}(\kappa, t) \) neglecting the Coulomb interaction; later we will show that the effect of the Coulomb term is mainly an enhancement of the interband polarization (see Sec. 5.5).

In order to explain the shape and motion of \( \mathcal{N}^{(a)}(\kappa, t) \), we consider first the contribution from \( \tilde{P}^{(a)}_{cv}(\kappa, t) \) to Eq. (5.60). In the independent particle approximation the solution to Eq. (5.56) can be written as
\[ \tilde{P}^{(a)}_{cv}(\kappa, t) = \frac{i}{\hbar} \int_{t_1}^t C^{\text{opt}, a}(t') \tilde{\Sigma}^a_{cv}(\kappa, t') dt'. \]  

(5.61)

In the integrand of this expression, the optical field envelope is centered at \( t' = 0 \) but the term with the transformed dipole moment matrix, \( \tilde{\Sigma}^a_{cv}(\kappa, t') \), is centered at a value of \( t' \) that depends on \( \kappa^z \) (see Eq. (5.58)). Therefore, when we integrate over \( t' \), the distribution of \( \tilde{P}^{(a)}_{cv}(\kappa, t) \) is not centered at \( \kappa = 0 \) for all times, as can be seen in Fig. 5.4; there is a visible shift, in the positive \( \kappa^z \) direction, of the center of the distribution for times
Figure 5.6: Franz-Keldysh spectrum for a 66 kV/cm dc field calculated in the two-band model. (a) Absorption coefficient with Coulomb interaction (solid line) and without (dashed line). (b) Difference with respect to the zero-field absorption in the independent particle approximation for $\alpha(\omega)$ calculated with Coulomb interaction (solid line) and without (dashed line). (c) Ratio between the absorption coefficient with and without Coulomb interaction; the inset shows the energy range from 1.6 to 1.9 eV in more detail.

$t < 0$. The reason for this shift is that $\bar{A}_C^a(\kappa, t')$ contributes more significantly for $\kappa^z > 0$ when the upper limit of the integral in Eq. (5.61) is negative; only when $t$ is positive and sufficiently large, is there a balance between the contributions from positive and negative $\kappa^z$, and the center of the distribution of $|\tilde{\mathcal{P}}_C^a(\kappa, t)|$ remains essentially at $\kappa^z = 0$.

The phase factor in Eq. (5.60) contributes oscillations to $\mathcal{R}^a(\kappa, t)$, which are noticeable in Fig. 5.5. The frequency of the oscillation increases with time as expected for accelerated carriers, but the center of the oscillations, where they are slower, moves in time and does not coincide with the center of the distribution of $|\tilde{\mathcal{P}}_C^a(\kappa, t)|$ for all times; furthermore, the center of $\tilde{\Theta}_C^a(\kappa + \epsilon t \hat{e}_{dc})$ in Eq. (5.60) also moves in time due to the shift by $\epsilon t \hat{e}_{dc}$. As a result, the oscillations of $\mathcal{R}^a(\kappa, t)$ for times $t > 0$ are centered at $\kappa^z < 0$ (for instance, see $t = 3\tau$ in Fig. 5.5). The motion of the center of the oscillations can be
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illustrated for low dc fields such that the approximation

\[ \int_0^t (\omega_{cv}(\boldsymbol{\kappa} + \epsilon' t \hat{e}^{dc}) - \omega_o) \, dt' \approx (\omega_{cv}(\boldsymbol{\kappa} + \epsilon' t \hat{e}^{dc}) - \omega_o) \, t \quad (5.62) \]

is valid. In this case it is clear that the center of the oscillations will move in the \( \kappa_z \) direction at a rate given by \( \epsilon \). Although in our calculations \( \epsilon \) is not sufficiently small for Eq. (5.62) to be valid, Fig. 5.5 illustrates that the center of the oscillations still moves in the \( \kappa_z \) direction.

The contours in Figs. 5.4 and 5.5 show the differences for \( \mathfrak{N}^{(a)}(\boldsymbol{\kappa}, t) \) between the two-band and 14-band models. Overall, their shapes are similar, but the 14-band model clearly displays some distortions due to the non-parabolicity of the band energies and the more complicated structure of the transformed dipole moment matrix elements; for instance, note the significant differences in \( |\mathfrak{N}^{(a)}(\boldsymbol{\kappa}, t)| \) at times when the pulse has stopped driving the system and carriers are simply accelerated by the dc field (see \( t = 3\tau \) in Fig. 5.4).

Once the interband polarization, Eq. (5.55), is calculated in time domain, we proceed to calculate the absorption coefficient \( \alpha(\omega) \) as described in Sec. 5.3. In the next section we discuss the results for the absorption coefficient with and without the Coulomb interaction, for different dc fields as calculated using the band models just described.

5.5 Results for different configurations

In this section we study the absorption spectra calculated from the two models discussed in Sec. 5.4 and examine the effect of the Coulomb interaction. The first set of results corresponds to \( E^{dc} = 66 \text{ kV/cm} \) (\( \epsilon = 1/(\text{ps } \text{Å}) \)), which is the most extensively discussed field in the work of Wahlstrand and Sipe [93]. Here we show how the excitonic effects modify their results. We also consider a lower dc field, \( E^{dc} = 44 \text{ kV/cm} \) (\( \epsilon = 2/(3 \text{ ps } \text{Å}) \)), where the Coulomb interaction modifies the absorption spectrum more significantly because the force due to \( E^{dc} \), which pulls apart the electron-hole pair, is weaker.
Figure 5.7: Franz-Keldysh spectrum for a 66 kV/cm dc field pointing along [001] calculated in the 14-band model. (a) Absorption coefficient with Coulomb interaction (solid lines) and without (dashed lines) for light polarized along [001] (red lines) and [100] (blue lines). The spectra are offset vertically for clarity. [(b) and (c)] Difference with respect to the zero-field absorption in the independent particle approximation for $\alpha(\omega)$ calculated with Coulomb interaction (solid lines) and without (dashed lines), for light polarized along [001] and [100].
The absorption coefficient for $E_{dc} = 66$ kV/cm in the parabolic two-band model is shown in Fig. 5.6a. Note the absorption tail below the band gap and oscillations above it, the typical features of the Franz-Keldysh effect (see Sec. 5.1). In order to examine how the dc field modifies the zero-field absorption, we plot the difference between the absorption coefficient (with and without Coulomb interaction) and the zero-field absorption coefficient in the independent particle approximation (see Fig. 5.6b). Without Coulomb interaction this difference is simply the *differential electroabsorption*, and our numerical calculations agree with the Airy function result [2, 93],

$$
\Delta\alpha(\omega) \propto \frac{1}{\pi} \left\{ \left[ \text{Ai}'(\hat{E}_\Omega) \right]^2 - \hat{E}_\Omega \text{Ai}^2(\hat{E}_\Omega) \right\} - (-\hat{E}_\Omega)^{1/2} \theta(-\hat{E}_\Omega),
$$

(5.63)

where $\hat{E}_\Omega \equiv (E_G - \hbar \omega)/(\hbar \Omega_{cv})$ is the energy relative to the band gap scaled by the electro-optic function $\Omega_{cv} \equiv [\hbar e^2/(2m_{cv}^\text{red}(0))]^{1/3}$ (see Sec. 5.4.1), and $\theta(\cdot)$ is the Heaviside step function. The Coulomb interaction enhances the absorption coefficient, especially near the band gap, as can be seen in the ratio between the Franz-Keldysh spectra with and without electron-hole interaction plotted in Fig. 5.6c; at higher energies the enhancement factor becomes flatter. Our results are slightly different from previous two-band model calculations with Coulomb interaction that consider the contributions from the hydrogenic exciton wavefunctions only at the origin [98–100]. In our scheme this would require fixing the dipole moment matrix element to the value at the $\Gamma$ point [2],

$$
\mu_{cv}(k) = \frac{e v_{cv}(0)}{i \omega_{cv}(0)},
$$

(5.64)

instead of fixing only the velocity matrix element (see Eq. (5.41)). The numerical calculations assuming Eq. (5.64) are more demanding in our scheme because the dipole moment matrix element does not decrease away from the $\Gamma$ point. The absorption coefficient in both cases is essentially the same up to a numerical factor, the enhancement being larger for (5.64).

In the 14-band model the absorption coefficient displays additional features as shown in Fig. 5.7a for [001] and [100] polarized light; in both cases the dc field is oriented
Figure 5.8: Ratio between the absorption coefficient with and without Coulomb interaction calculated in the 14-band model as in Fig. 5.7. Two light polarizations are shown, along [100] (dash-dotted blue line) and [001] (solid red line). The inset shows the energy range from 1.6 to 1.9 eV in more detail.

along [001]. For example, there is a dependence on the polarization of the optical field, which can be seen more easily in the difference with respect to the zero-field absorption (compare Figs. 5.7b and c). Such dependence has been observed experimentally [113] and discussed in the independent particle approximation [91, 93, 94], but we also observe that the enhancement of the absorption coefficient due to the Coulomb interaction, plotted in Fig. 5.8, depends on the optical polarization, despite the Coulomb potential being isotropic. Even though the overall behavior of the enhancement is similar for the optical polarization perpendicular and parallel to the dc field, the perpendicular configuration is favored below the band gap and the enhancement factor displays oscillations that do not coincide for the two optical polarizations. The difference between the absorption in these two cases for the independent particle calculation (see Fig. 5.9) oscillates around a zero difference above the band gap and shows that the absorption is stronger for the parallel polarization below the band gap. Including the Coulomb interaction not only amplifies the difference below the band gap and the oscillations above it, as expected for an isotropic enhancement, but it also causes a phase shift and a separation from
the zero difference as we move to higher energies. Experiments have confirmed the polarization anisotropy for low-temperature grown GaAs [113], showing that the parallel configuration leads to higher absorption below the band gap (1.52 eV in our case) and different Franz-Keldysh oscillations above it, especially for energies close to the band gap; these experiments, however, do not show a significant polarization anisotropy near the energy of the split-off valence band to conduction band transition (1.86 eV in our case). This last observation is in disagreement with our predictions including Coulomb interaction, as can be seen in Fig. 5.9, where the anisotropy for energies near the split-off to conduction band transition can be even larger than for energies near the band gap. There are various possible reasons for this discrepancy; for instance, inhomogeneities of the electric field inside the sample [155] and temperature effects can potentially wash out the Coulomb enhancement of the anisotropy.

The enhancement of the absorption coefficient due to the Coulomb interaction can be traced back to the interband polarization. We illustrate this point in Fig. 5.10, where $|\bar{P}_{cv}^{(x)}(\kappa, t)|$ and $|\bar{S}_{cv}^{(x)}(\kappa, t)|$ for the the two-band model (Fig. 5.6) and the 14-band model in the perpendicular configuration (Fig. 5.7) are plotted in the moving frame for fixed $\kappa_\perp = 0\hat{x} + 0\hat{y}$, as they evolve in time. Note that $|\bar{P}_{cv}^{(x)}(\kappa, t)|$ is peaked at values of $\kappa^z$ such that the energy difference between the bands $c$ and $v$ is tuned to the energy
associated with the center frequency of the pulse, $\hbar \omega_0$. Since we have not included dephasing, $|\overrightarrow{P}_{cv}(\kappa, t)|$ remains essentially unchanged after the pulse has stopped driving the system. The behavior of $|\overrightarrow{S}_{cv}(\kappa, t)|$ is quite different; although it has the same two peaks present in the interband polarization, the Coulomb term decreases significantly and eventually vanishes when the pulse is not acting. Furthermore, one of the peaks lasts for a longer time before it disappears. In order to explain these two observations, we consider $\overrightarrow{P}_{cv}(k, t)$ and $\Sigma_{cv}^P(k, t)$, both in the lab frame and including the phase introduced in Eq. (5.55). Clearly, this phase oscillates faster for values of $k$ and $t$ where the energy difference is detuned from $\hbar \omega_0$. In the Coulomb integral Eq. (5.37) (see also Eq. (6.6) in Chapter 6), the contribution from $\overrightarrow{P}_{cv'}(k, t)$ is smaller when the interband polarization oscillates faster; this occurs when $\overrightarrow{P}_{cv'}(k, t)$ has left the vicinity of the $k$ points where the energy difference is close to $\hbar \omega_0$. The insets in Figs. 5.10c and 5.10f show the shape of $|\Sigma_{cv}^P(k, t)| = |\overrightarrow{S}_{cv}(\kappa - \epsilon \hat{e}_d, t)|$ in the lab frame, which results in one peak lasting longer than the other in the moving frame. Consequently, the Coulomb term enhances the peaks of $|\overrightarrow{P}_{cv}(\kappa, t)|$ asymmetrically, as shown in Fig. 5.10b and Fig. 5.10e. The peak that is enhanced the most is also broadened, which is not surprising considering that the Coulomb interaction attempts to keep the electron-hole pair together, localizing its wavefunction in real space.

We also note that the absorption spectrum with electron-hole interaction can be modified by introducing a statically screened potential

$$U_s(q) = \frac{4\pi e^2}{\epsilon_b} \frac{1}{q^2 + \kappa_s^2},$$

(5.65)

where $\kappa_s$ is the inverse of the screening length of the long-ranged bare Coulomb interaction [2]. The screening reduces the Coulomb enhancement and shifts the peaks of the absorption coefficient to higher energies, especially near the band gap; as we would expect, both changes are in the direction of the independent particle result. We illustrate this observation in Fig. 5.11, where the absorption coefficient for 66 kV/cm dc field and [100] polarization in the 14-band model is plotted with and without screening. Even
Figure 5.10: Time evolution of $|\bar{P}^{(x)}_{cv}(\kappa, t)|$ in the independent particle approximation (panels (a) and (d)) and including Coulomb interaction (panels (b) and (e)) in arbitrary units for a 66 kV/cm dc field oriented along the [001] direction and light polarized along the [100] direction, as calculated using the two-band and 14-band models. The horizontal and vertical axes represent time and wave vector along the $\hat{z}$ direction in the moving frame, respectively; the coordinates perpendicular to the dc field are fixed at $\kappa^x = 0$ and $\kappa^y = 0$. We also include plots of $|\mathcal{G}^{(x)}_{cv}(\kappa, t)|$ (panels (c) and (f), in arbitrary units) in the moving frame; the insets in these plots show $|\Sigma^{P(x)}_{cv}(\kappa, t)|$ in the lab frame, where $\kappa^z$ is replaced by $k^z$ for the vertical axis. [(a)-(c)] Two-band model with a pulse duration of $\tau = 8$ fs and center frequency such that $\hbar \omega_o = 1.719$ eV. [(d)-(f)] 14-band model with a pulse duration of $\tau = 16$ fs and center frequency such that $\hbar \omega_o = 1.619$ eV; the two bands chosen in this case are the lowest conduction band and the highest valence band.
for arbitrarily large $\kappa_s$, we still have $U(q)/U_s(q) \to 1$ as $q \to \infty$, so deviations of the absorption coefficient from that in the absence of the Coulomb interaction persist.

Finally, we consider the effect of a weaker dc field. At the independent particle level, we expect the oscillations of the differential absorption $\Delta \alpha(\omega)$ to have a smaller amplitude and a shorter period. When the optical polarization is perpendicular to the dc field, the shorter period of the oscillation allows us to observe its beating due to the different effective masses of the heavy and light holes, before the appearance of the
Figure 5.12: Franz-Keldysh spectrum for a 44 kV/cm dc field calculated in the two-band model. (a) Absorption coefficient with Coulomb interaction (solid line) and without (dashed line). (b) Difference with respect to the zero-field absorption in the independent particle approximation for $\alpha(\omega)$ calculated with Coulomb interaction (solid line) and without (dashed line). (c) Ratio between the absorption coefficient with and without Coulomb interaction; the inset shows the energy range from 1.6 to 1.8 eV in more detail.

‘bump’ associated with the split-off bands [93, 156]. For these reasons, we choose the value $E_{dc} = 44$ kV/cm for the dc field, still oriented along the [001] direction, and we set the optical polarization along the [100] direction in Figs. 5.12 and 5.13, where the absorption coefficient is calculated in the two-band and 14-band models, respectively. The overall behavior is very similar to the results obtained for the stronger field presented in Figs. 5.6 and 5.7 with the same optical polarization; however, the Coulomb enhancement increases near the band edge, roughly for energies below 1.6 eV (compare 5.6c and 5.12c for the two-band model, and Figs. 5.8 and 5.13c for the 14-band model). Note that the Coulomb interaction enhances the absorption at higher energies in a similar way for the two fields.
5.6 Conclusion

We have presented a theoretical approach for studying the Franz-Keldysh effect in the linear response regime. Our treatment represents an improvement on previous calculations in the independent particle approximation by including the electron-hole interaction at a Hartree-Fock level. We have kept the features associated with realistic band structure calculations from $k \cdot p$ models, properly accounting for the interband coupling away from the $\Gamma$ point [90, 91, 93]. We have also improved the expressions derived by Wahlstrand and Sipe by using the length gauge that removes divergent terms proportional to $1/\omega$, such as Eq. (51) in their work [93], without relying on sum-rules [26]; this feature could be used in situations where the dc field or the optical pulse are replaced by excitations with frequencies below the optical range, for instance, in the terahertz regime [70, 124, 125, 152, 157]. Furthermore, the calculation of the interband polarization in our approach is not only an intermediate step in finding the absorption coefficient but it has its own advantages. It illustrates the physics of the injection process and it becomes relevant in the analysis of experiments with pulsed excitation [115].

Regarding the effects of the Coulomb interaction, our calculations show that the absorption spectrum with and without Coulomb interaction are qualitatively similar. The most noticeable effect is the enhancement of the absorption lineshape, especially near the band edge; this is accompanied by a slight displacement of the Franz-Keldysh oscillations to lower energies. The Coulomb enhancement depends on the strength of the dc field, which determines how easily the electron and hole in an exciton are pulled apart from each other; as expected, weaker dc fields lead to higher enhancement.

Additionally, we studied the dependence on the orientation of the optical field fixing the dc field along the [001] direction and using parallel and perpendicular configurations for the optical polarization; such configurations are significantly different due to the heavy hole-light hole beat in the perpendicular case [156]. This feature is preserved in the Coulomb case, but a more detailed comparison shows that the perpendicular
Figure 5.13: Franz-Keldysh spectrum for [100] polarized light and a 44 kV/cm dc field pointing along [001], calculated in the 14-band model. (a) Absorption coefficient with Coulomb interaction (solid blue line) and without (dashed blue line). (b) Difference with respect to the zero-field absorption in the independent particle approximation for $\alpha(\omega)$ calculated with Coulomb interaction (solid blue line) and without (dashed blue line). (c) Ratio between the absorption coefficient with and without Coulomb interaction; the inset shows the energy range from 1.6 to 1.8 eV in more detail.
configuration is favored by the Coulomb interaction (see Fig. 5.8). This result motivates a closer study of the optical polarization dependence in the Franz-Keldysh effect, with experimental techniques where the optical polarization can be easily modified relative to the dc field [113, 115]. A possible approach is to measure the difference between the absorption coefficient for two optical polarizations, which we illustrated in Fig. 5.9, noticing a significant correction due to the Coulomb interaction.

We believe that these calculations show how including both interband coupling and the Coulomb interaction lead to an advance in our understanding of the Franz-Keldysh effect. As experimental techniques are improved [113, 115–118, 156], we expect that gradually more detailed features in the Franz-Keldysh effect will be observed, justifying analysis beyond the simple effective mass approximation. Finally, we point out that the framework presented here is not limited to bulk semiconductors, and it can be extended to systems of different dimensionality [121, 123]; in addition, there are potential improvements to the treatment of the Coulomb interaction with more sophisticated self-energies.
Chapter 6

Numerical calculation of the Franz-Keldysh effect

In this chapter we discuss in more detail the numerical procedures for the calculations described in the previous chapter. In our numerical approach, the calculations for the Franz-Kelsdysh effect are divided in three main steps, which are performed separately. First, we find the required band energies and matrix elements using a variation of the usual $\mathbf{k} \cdot \mathbf{p}$ method (see Sec. 5.4.2). Next, we propagate the interband polarization in time (see Sec. 5.4.3), calculating simultaneously the contributions to the Fourier transform $\tilde{P}_{cv}^{(a)}(\mathbf{k}, \omega - \omega_o)$ required for the absorption coefficient (see Sec. 5.3). The last step is the calculation of the integral for the injection rate $\eta^{ab}(\omega)$ in Eq. (5.33).

The specific implementation of the numerical procedures described in this chapter was done in a C++ program, using libraries such as GSL\textsuperscript{1} and FFTW3\textsuperscript{2} for matrix diagonalization, interpolation, and Fast Fourier Transforms. Instead of describing the program in detail, we present an overview of the general features of the calculation, which can be implemented in any programming language.

\textsuperscript{1}For documentation see: http://www.gnu.org/software/gsl/.
\textsuperscript{2}For documentation see: http://www.fftw.org/.
Figure 6.1: Schematic illustration of the coordinate system in reciprocal space. The $k_\perp$-coordinates lie on the starting plane (shown in green), which crosses the $\Gamma$ point ($k = 0$); the position relative to this plane is given by the $k_\parallel$-coordinate.

The chapter is organized as follows. In Sec. 6.1 we discuss some general features of the numerical scheme, including the setup of the grids in reciprocal space and the use of parallelization. In Sec. 6.2 we describe the procedure for calculating the required band energies and matrix elements. Finally, in Sec. 6.3 we present the aspects related to the calculation of the interband polarization and the absorption coefficient.

### 6.1 General aspects

All the steps of the calculation are performed in reciprocal space, except for some where Fourier transforms to real space are employed (see Sec. 6.3.2); this choice was motivated
by the use of $\mathbf{k} \cdot \mathbf{p}$ models to capture the details of the band structure. As discussed in Sec. 5.4.2, the dc field establishes a special direction in which the matrix elements need to be calculated so that the phase is well-defined along lines parallel to the dc field. In the numerical calculation, the difference between wave vectors perpendicular and parallel to the dc field is reflected in the setup of the grids and the structure of the calculation. As shown in Fig. 6.1, there is a “starting plane” perpendicular to the dc field and crossing the $\Gamma$ point, where the position of each grid point is given by a wave vector $\mathbf{k}_\perp$; for points that do not lie on the starting plane we use the coordinate $k_\parallel$ to locate them.

In this section we describe briefly two important aspects of the setup for the calculation: the grid of points in reciprocal space (Sec. 6.1.1) and the use of parallelization to speed up the computation (Sec. 6.1.2).

### 6.1.1 Grids

The grid in reciprocal space is treated separately for the lines parallel to the dc field and the starting plane perpendicular to it (see Fig. 6.1). The perpendicular grid is a square grid limited by $K_{\max}^\perp$,

$$-K_{\max}^\perp < k^x < K_{\max}^\perp \quad \text{and} \quad -K_{\max}^\perp < k^y < K_{\max}^\perp \quad (\text{for } \hat{\mathbf{e}}_{\text{dc}} = \hat{z}),$$

(6.1)

calculated with different levels of precision, as illustrated in Fig. 6.2. The lowest level of precision has seven equidistant points in each perpendicular direction (black points in Fig. 6.2); successive levels add points halfway between the points from the previous level (for example, the red points in Fig. 6.2). In the 14-band calculations we use $63 \times 63$ $\mathbf{k}_\perp$-points and $K_{\max}^\perp = 0.1 \, \text{Å}^{-1}$ on the starting plane, while in the two-band calculations we use $127 \times 127$ $\mathbf{k}_\perp$-points and $K_{\max}^\perp = 0.2 \, \text{Å}^{-1}$. In both cases we check convergence and compare our results in the independent particle limit with earlier calculations [2, 93] to ensure that the $\mathbf{k}_\perp$-grid is appropriate.

Once the band energies and required matrix elements are calculated (see Sec. 6.2),
they are stored in binary files organized by level of precision in $k_\perp$ so that only the data necessary for the chosen level is loaded when calculating the interband polarization and the absorption coefficient. After the level is chosen, it remains fixed throughout the rest of the calculation and we do not use interpolations in the perpendicular directions.

The direction parallel to the dc field is treated differently with a finer grid; in addition, the grid does not remain fixed during the calculation. A fine grid is used for evaluating the matrix elements in the range

$$-K_{\|, \max}^\max < k_{\|} < K_{\|, \max}^\max$$

(for our calculations with GaAs we set $K_{\|, \max}^\max = 0.5 \text{ Å}^{-1}$), and the results are stored in binary files. When the calculated matrix elements are read from these files, an interpolation of them along the parallel direction is used to evaluate the matrix elements at any desired point within the original boundaries, Eq. (6.2). This gives us full flexibility when
setting the density of the $k_{\parallel}$-grid for the calculation of the interband polarization and the absorption coefficient; typically, we choose a maximum of about 800 points along the parallel direction.\footnote{In the moving frame we actually use less points for $\kappa_{\parallel}$, but it is still necessary to evaluate the band energies and matrix elements in the original lab frame grid for $k_{\parallel}$ (see Sec. 6.3).} For most of the calculation this grid remains fixed, except for the determination of the Coulomb term $\mathcal{S}^{(a)}_{cv}(\kappa, t)$, which requires the interband polarization $\bar{P}^{(a)}_{cv}(k, t)$ instead of the slowly varying $\bar{P}^{(a)}_{cv}(\kappa, t)$ (see Sec. 5.4.3); therefore, in the calculation of the Coulomb term we allow for a different choice of the grid, interpolating from the original grid in order to calculate the points in the new one (see Sec. 6.3.2).

### 6.1.2 Parallelization

Due to the coupling induced by the Coulomb term, the solution of Eq. (5.56) for the interband polarization must be calculated simultaneously for all the relevant $\kappa$-points in the grid. In the independent particle calculation it is possible to find the contributions to the interband polarization and the absorption coefficient from different $k_{\perp}$-points separately, splitting the work among many computers as described by Wahlstrand [93]. In the excitonic case, we cannot structure the parallelization in this way, but we can parallelize some procedures inside each step of the time propagation of the interband polarization. Following the same philosophy of separating the wave vectors in their components perpendicular and parallel to the dc field, we always parallelize over $k_{\perp}$; in some cases we parallelize over bands too. In order to implement the parallelization we use the application programming interface (API) provided by OPEN-MP®. In the next sections we mention when parallelization is used.
6.2 Calculation of the matrix elements

The essential parts of the calculation of the matrix elements were developed by J. K. Wahlstrand for earlier calculations of the Franz-Keldysh effect in the independent particle approximation [93]. We adapted his scheme, designed for the velocity gauge, to the matrix elements required in the length gauge; therefore, some matrix elements had to be redefined and built from the ones he implemented. A major difference with respect to Wahlstrand’s approach is the intermediate calculation of the interband polarization before the absorption coefficient; this additional step is required in our case, since the absorption coefficient cannot be written directly in terms of the matrix elements from the $\mathbf{k} \cdot \mathbf{p}$ calculation, as can be done in the independent particle case. For this reason, and since the calculation is quite demanding, it is convenient to calculate the matrix elements separately and store them for future use.

The starting point of the calculation is the numerical diagonalization of the $\mathbf{k} \cdot \mathbf{p}$ Hamiltonian, $\hat{H}_\mathbf{k}$ (see Eq. (5.46)). The band energies $\hbar \omega_n(k)$ (eigenvalues of $\hat{H}_\mathbf{k}$) are calculated over the entire $\mathbf{k}$-grid described in Sec. 6.1.1, but the $\Gamma$-basis coefficients $C_{n_1n_2}(\mathbf{k})$ (eigenvectors of $\hat{H}_\mathbf{k}$, see Eq. (5.44)) are calculated on the starting plane only, assuming no phase relation between $k_\perp$-points.

The next step is to find the coefficients $C_{n_1n_2}(k_\perp + k_\parallel \hat{e}^{dc})$ and the dipole moment matrix elements $\mu_{n_1n_2}(k_\perp + k_\parallel \hat{e}^{dc})$ along lines parallel to the dc field. We solve numerically Eq. (5.50) moving in the positive and negative $k_\parallel$ directions starting on the $k_\parallel = 0$ plane (see Fig. 6.1). For each fixed $k_\perp$ this is an ordinary differential equation, solved using an adaptive Runge-Kutta-Fehlberg method [158]. With the same approach, we solve Eq. (5.23) for the interband coupling matrix elements $\hat{M}_{n_1n_2}(k_\perp + k_\parallel \hat{e}^{dc})$. Using the dipole moment and interband coupling matrix elements we calculate the transformed dipole moment matrix $\bar{\Theta}(\mathbf{k})$, Eq. (5.26).

The Coulomb integral Eq. (5.37) requires the transformed overlap matrix elements $K_{n_1n_2}(\mathbf{k}_1, \mathbf{k}_2)$. These were not considered in the independent particle calculation, but they
can still be calculated from the aforementioned matrix elements. Note that the overlap matrix elements depend on two wave vectors; thus, storing them for every possible pair of wave vectors in the grid requires a large amount of memory and becomes impractical. An alternative is to split the matrix $K(k_1, k_2)$ as

$$K(k_1, k_2) = R^\dagger(k_1)R(k_2), \quad (6.3)$$

where

$$R(k) \equiv C(k)\bar{M}(k), \quad (6.4)$$

and store only the “split” overlap matrix elements $R_{n_1n_2}(k)$ evaluated on the full original $k$-grid. These matrix elements, along with the band energies $\hbar\omega_n(k)$ and the transformed dipole moment matrix elements $\bar{\Theta}_{cv}(k)$, are stored in binary files, which can be reused as necessary in calculations of the interband polarization and absorption coefficient with different $k$-grids and optical polarizations (see Sec. 5.5).

### 6.3 Calculation of the interband polarization and the absorption coefficient

We solve numerically Eq. (5.56) in order to find the time evolution of the interband polarization. Recall that $\bar{P}_{cv}^{(a)}(\kappa, t)$ is the slowly varying interband polarization in the moving frame, introduced in Sec. 5.4.3 with the purpose of optimizing the numerical calculation. There are two main advantages of using $\bar{P}_{cv}^{(a)}(\kappa, t)$ instead of its predecessor, $\bar{P}_{cv}^{(a)}(k, t)$, which satisfies Eq. (5.36). First, the gradient term in Eq. (5.36) becomes a simple translation in reciprocal space of the arguments in $\Sigma_{cv}^{(a)}(\kappa + \epsilon\hat{e}_d^c, t)$ and $\bar{\Theta}_{cv}^{a}(\kappa + \epsilon\hat{e}_d^c)$ (see Eqs. (5.57) and (5.58)); this translation occurs at a constant rate in time, controlled by the reduced electric field $\epsilon$, which remains constant during the calculation. The additional advantage is the removal of the band energy term from Eq. (5.36), which can cause numerical problems in the regions of reciprocal space where the energy difference $\hbar(\omega_{cv}(k) - \omega_o)$
becomes significant and causes fast oscillations; note that in solving Eq. (5.56) the energy only enters as a phase, which can be calculated accurately by simple interpolation.

In this final section, we describe the basic structure of the time propagation of the interband polarization, explaining how the energies and matrix elements discussed in Sec. 6.2 enter the time stepping (Sec. 6.3.1). A significant part of the time stepping is the calculation of the Coulomb term $S^{(a)}_{cv}(\kappa, t)$, which we describe separately in Sec. 6.3.2. We end with some remarks about the calculation of the absorption coefficient from the interband polarization in Sec. 6.3.3.

### 6.3.1 Time propagation of the interband polarization

The results presented in the previous chapter were calculated using the Runge-Kutta fourth order method in its simplest version without step size control [159]. However, the structure we describe here is not particular to this choice of stepping method, and therefore the calculation can be implemented in other stepping schemes.

In our discussion we will move between the lab-frame ($k$-coordinates) and the moving frame ($\kappa$-coordinates); the interband polarization in the lab-frame is $\bar{P}^{(a)}_{cv}(k, t)$, and the one in the moving frame is $\bar{P}^{(a)}_{cv}(\kappa, t)$. The Gaussian envelope function Eq. (5.38) for the optical pulse allows us to estimate a range of $k$-points where the interband polarization is significant so that we can safely ignore the points outside this range, which we simply call the “range of the interband polarization.” At $t = 0$ the range of the interband polarization in the lab frame coincides with the one in the moving frame; we denote this range by $[k^{\text{min}}, k^{\text{max}}]$ in the direction parallel to the dc field. Typically, the range of the interband polarization covers about 400 $\kappa_{\parallel}$-points. Since the calculation starts at $t_0$ and ends at $t_3$ (see Fig. 5.2), the range of required wave vectors in the lab frame for the entire

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4This range can be clearly seen in the examples in Figs. 5.4, 5.5, and 5.10. The range of the interband polarization is essentially determined by the duration $\tau$ and the center frequency $\omega_0$ of the pulse. Shorter pulses excite a broader range of energies $\hbar\omega_{cv}(k)$ around the center energy $\hbar\omega_0$; therefore, for shorter pulses we require a broader range of the interband polarization.
Figure 6.3: Schematic illustration of the $k_\parallel$-grid (lab frame, shown in black) and the $\kappa_\parallel$-grid (moving frame, shown in purple). At $t = 0$ the two frames coincide, but after every time step the $\kappa_\parallel$-grid moves one step to the right in the original $k_\parallel$-grid (for $\epsilon > 0$). Even though the range of the interband polarization between $\kappa_\parallel = k_\parallel^{\text{min}}$ and $\kappa_\parallel = k_\parallel^{\text{max}}$ remains fixed in the moving frame, the motion of the interband polarization probes all the points in the original $k_\parallel$-grid in the range $[k_\parallel^{\text{min}} + \epsilon t_0, k_\parallel^{\text{max}} + \epsilon t_3]$, where the required matrix elements must be calculated. For simplicity, we only show a few time steps and $k_\parallel$-points; in the actual calculation the number of grid points is significantly larger.

calculation is $[k_\parallel^{\text{min}} + \epsilon t_0, k_\parallel^{\text{max}} + \epsilon t_3]$; clearly, this range must be within the limits set by $K_\parallel^{\text{max}}$ for the calculated matrix elements (see Sec. 6.2). The relation between the grids for the lab and moving frames is illustrated in Fig. 6.3 for the direction parallel to the dc field; note that the step of the grid in reciprocal space, $\Delta k_\parallel = \epsilon \Delta t$, is set by the time step $\Delta t$, because we require the $\kappa$-grid to coincide with points of the $\mathbf{k}$-grid at every time step.

In preparation for the calculation of the interband polarization, the required band energies and matrix elements are loaded from binary files (see Sec. 6.2). Since the calculation is performed in the moving frame, the band energies $\hbar \omega_n(k)$, the transformed dipole moment matrix $\bar{\Theta}_{cv}(k)$, and the matrix $R(k)$ are evaluated over different ranges of wave vectors for each time step (purple dots in Fig. 6.3). Only the transformed
The loaded data for the energies and the \( R(\mathbf{k}) \) is used to build interpolating functions along the direction parallel to the dc field, which are then transferred to the stepping function. We use interpolating functions instead of the originally calculated points because this facilitates the accurate integration of the band energy for the phase factor \( \exp[-i \int_{0}^{t} (\omega_{cv}(\mathbf{k} + \epsilon t \hat{e}^{dc}) - \omega_{o}) \, dt'] \) and it allows us to calculate the Coulomb term in a grid specified separately (see Sec. 6.3.2).

For the time stepping we call a function that calculates the estimates required by the Runge-Kutta fourth order method \([159]\); these estimates are combined at the end of each time step in order to update the interband polarization. The function works in parallel over bands and \( \mathbf{k}_{\perp} \)-points; the input required for the intermediate steps is the interpolation function for the energy phase factor (properly updated for the current time step), the transformed dipole \( \bar{\Theta}_{cv}(\mathbf{k}) \) (already calculated), and the Coulomb term (calculated with a different function described in Sec. 6.3.2).

Since storing the interband polarization \( \bar{\mathbf{P}}_{cv}^{(a)}(\mathbf{k}, t) \) for all the time steps would require a significant amount of memory, we take advantage of the fact that the Fourier transform of \( \bar{P}_{cv}^{(a)}(\mathbf{k}, t) \) in time (see Eq. (5.30)) can be split as

\[
\bar{P}_{cv}^{(a)}(\mathbf{k}, \omega) = \int_{-\infty}^{\infty} \bar{P}_{cv}^{(a)}(\mathbf{k}, \omega - \omega_{o}) e^{i(\omega - \omega_{o})t} \, dt \approx \int_{t_{0}}^{t_{0} + \Delta t} + \int_{t_{0} + \Delta t}^{t_{0} + 2\Delta t} + \cdots + \int_{t_{0} + (N-1)\Delta t}^{t_{3}} \bar{P}_{cv}^{(a)}(\mathbf{k}, t) e^{i(\omega - \omega_{o})t} \, dt, \quad (6.5)
\]

for \( N \) time steps in between \( t_{0} \) and \( t_{3} \). Therefore, after finding the interband polarization \( \bar{\mathbf{P}}_{cv}^{(a)}(\mathbf{k}, t) \) at each time step, we transform it to \( \bar{P}_{cv}^{(a)}(\mathbf{k}, t) \) and calculate its contribution to \( \bar{P}_{cv}^{(a)}(\mathbf{k}, \omega - \omega_{o}) \), parallelizing over bands and \( \mathbf{k}_{\perp} \).

### 6.3.2 Coulomb term

The calculation of the Coulomb term \( \mathcal{E}_{cv}^{(a)}(\mathbf{k}, t) \) is the the most demanding part of the numerical computation because it requires one to calculate the convolution Eq. (5.37) at
each time step (and also for the intermediate estimates in Runge-Kutta schemes of \( n \)th order). Naturally, calculating the integral Eq. (5.37) directly is not the most efficient approach; thus, we use some additional processing to optimize the calculation.

First, it is necessary to create an interpolation of \( \tilde{\mathbf{P}}_{cv}^{(a)}(\kappa, t) \) (or its intermediate estimate inside a Runge-Kutta step), which is used to evaluate \( \tilde{\mathbf{P}}_{cv}^{(a)}(\kappa, t) \) in a new grid, set independently from the original \( k \)-grid;\(^5\) we refer to this new grid as the “Coulomb grid.” The matrix \( R(\kappa) \) is also evaluated in this grid. Then we calculate

\[
\mathbf{e}_{n_1n_2}^{(a)}(\kappa, t) \equiv \int \frac{dq}{(2\pi)^3} U(q) \sum_{c'v'} R_{n_1c'}(\kappa - q) \tilde{\mathbf{P}}_{c'v'}^{(a)}(\kappa - q, t) R_{v'n_2}^\dagger(\kappa - q),
\]

using the Fourier transform of \( \sum_{c'v'} R_{n_1c'}(\kappa) \tilde{\mathbf{P}}_{c'v'}^{(a)}(\kappa, t) R_{v'n_2}^\dagger(\kappa) \) and of the Coulomb potential \( U(q) \);\(^6\) the output is evaluated in the original \( k \)-grid. We use a Fast Fourier Transform implementation [148, 159], which can run in parallel over the Coulomb grid to speed up the calculation for large numbers of grid points.\(^7\) The Coulomb term \( \mathbf{G}_{cv}^{(a)}(\kappa, t) \) can be found from \( \mathbf{e}_{n_1n_2}^{(a)}(\kappa, t) \) using

\[
\mathbf{G}_{cv}^{(a)}(\kappa, t) = e^{i \int_0^t (\omega_{cv}(\kappa + \epsilon t \mathbf{e}^{dc}) - \omega_0) dt'} \sum_{n_1n_2} \left[ R_{cn_1}^\dagger(\kappa + \epsilon t \mathbf{e}^{dc}) \mathbf{e}_{n_1n_2}^{(a)}(\kappa + \epsilon t \mathbf{e}^{dc}, t) R_{n_2v}(\kappa + \epsilon t \mathbf{e}^{dc}) \right. \\
+ \left. R_{cn_1}^\dagger(\kappa + \epsilon t \mathbf{e}^{dc}) \mathbf{e}_{n_1n_2}^{(a)\dagger}(\kappa + \epsilon t \mathbf{e}^{dc}, t) R_{n_2v}(\kappa + \epsilon t \mathbf{e}^{dc}) \right].
\]

Since \( \mathbf{e}_{n_1n_2}^{(a)}(\kappa, t) \) is a matrix over all the \( N_B \) bands of the \( \mathbf{k} \cdot \mathbf{p} \) model, storing it requires a large amount of memory. In order to reduce the memory usage, we run the calculation

\(^5\)Typically, we choose the Coulomb grid to be finer than the original grid in order to resolve the oscillations due to the energy phase in Eq. (5.55) appropriately.

\(^6\)The divergence of the bare Coulomb potential at \( q = 0 \) is avoided with a simple lower cut-off at the value of \( U(\sqrt{3(\Delta k^\perp)^2}) \), where \( \Delta k^\perp \) is step used in the rectangular grid for \( k^\perp \). The error introduced by this cut-off was reduced by decreasing \( \Delta k^\perp \) until no significant modification in the absorption spectrum was found.

\(^7\)Additionally, note that the Coulomb term \( \mathbf{G}_{cv}^{(a)}(\kappa, t) \) couples the interband polarization for all possible pairs of conduction and valence bands; in order to reduce the number of pairs involved in the numerical calculation for the 14-band model, we neglect the contributions from the interband polarization associated with the six upper conduction bands (see Fig. 5.3); these contributions will oscillate much faster due to their energy separation with respect to the valence bands.
of Eq. (6.6) in a loop over the index $n_1$ finding

$$S^{(a)}_{\text{left}}(\kappa,t) = \sum_{n_1} R^\dagger_{cn_1} (\kappa + \epsilon t \hat{e}_d) \mathcal{C}^{(a)}_{n_1n_2} (\kappa + \epsilon t \hat{e}_d, t),$$

$$S^{(a)}_{\text{right}}(\kappa,t) = \sum_{n_1} (R^\dagger_{vn_1} (\kappa + \epsilon t \hat{e}_d) \mathcal{C}^{(a)}_{n_1n_2} (\kappa + \epsilon t \hat{e}_d, t))^*.$$

for fixed $n_2$. After going through the loop we get two matrices of size $N_C \times N_B$ and $N_B \times N_V$, where $N_V$ ($N_C$) is the number of valence (conduction) bands where the interband polarization is evaluated (see footnote 7). Finally, these matrices are multiplied by the corresponding matrix elements of $R(\mathbf{k})$ and the energy phase to complete Eq. (6.7),

$$S^{(a)}_{cv}(\kappa,t) = e^{i \int_0^t (\omega_{cv}(\kappa + \epsilon \mathbf{t} \hat{e}_d) - \omega_0) dt'} \sum_{n_2} \left[ S^{(a)}_{\text{left}}(\kappa,t) R_{n_2v}(\kappa + \epsilon \mathbf{t} \hat{e}_d) + R^\dagger_{cn_2} (\kappa + \epsilon \mathbf{t} \hat{e}_d) S^{(a)}_{\text{right}}(\kappa,t) \right].$$

We also use parallelization over $k_\perp$-points in the calculation of Eqs. (6.8)-(6.10).

Even after this optimization, the numerical calculations are very demanding when the Coulomb term is included. For example, in the 14-band model using 44 AMD Opteron™ 6176 SE processors in parallel, each time step takes about 1100 s for $E^{dc} = 66$ kV/cm. For lower dc fields the calculation is even more time consuming, since the required step sizes in time and $k_\parallel$ are smaller [93].

### 6.3.3 Absorption coefficient

After the Fourier transform of the interband polarization, $\tilde{P}^{(a)}_{cv}(\mathbf{k},\omega - \omega_0)$, is calculated, it is simple to find the linear response function $\tilde{X}^{(a)}_{cv}(\mathbf{k},\omega)$ from Eq. (5.39). The final step is to calculate the integral Eq. (5.33) over the $\mathbf{k}$-grid. Once more, we treat differently the directions parallel and perpendicular to the dc field. For the parallel direction we find an interpolation function for each line (see Fig. 6.1), which can be easily integrated as we did for the energy phase mentioned in Sec. 6.3.1. The contributions from each line parallel to the dc field are then added using a two-dimensional trapezoidal rule [159].
Chapter 7

Conclusion

In this thesis we have discussed inter- and intraband phenomena associated with the motion of particles in a periodic potential and subject to constant and uniform forces. Such forces can be provided by an electric field in the example of charged carriers in a crystal, or by other means, such as the gravitational force or gradients in a magnetic trap, in the example of ultracold neutral atoms in optical lattices. Naïvely one would distinguish between inter- and intraband effects using the energy bands and associated Bloch states obtained from diagonalization of the Hamiltonian involving the unperturbed periodic potential; intraband phenomena would be those not requiring physical quantities associated with more than one band. This simple approach is not sufficient because the applied forces that drive what is undoubtedly intraband motion – for instance, Bloch oscillations – inevitably also couple the original bands characterizing the unperturbed periodic potential.

The interband coupling induced by a weak force slowly varying in time and space has a particular form, and can be used to redefine the Bloch states associated with the unperturbed periodic potential. We studied the dynamics of wave packets of these modified Bloch states associated with one of the original bands; the response of this type of wave packet to an applied force is very different from the response of wave packets
formed by the original Bloch states from the same band. A particle described by a wave packet prepared in one of the original Bloch bands responds initially to a force as a free particle. In contrast, a particle described by a wave packet of modified Bloch states, associated with the same original band, responds according to the usual effective mass theorem and anomalous transport, derived from the usual semiclassical theory of wave packet dynamics.

As discussed in Chapter 1, dc fields also modify optical absorption, as in the Franz-Keldysh effect. Here the fact that the dc field couples the original Bloch bands also plays an important role, as shown in the calculations of the Franz-Keldysh effect presented in this thesis. We combined a full account of this coupling (calculated within $k \cdot p$ models) with the inclusion of the electron-hole interaction, developing a theoretical framework and a numerical approach appropriate for calculations with realistic band models.

In Chapter 2 we derived semianalytical expressions for the dynamics of wave packets prepared in one band and subject to a uniform force, which is suddenly applied and remains constant afterwards. We found that the usual semiclassical description requires corrections due to the initial condition of the wave packet. These corrections lead not only to an initial response with the bare mass but also to dynamical oscillations about the usual expressions from the semiclassical theory; therefore, it is convenient to introduce dynamical versions of the inverse effective mass tensor, the group velocity, and the anomalous velocity, which can replace their usual counterparts when the force is applied suddenly instead of slowly in time. We also found it necessary to introduce a dynamical anomalous acceleration to fully describe the modifications to the acceleration.

The experimental observation of the dynamics described in Chapter 2 is challenging in typical solid-state systems, but it is more accessible in optical lattices, which provide a highly tunable and clean potential for ultracold atoms. In Chapters 3 and 4 we illustrated the dynamics of the effective mass and the anomalous velocity in the context of experiments with ultracold atoms in optical lattices. In the one-dimensional case discussed in
Chapter 3, anomalous transport is not present, and effects associated with the dynamical inverse effective mass can be studied in isolation. We showed simulations with various parameters of the wave packet and the lattice; our results motivated the experiments that confirmed the dynamics of the inverse effective mass in this type of lattice [68]. In the two-dimensional case, we expect the dynamics to be richer because topological properties of the lattice enter the scene; we presented simulations where oscillations associated with the dynamics of the anomalous transport are significant, complementing the results from the one-dimensional case. For two dimensions, experiments confirming these dynamics have not been carried out yet, but recent progress in two-dimensional optical lattices suggests that such experiments can be performed in the near future. Moreover, advances in attosecond science applied to solid-state systems are opening possibilities to observe and control ultrafast dynamics of charged carriers in this type of system; thus, the results of our study can also become relevant in the context of solid-state physics.

In Chapter 5 we turned our attention to the modification of optical absorption by the presence of a dc field, the Franz-Keldysh effect. We improved previous descriptions by including both interband coupling due the dc field and excitonic effects due to the electron-hole interaction. We proposed a scheme in which the time evolution of the interband polarization is calculated as an intermediate step before the absorption coefficient. Our results confirmed expectations following from simpler models, such as the parabolic two-band model, when the electron-hole interaction is included; the main prediction of these simpler models is an enhancement of the absorption coefficient, which we observed with a more sophisticated 14-band model for bulk GaAs. More interestingly, we found that the particular features predicted by independent particle calculations with the 14-band model are not washed out by the Coulomb interaction, but they are more visible. One of these features, which can motivate further research in this area, is the dependence on the polarization of the optical field relative to the dc field. In this regard, we found that the Coulomb interaction modifies the difference between the absorption
coefficient for optical polarizations parallel and perpendicular to the dc field calculated in the independent particle approximation.

The calculations of the Franz-Keldysh effect presented in Chapter 5 were numerically challenging because our goal was to use realistic many-band models in order to consider properly the effects of the interband coupling. In the independent particle case, lines in reciprocal space parallel to the dc field can be treated separately when calculating the interband polarization and the absorption coefficient; this feature simplifies the computation as the work can be split into separate calculations that can be run in parallel, independently of each other. However, when the Coulomb interaction is included, it is necessary to calculate a convolution integral where the Coulomb potential couples each point of the grid with its neighbors, and so it is not possible to consider the lines parallel to the dc field as independent. Our strategy to deal with this and other issues of the numerical calculation of the Franz-Keldysh effect was described in Chapter 6.

The work presented here opens new directions in the study of transport and optical phenomena of particles in periodic potentials. The observation of the dynamics of the inverse effective mass in one-dimensional optical lattices is an incentive for future experiments not only in optical lattices of higher dimensionality but also in solid-state systems. Additionally, since our results for the dynamics of wave packets are restricted to the non-interacting regime, an interesting direction for future research is the effect of interactions between particles on the dynamics of their effective mass and anomalous velocity. Finally, our work on the Franz-Keldysh effect constitutes a theoretical improvement aimed at more detailed comparisons between theory and experiment. Regarding this point, the results from our numerical calculations suggest that aspects of the interplay between the band structure features and the electron-hole interaction need further investigation; one example is the effect of the Coulomb interaction on the polarization anisotropy predicted by independent particle calculations.
Appendix A

Wannier’s decoupling procedure

In this appendix we sketch the method developed by Wannier in [43] to decouple the bands to any order in the force $F$. We can rewrite Eq. (2.46) as

$$\left[ \mathcal{H}_o - \mathbf{F} \cdot (\mathbf{r} + i \nabla_k) \right] \phi_{nk}(\mathbf{r}) = W_n(k) \phi_{nk}(\mathbf{r}),$$

(A.1)

where

$$\mathcal{H}_o \equiv -\frac{\hbar^2}{2m} \nabla^2 + V(\mathbf{r}) \quad \text{and} \quad \phi_{nk}(\mathbf{r}) \equiv \langle \mathbf{r} | \phi_{nk} \rangle$$

(A.2)

are the coordinate representations of the unperturbed Hamiltonian operator $\hat{H}_o$ and the modified Bloch state $|\phi_{nk}\rangle$, respectively (see Eqs. (2.2) and Eq. (2.42)). Note that equation (A.1) takes the form of an eigenvalue problem, but with the peculiarity that both the operator (acting on $\phi_{nk}(\mathbf{r})$) and $W_n(k)$ depend on $k$.

The parameter $\tilde{F}$ introduced in Eq. (3.30) is appropriate to characterize how strong the external force is with respect to the lattice potential. For convenience, we use the other dimensionless variables defined in (3.29), and we also introduce

$$\hat{\mathcal{H}}_o \equiv \frac{\mathcal{H}_o}{E_R}, \quad \hat{W}_n(\mathbf{k}) \equiv \frac{W_n(k)}{E_R}, \quad \hat{\mathbf{r}} \equiv k_R \mathbf{r}, \quad \hat{\psi}_{nk}(\hat{\mathbf{r}}) \equiv \psi_{nk}(\mathbf{r}), \quad \text{and} \quad \hat{U}_{n_1n_2}(\mathbf{k}) \equiv U_{n_1n_2}(\mathbf{k}).$$

(A.3)

With these definitions Eq. (A.1) can be rewritten as

$$\sum_{n'} \left[ \hat{\mathcal{H}}_o - \hat{\mathcal{F}} \cdot (\hat{\mathbf{r}} + i \hat{\nabla}_{\mathbf{k}}) \right] \hat{\psi}_{n'k}(\hat{\mathbf{r}}) \hat{U}_{n'n}(\hat{\mathbf{k}}) = \hat{W}_n(\hat{\mathbf{k}}) \sum_{n'} \hat{\psi}_{n'k}(\hat{\mathbf{r}}) \hat{U}_{n'n}(\hat{\mathbf{k}}).$$

(A.4)
We attempt to solve this equation expressing

\[ U_{n_{1}n_{2}}(\mathbf{k}) \approx \sum_{\alpha} U_{n_{1}n_{2}}^{(\alpha)}(\mathbf{k}) \hat{F}^{\alpha} \quad \text{and} \quad \hat{W}_{n}(\mathbf{k}) \approx \sum_{\alpha} \hat{W}_{n}^{(\alpha)}(\mathbf{k}) \hat{F}^{\alpha} \]  

as power series in \( \hat{F} \). It is assumed that the zeroth order corresponds to the usual Bloch states and band energies. Thus we set

\[ \hat{U}_{n_{1}n_{2}}^{(0)}(\mathbf{k}) = \delta_{n_{1}n_{2}} \quad \text{and} \quad \hat{W}_{n}^{(0)}(\mathbf{k}) = \hat{E}_{n}(\mathbf{k}). \]  

Replacing the expansions from Eq. (A.5) in Eq. (A.4) and collecting terms with equal powers of \( \hat{F} \), we can find a recurrent system of equations. To first order, it is found that \( \hat{W}_{n}(\mathbf{k}) \) and \( \hat{U}_{n_{1}n_{2}}(\mathbf{k}) \) are given by Eq. (2.51) and (2.54) in the original variables \([39, 43]\).

Note that if \( \hat{F} \) is small we expect the parameter \( |\Delta_{n_{1}n_{2}}(\mathbf{k})| \), defined in Eq. (2.55), to be small; for instance, in the context of experiments with optical lattices (discussed in Chapters 3 and 4), \( \xi_{n_{1}n_{2}}(\mathbf{k}) \) is of the order of the lattice constant, while the energy difference is of the order of the recoil energy, and so we conclude that \( |\Delta_{n_{1}n_{2}}(\mathbf{k})| \) is of the order of \( \hat{F} \).
Appendix B

Derivation of the dynamical corrections

In this appendix we sketch the proofs of some of the main results presented in Chapter 2.

B.1 Matrix elements in the modified Bloch basis

The matrix elements of the momentum operator and the lattice force in the basis formed by the modified Bloch states were defined in Eqs. (2.64) and (2.65), respectively. Using the property $\Delta^\dagger(k) = -\Delta(k)$, we can rewrite them as

$$
\mathcal{P}_{n_1n_2}(k) \approx p_{n_1n_2}^a(k) + \sum_{n'_2} p_{n_1n'_2}(k) \Delta_{n'_2n_2}(k) - \sum_{n'_1} \Delta_{n_1n'_1}(k) p_{n'_1n_2}^a(k) \quad (B.1)
$$

and

$$
\mathcal{F}_{n_1n_2}^a(k) \approx i\omega_{n_1n_2}(k)p_{n_1n_2}^a(k) + \sum_{n'_2} i\omega_{n_1n'_2}(k)p_{n_1n'_2}(k) \Delta_{n'_2n_2}(k) - \sum_{n'_1} \Delta_{n_1n'_1}(k)i\omega_{n'_1n_2}(k)p_{n'_1n_2}^a(k) \quad (B.2)
$$

to first order in the force.

The diagonal elements ($n_1 = n_2 = n$) can be reduced to

$$
\mathcal{P}_{nn}^a(k) \approx p_{nn}^a(k) + \sum_{n'} (p_{nn'}^a(k)\Delta_{n'n}(k) - \Delta_{nn'}(k)p_{nn'}^a(k))
$$

$$
= p_{nn}^a(k) + \frac{m}{\hbar} \sum_{n' \neq n} 2 \text{Im} \left[ \xi_{nn'}^a(k)\xi_{nn'}^b(k) \right] F^b = p_{nn}^a(k) + m\nu_{nn}^{an,a}(k) \quad (B.3)
$$
and

\[ \mathcal{F}_{nn}^{a}(k) \approx \sum_{n'} (i\omega_{nn'}(k)p_{nn'}^a(k)\Delta_{n'n}(k) - \Delta_{nn'}(k)i\omega_{n'n}(k)p_{n'n}^a(k)) \]

\[ = \frac{1}{m} \sum_{n' \neq n} \frac{2 \text{Re}[p_{nn'}^a(k)p_{n'n}^b(k)]}{\hbar \omega_{nn'}(k)} F_b = \left( m \left[ \frac{1}{m_n^*(k)} \right]^{ab} - \delta^{ab} \right) F^b, \quad (B.4) \]

where we used Eq. (2.16) and the sum rules in Eqs. (2.68) and (2.69). Using Eqs. (B.3) and (B.4) for \( \mathcal{P}_{NN}^{a}(k) \) and \( \mathcal{F}_{NN}^{a}(k) \) in Eqs. (2.66) and (2.67) we recover the usual semiclassical results, Eqs. (2.70) and (2.71).

## B.2 Dynamical corrections

Since \( b_N(k,t) \) and \( b_{n \neq N}(k,t) \) are of zeroth and first order in \( \Delta(k) \), respectively, Eqs. (2.78) and (2.79) become

\[ \langle \hat{v}^a(t) \rangle \approx \frac{1}{m} \int_{BZ} dk |b_N(k,t)|^2 \mathcal{P}_{NN}^{a}(k) + \frac{1}{m} \sum_{n \neq N} \int_{BZ} dk (b_{N}^*(k,t)b_{n}(k,t) \mathcal{P}_{NN}^{a}(k) + c.c.) \]

(B.5)

and

\[ \langle \hat{a}^a(t) \rangle \approx \frac{F^a}{m} + \frac{1}{m} \int_{BZ} dk |b_N(k,t)|^2 \mathcal{F}_{NN}^{a}(k) \]

\[ + \frac{1}{m} \sum_{n \neq N} \int_{BZ} dk (b_{N}^*(k,t)b_{n}(k,t) \mathcal{F}_{NN}^{a}(k) + c.c.) , \quad (B.6) \]

keeping only terms up to first order. If we ignore the last term on the right-hand-side of each of these expressions, they reduce to the usual semiclassical results, Eqs. (2.70) and (2.71) as shown in the previous section. Now we consider the additional terms, which describe the dynamical oscillations induced by the sudden application of the force. Note that we only need to include the zeroth order contributions from \( \mathcal{P}_{NN}^{a}(k) \) and \( \mathcal{F}_{NN}^{a}(k) \), since \( b_{n \neq N}(k,t) \) is of first order; therefore, we can write

\[ b_{N}^*(k,t)b_{n}(k,t) \mathcal{P}_{NN}^{a}(k) \approx b_{N}^*(k,t)b_{n}(k,t)p_{NN}^a(k) \approx -|f_N(k)|^2 \Delta_{N}(k)e^{-i\gamma_{NN}(k,t)p_{NN}^a(k)} \]

\[ = -\frac{m}{\hbar} |f_N(k)|^2 \frac{\omega_{NN}(k)}{\omega_{NN}(k)} \frac{1}{\xi_{NN}^a(k)} \xi_{NN}^b(k) e^{-i\gamma_{NN}(k,t)} F^b \quad (B.7) \]
and

\[ b_N^a(k, t) b_n(k, t) \tilde{\xi}^a_{NN}(k) \approx b_N^a(k, t) b_n(k, t) i \omega_{NN}(k) p_{NN}^a(k) \]

\[ \approx -|f_N(\kappa)|^2 \Delta_{NN}(\kappa) e^{-i\gamma_{NN}(\kappa, t)} i \omega_{NN}(k) p_{NN}^a(k) \]

\[ = \frac{m}{\hbar} |f_N(\kappa)|^2 \left( \frac{\omega_{NN}(k)}{\omega_{NN}(\kappa)} \right)^2 \xi_{NN}^a(k) \xi_{nn}^b(k) e^{-i\gamma_{NN}(\kappa, t)} F^b, \] (B.8)

where we used Eqs. (2.16) and (2.75). When we combine these expressions with their complex conjugates we find

\[ b_N^a(k, t) b_n(k, t) \Xi_{NN}^a(k) + \text{c.c.} \approx -\frac{m}{\hbar} |f_N(\kappa)|^2 \left( \frac{\omega_{NN}(k)}{\omega_{NN}(\kappa)} \right)^2 2 \text{Im} \left[ \xi_{NN}^a(k) \xi_{nn}^b(k) e^{-i\gamma_{NN}(\kappa, t)} \right] F^b \] (B.9)

and

\[ b_N^a(k, t) b_n(k, t) \tilde{\xi}^a_{NN}(k) + \text{c.c.} \approx \frac{m}{\hbar} |f_N(\kappa)|^2 \left( \frac{\omega_{NN}(k)}{\omega_{NN}(\kappa)} \right)^2 2 \text{Re} \left[ \xi_{NN}^a(k) \xi_{nn}^b(k) e^{-i\gamma_{NN}(\kappa, t)} \right] F^b. \] (B.10)

After summing each of these expressions over all the bands \( n \neq N \), we can write

\[ \sum_{n \neq N} (b_N^a(k, t) b_n(k, t) \Xi_{NN}^a(k) + \text{c.c.}) \approx m |f_N(\kappa)|^2 \left( -\frac{1}{\hbar} \mathcal{J}_N^{ab}(k, t) F^b \right) \] (B.11)

and

\[ \sum_{n \neq N} (b_N^a(k, t) b_n(k, t) \tilde{\xi}^a_{NN}(k) + \text{c.c.}) \approx m |f_N(\kappa)|^2 \left( -\frac{1}{m} \mathcal{K}_N^{ab}(k, t) F^b \right), \] (B.12)

where \( \mathcal{J}_N^{ab}(k, t) \) and \( \mathcal{K}_N^{ab}(k, t) \) are given by Eqs. (2.83) and (2.84), respectively. Note that the terms inside the parentheses in Eqs. (B.11) and (B.12) are precisely the definitions of \( \mathcal{V}_n^a(k, t) \) and \( \mathcal{A}_N^{ab}(k, t) \) (see Eq. (2.82)); therefore, we have

\[ \frac{1}{m} \sum_{n \neq N} \int_{BZ} dk (b_N^a(k, t) b_n(k, t) \Xi_{NN}^a(k) + \text{c.c.}) \approx \int_{BZ} dk |f_N(\kappa)|^2 \mathcal{V}_n^a(k, t) \] (B.13)

and

\[ \frac{1}{m} \sum_{n \neq N} \int_{BZ} dk (b_N^a(k, t) b_n(k, t) \tilde{\xi}^a_{NN}(k) + \text{c.c.}) \approx \int_{BZ} dk |f_N(\kappa)|^2 \mathcal{A}_N^{ab}(k, t) \] (B.14)

to first order in the force. After replacing Eqs. (B.13) and (B.14) in Eqs. (B.5) and (B.6), we recover the expectation values with the dynamical corrections, Eqs. (2.80) and (2.81).
B.3  Decomposition of the dynamical corrections

The decomposition of the tensors $J_{N}^{ab}(k, t)$ and $K_{N}^{ab}(k, t)$ in symmetric and antisymmetric parts (see Eq. (2.86)) is given by

$$
\tilde{J}_{N}^{ab}(k, t) \equiv \frac{1}{2} \left( J_{N}^{ab}(k, t) \pm J_{N}^{ba}(k, t) \right) \quad \text{and} \quad \tilde{K}_{N}^{ab}(k, t) \equiv \frac{1}{2} \left( K_{N}^{ab}(k, t) \pm K_{N}^{ba}(k, t) \right),
$$

(B.15)

where the upper bar and plus sign correspond to the symmetric part, and the lower tilde and minus sign correspond to the antisymmetric part. Using the definitions Eqs. (2.83) and (2.84), we can write

$$
\tilde{J}_{N}^{ab}(k, t) = \sum_{n \neq N} \text{Im} \left[ \xi_{Nn}(k) \xi_{nN}(\kappa)e^{-i\gamma_{N}(\kappa,t)} \mp \xi_{Nn}(\kappa)e^{-i\gamma_{N}(\kappa,t)} \xi_{nN}(k) \right] \frac{\omega_{nN}(k)}{\omega_{nN}(\kappa)}
$$

(B.16)

and

$$
\tilde{K}_{N}^{ab}(k, t) = -\frac{m}{\hbar} \sum_{n \neq N} \text{Re} \left[ \xi_{Nn}(k) \xi_{nN}(\kappa)e^{-i\gamma_{N}(\kappa,t)} \mp \xi_{Nn}(\kappa)e^{-i\gamma_{N}(\kappa,t)} \xi_{nN}(k) \right] \frac{(\omega_{nN}(k))^2}{\omega_{nN}(\kappa)},
$$

(B.17)

which reduce to Eqs. (2.88) and (2.89) with the definition of $X_{Nn}^{\pm,ab}(k, t)$ in Eq. (2.87).

B.4  Time derivative of the velocity terms

In order to check the consistency of the pairs of expressions found for the velocity and the acceleration of the wave packet $|\tilde{\phi}_{N}(t)\rangle$ (Eqs. (2.70) and (2.71)) and of the wave packet $|\Psi(t)\rangle$ (Eqs. (2.80) and (2.81)), we show explicitly that the time derivative of the velocity terms leads to the corresponding acceleration terms to first order in the force. For calculating these derivatives it will be useful to consider the time derivative of integrals of the form

$$
\mathcal{I}(t) \equiv \int_{BZ} d\kappa \ h(\kappa) j(\kappa, t),
$$

(B.18)

where $h(\kappa)$ and $j(\kappa, t)$ are functions with the periodicity of the reciprocal lattice, $h(\kappa + G) = h(\kappa)$ and $j(\kappa + G, t) = j(\kappa, t)$; the moving-frame wave vector $\kappa$ depends on time,
and it is defined in Eq. (2.47). We can write

\[
\frac{d}{dt} I(t) = \int_{BZ} dk \frac{\partial}{\partial t} (h(\kappa)) j(k, t) + \int_{BZ} dk h(\kappa) \frac{\partial}{\partial t} j(k, t) \\
= -\frac{1}{\hbar} \int_{BZ} dk \left( F \cdot \nabla_k h(\kappa') \right) j(k', t) + \int_{BZ} dk h(\kappa) \frac{\partial}{\partial t} j(k, t) \\
= -\frac{1}{\hbar} F^b \int_{BZ} dk \left( \frac{\partial}{\partial k^b} h(\kappa) \right) j(k, t) + \int_{BZ} dk h(\kappa) \frac{\partial}{\partial t} j(k, t) \\
= \int_{BZ} dk h(\kappa) \frac{1}{\hbar} \frac{\partial}{\partial k^b} j(k, t) F^b + \int_{BZ} dk h(\kappa) \frac{\partial}{\partial t} j(k, t),
\]

(B.19)

where we used the Green’s theorem for periodic functions in the last step (see Appendix I of [30]).

First, we use this result to prove Eq. (2.72) setting \( h(\kappa) = |\bar{b}_N(\kappa)|^2 \) and \( j(k, t) = v_{N}^{g,a}(k) \). In this case, \( j(k, t) \) is independent of time; therefore, only the first term in Eq. (B.19) contributes, and clearly we have

\[
\frac{1}{\hbar} \frac{\partial}{\partial k^b} j(k, t) = \frac{1}{\hbar} \frac{\partial}{\partial k^b} v_{N}^{g,a}(k) = \left[ \frac{1}{m_N^*(k)} \right]^{\gamma}_{ab}.
\]

(B.20)

If instead of the local group velocity we use the local anomalous velocity, \( j(k, t) = v_{N}^{a,n,a}(k) \), then \( dI(t)/dt \) is of second order in the force; thus, the time derivative of the anomalous velocity does not contribute to Eq. (2.71).

The connection between Eqs. (2.80) and (2.81) is slightly more complicated because of the additional term \( V_{N}^a(k, t) \). In this case, we set \( h(\kappa) = |f_N(\kappa)|^2 \) and \( j(k, t) = V_{N}^a(k, t) \) in Eq. (B.19). Note that since \( V_{N}^a(k, t) \) is already of first order in the force, the first term in Eq. (B.19) does not contribute; the second term, does contribute because of the time dependence of \( V_{N}^a(k, t) \). This time dependence comes from the moving-frame wave vector \( \kappa \) and from the explicit time dependence of the phase \( \gamma_{nN}(k, t) \) in Eq. (2.83); however, the time derivative of \( \kappa \) is proportional to the force, and consequently it does
not contribute to first order in the force. Hence, we can write
\[
\frac{\partial}{\partial t} j(k, t) = -\frac{1}{\hbar} \frac{\partial}{\partial t} J^a_b(k, t) F^b
\]
\[
\approx -\frac{1}{\hbar} \sum_{n \neq N} \frac{\omega_{nN}(k)}{\omega_{nN}(\kappa)} 2 \text{Im} \left[ \xi^a_{nN}(k) \xi^b_{nN}(\kappa) \frac{\partial}{\partial t} (e^{-i\gamma_{nN}(\kappa, t)}) \right] F^b
\]
\[
\approx -\frac{1}{\hbar} \sum_{n \neq N} \frac{\omega_{nN}(k)}{\omega_{nN}(\kappa)} 2 \text{Im} \left[ \xi^a_{nN}(k) \xi^b_{nN}(\kappa) (-i\omega_{nN}(k)e^{-i\gamma_{nN}(\kappa, t)}) \right] F^b
\]
\[
= -\frac{1}{m} \tilde{K}^a_b(k, t) F^b = A^a_N(k, t),
\]
and we recover Eq. (2.81) from the time derivative of Eq. (2.80) (to first order in the force).

Following similar steps to those leading to Eq. (B.21) where \( j(k, t) = V^a_N(k, t) = -J^a_b(k, t) F^b / \hbar \), we can show that for \( j(k, t) = -\tilde{J}^a_b(k, t) F^b / \hbar \) we have
\[
\frac{\partial}{\partial t} j(k, t) = -\frac{1}{\hbar} \frac{\partial}{\partial t} \tilde{J}^a_b(k, t) F^b
\]
\[
\approx -\frac{1}{\hbar} \sum_{n \neq N} \frac{\omega_{nN}(k)}{\omega_{nN}(\kappa)} \text{Im} \left[ \xi^a_{nN}(k) \xi^b_{nN}(\kappa) \frac{\partial}{\partial t} (e^{-i\gamma_{nN}(\kappa, t)}) \right]
\]
\[
\mp \xi^a_{nN}(\kappa) \frac{\partial}{\partial t} (e^{-i\gamma_{nN}(\kappa, t)}) \xi^b_{nN}(k) F^b
\]
\[
\approx -\frac{1}{\hbar} \sum_{n \neq N} \frac{\omega_{nN}(k)}{\omega_{nN}(\kappa)} \text{Im} \left[ \xi^a_{nN}(k) \xi^b_{nN}(\kappa) (-i\omega_{nN}(k)e^{-i\gamma_{nN}(\kappa, t)}) \right]
\]
\[
\mp \xi^a_{nN}(\kappa) (-i\omega_{nN}(k)e^{-i\gamma_{nN}(\kappa, t)}) \xi^b_{nN}(k) F^b
\]
\[
= -\frac{1}{m} \tilde{K}^a_b(k, t) F^b.
\]
Using \( h(\kappa) = |f_N(\kappa)|^2 \) again, Eq. (B.22) serves to prove Eqs. (2.98) and (2.102), which correspond to the contributions to the expectation value of the acceleration in the decomposition Eq. (2.101).
Appendix C

Gauge-independent dynamical equation
for the lesser Green function $G^<(k, t)$

In this appendix we derive Eq. (5.8) starting with the formalism of non-equilibrium Green functions and using a basis of Wannier functions modified to obtain gauge-independent expressions [23, 124, 125, 152, 160]. This derivation presents a framework to deal with more general problems than the one assumed in Eq. (5.8), but we show how such a framework reduces to the simple case.

For a general non-equilibrium situation we introduce the matrix Green function

$$
\mathcal{G}(r_1, t_1; r_2, t_2) \equiv \begin{pmatrix}
G_c(r_1, t_1; r_2, t_2) & G^<(r_1, t_1; r_2, t_2) \\
G^>(r_1, t_1; r_2, t_2) & G_c(r_1, t_1; r_2, t_2)
\end{pmatrix},
$$

(C.1)

which contains the lesser Green function Eq. (5.1) and three more types of Green functions in real time:

\begin{align*}
G^>(r_1, t_1; r_2, t_2) &\equiv \frac{1}{i\hbar} \langle \hat{\Psi}(r_1, t_1) \hat{\Psi}^\dagger(r_2, t_2) \rangle, \quad (C.2) \\
G_c(r_1, t_1; r_2, t_2) &\equiv \theta(t_2 - t_1)G^<(r_1, t_1; r_2, t_2) + \theta(t_1 - t_2)G^>(r_1, t_1; r_2, t_2), \quad (C.3) \\
G_c(r_1, t_1; r_2, t_2) &\equiv \theta(t_1 - t_2)G^<(r_1, t_1; r_2, t_2) + \theta(t_2 - t_1)G^>(r_1, t_1; r_2, t_2). \quad (C.4)
\end{align*}

For the last two, $\theta(\cdot)$ denotes the Heaviside step function. The matrix Green function...
satisfies the Dyson equation
\[
\left[i\hbar \frac{\partial}{\partial t_1} - \mathcal{H}_{\text{m.c.}}(\mathbf{r}_1, t_1)\right] \check{\mathcal{G}}(\mathbf{r}_1, t_1; \mathbf{r}_2, t_2) - \int \check{\Sigma}(\mathbf{r}_1, t_1; \mathbf{r}_3, t_3) \check{\mathcal{G}}^< (\mathbf{r}_3, t_3; \mathbf{r}_2, t_2) d\mathbf{r}_3 dt_3 \\
= \delta(\mathbf{r}_1 - \mathbf{r}_2)\delta(t_1 - t_2) \check{\tau}_3 \tag{C.5}
\]
and its adjoint, where
\[
\mathcal{H}_{\text{m.c.}}(\mathbf{r}, t) \equiv \frac{1}{2m} \left( \frac{\hbar}{i} \nabla_\mathbf{r} - \frac{e}{c} \mathbf{A}(\mathbf{r}, t) \right)^2 + V(\mathbf{r}) + eA_4(\mathbf{r}, t) \tag{C.6}
\]
is the coordinate representation of the minimal coupling Hamiltonian introduced in Eq. (1.1) (see Chapter 1). We also include a self-energy \(\check{\Sigma}(\mathbf{r}_1, t_1; \mathbf{r}_2, t_2)\), which contains the many-body effects. The third Pauli matrix,
\[
\check{\tau}_3 \equiv \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \tag{C.7}
\]
keeps track of the correct combination of Green functions in \(\check{\mathcal{G}}(\mathbf{r}_1, t_1; \mathbf{r}_2, t_2)\) [160].

It is convenient to use a gauge-independent formalism where Eq. (C.5) and its adjoint are formulated in terms of the electromagnetic fields instead of the potentials in \(\mathcal{H}_{\text{m.c.}}(\mathbf{r}, t)\). Following the approach of Kita and Yamashita [23], we introduce modified Wannier functions [161]
\[
W'_\nu(\mathbf{r}, t) \equiv e^{iI_{\mathbf{rR}}(t)} W_\nu(\mathbf{r}), \tag{C.8}
\]
where
\[
W_\nu(\mathbf{r}) \equiv \sqrt{\frac{\text{V}_{\text{cell}}}{(2\pi)^3}} \int_{\text{BZ}} d\mathbf{k} \psi_{n_k}(\mathbf{r}) e^{-i\mathbf{k} \cdot \mathbf{R}} \tag{C.9}
\]
are the usual Wannier functions [162], labeled by band index and lattice vector with \(\nu \equiv (n, \mathbf{R})\). In Eq. (C.9) we denote the volume of the unit cell by \(\text{V}_{\text{cell}}\) and use BZ for integration over the (first) Brillouin zone (see Sec. 2.1 in Chapter 2). The additional Peierls phase in Eq. (C.8) is given by
\[
I_{\mathbf{rR}}(t) \equiv \frac{e}{\hbar c} \int_{\mathbf{R}}^{\mathbf{r}} \mathbf{A}(\mathbf{r}', t) \cdot d\mathbf{r}' \tag{C.10}
\]
where the integration is along the straight line from \( R \) to \( r \) [163].

For situations where the only applied field is a uniform electric field \( E(t) \), we can start with a vector potential gauge such that

\[
A_4(r, t) = 0 \quad \text{and} \quad E(t) = -\frac{1}{c} \frac{\partial}{\partial t} A(t). \tag{C.11}
\]

In this case the \( W'_\nu(r, t) \) are orthogonal because \( A(t) \) is uniform.\(^1\) In order to make the Green function in the representation of the modified Wannier functions gauge-independent, we use the two-time Peierls phase

\[
\mathcal{I}(R_1, t_1; R_2, t_2) \equiv \frac{e}{\hbar c} \frac{R_1 - R_2}{t_1 - t_2} \int_{t_2}^{t_1} A(t) \cdot dt, \tag{C.12}
\]

which is a particular case of the general definition given by Kita and Yamashita [23]. Thus, we introduce the gauge-independent matrix Green function

\[
\tilde{G}_{\nu_1 \nu_2}(t_1, t_2) \equiv e^{-i\mathcal{I}(R_1, t_1; R_2, t_2)} \int W'^{\nu_1}_{\nu_1}(r_1, t_1) \tilde{G}(r_1, t_1; r_2, t_2) W'^{\nu_2}_{\nu_2}(r_2, t_2) dr_1 dr_2, \tag{C.13}
\]

which satisfies the Dyson equation

\[
i\hbar \frac{\partial}{\partial t_1} \tilde{G}_{\nu_1 \nu_2}(t_1, t_2) - \sum_{\nu_3} \int dt_3 \delta(t_1 - t_3) \left[ \frac{\hbar \phi_c \delta_{\nu_1 \nu_3}}{t_1 - t_2} \right. \\
\left. + e^{i\phi_c} (\beta_{\nu_1 \nu_3}(t_1) + \sum_{\nu_3} \nu_3(t_1)) \right] \tilde{G}_{\nu_1 \nu_2}(t_3, t_2) = \delta_{\nu_1 \nu_2} \delta(t_1 - t_2) \tau_3 \tag{C.14}
\]

and its adjoint. The function \( \phi_c \) is a gauge-independent combination of phases in a closed circuit in space-time [164],

\[
\phi_c \equiv \mathcal{I}(R_1, t_1; R_3, t_3) + \mathcal{I}(R_3, t_3; R_2, t_2) + \mathcal{I}(R_2, t_2; R_1, t_1). \tag{C.15}
\]

Additionally in Eq. (C.14), we introduced the single-particle energy

\[
\beta_{\nu_1 \nu_2}(t) \equiv \int W'^{\nu_1}_{\nu_1}(r) \left[ H_o - eE(t) \cdot (r - R_2) \right] W_{\nu_2}(r) dr \tag{C.16}
\]

\(^1\)There are strategies to deal with the more general case where the modified Wannier functions are not orthogonal due to a non-uniform vector potential \( A(r, t) \). See the discussion in [23].
Appendix C. Dynamical equation for the lesser Green function

(compare with Eq. (5.9) in Chapter 5), where \( \mathcal{H}_o \) is the coordinate representation of the unperturbed Hamiltonian \( \hat{\mathcal{H}}_o \) (see Eq. (A.2) in Appendix A), and for simplicity we assumed a self-energy singular in time,

\[
\tilde{\Sigma}(\mathbf{r}_1, t_1; \mathbf{r}_2, t_2) = \tilde{\Sigma}(\mathbf{r}_1, t_1) \delta(t_1 - t_2),
\]

which was projected on the modified Wannier function basis similarly to Eq. (C.13),

\[
\tilde{\Sigma}_{\nu_1 \nu_2}(t) \equiv \lim_{t_1, t_2 \to t} e^{-it\mathbf{r}(\mathbf{R}_1, t_1; \mathbf{R}_2, t_2)} \int W_{\nu_1}'(\mathbf{r}_1, t_1) \tilde{\Sigma}(\mathbf{r}_1, \mathbf{r}_2; t_1) W_{\nu_2}'(\mathbf{r}_2, t_2) \, d\mathbf{r}_1 d\mathbf{r}_2.
\]

In the Hartree-Fock approximation used here (see Eq. (5.2)) we can write

\[
\tilde{\Sigma}_{\nu_1 \nu_2}(t) = \Sigma_{\nu_1 \nu_2}(t) \tilde{\tau}_3,
\]

which decouples the four elements of the matrix Green function in Eq. (C.14) because it is proportional to \( \tilde{\tau}_3 \). There are further simplifications in the equal time limit, since the phase factor multiplying the single-particle and self-energy terms vanishes. Thus, we take the difference between Eq. (C.14) and its adjoint in the equal time limit for the lesser Green function,

\[
\left[ i\hbar \frac{\partial}{\partial t} + e(\mathbf{R}_1 - \mathbf{R}_2) \cdot \mathbf{E}(t) \right] G^<_{\nu_1 \nu_2}(t) - \sum_{\nu_3} \left[ (\beta_{\nu_1 \nu_3}(t) + \Sigma_{\nu_1 \nu_3}^{\text{ex}}(t)) G^<_{\nu_3 \nu_2}(t) 
- G^<_{\nu_1 \nu_3}(t) (\beta_{\nu_3 \nu_2}(t) + \Sigma_{\nu_3 \nu_2}^{\text{ex}}(t)) \right] = 0, \tag{C.20}
\]

where

\[
G^<_{\nu_1 \nu_2}(t) \equiv \lim_{t_1, t_2 \to t} G^<_{\nu_1 \nu_2}(t_1, t_2). \tag{C.21}
\]

The single-particle energy, Eq. (C.16), depends on the lattice vectors only through the relative coordinate \( \mathbf{R} \equiv \mathbf{R}_1 - \mathbf{R}_2 \); therefore, we can write

\[
\beta_{n_1 n_2}(\mathbf{R}, t) = \int W^*_n(\mathbf{r} - \mathbf{R}) [\mathcal{H}_o - e\mathbf{E}(t) \cdot \mathbf{r}] W_{n_2}(\mathbf{r}) \, d\mathbf{r} \tag{C.22}
\]

for \( \beta_{\nu_1 \nu_2}(t) \). Note that \(-e\mathbf{E}(t) \cdot \mathbf{r}\) could be replaced by \(-e\mathbf{E}(t) \cdot (\mathbf{r} - \mathbf{R})\), since Wannier functions at different lattice sites are orthogonal. In Eq. (C.22) we denoted the Wannier
function for band \( n \) and \( \mathbf{R} = 0 \) by \( W_n(r) \). Furthermore, if we assume that \( G_{\nu_1,\nu_2}^<(t) \) also depends on the lattice vectors only through the relative coordinate, it can be shown that the same property holds for the self-energy \( \Sigma_{\nu_1,\nu_2}^{ex}(t) \). Thus, we can simply write \( G_{n_1 n_2}^<(\mathbf{R},t) \) for \( G_{\nu_1,\nu_2}^<(t) \) and

\[
\Sigma_{n_1 n_2}(\mathbf{R},t) = i\hbar \sum_{\nu'_1\nu'_2} U_{n_1 n_2}^{\nu'_1\nu'_2}(\mathbf{R}) G_{n'_1 n'_2}^<(\mathbf{R}'_1 - \mathbf{R}'_2 + \mathbf{R},t) \tag{C.23}
\]

for \( \Sigma_{\nu_1,\nu_2}^{ex}(t) \). In Eq. (C.23) we introduced the matrix element of the Coulomb interaction in the Wannier function basis as

\[
U_{n_1 n_2}^{\nu_1'\nu_2'}(\mathbf{R}) = \int W_{n_1}^*(r_1) W_{\nu_1'}(r_1) U(r_1 - r_2 + \mathbf{R}) W_{\nu_2'}^*(r_2) W_{n_2}(r_2) d\mathbf{r}_1 d\mathbf{r}_2. \tag{C.24}
\]

At this point we move to reciprocal space using the Fourier transform of \( G_{n_1 n_2}^<(\mathbf{R},t) \) according to

\[
G_{n_1 n_2}(\mathbf{k},t) = \sum_{\mathbf{R}} G_{n_1 n_2}^<(\mathbf{R},t) e^{-i\mathbf{k} \cdot \mathbf{R}}, \tag{C.25}
\]

which is equivalent to the Green function introduced in Eq. (5.6). Similarly, the energy terms, \( \beta_{n_1 n_2}(\mathbf{R},t) \) and \( \Sigma_{n_1 n_2}(\mathbf{R},t) \), become

\[
\beta_{n_1 n_2}(\mathbf{k},t) = \sum_{\mathbf{R}} \beta_{n_1 n_2}(\mathbf{R},t) e^{-i\mathbf{k} \cdot \mathbf{R}} \quad \text{and} \quad \Sigma_{n_1 n_2}(\mathbf{k},t) = \sum_{\mathbf{R}} \Sigma_{n_1 n_2}(\mathbf{R},t) e^{-i\mathbf{k} \cdot \mathbf{R}}. \tag{C.26}
\]

Using Eq. (C.9) and (C.23) we can write the matrix for the self-energy, whose elements are given by \( \Sigma_{n_1 n_2}(\mathbf{k},t) \), as

\[
\Sigma(\mathbf{k},t) = i\hbar \int \frac{d\mathbf{q}}{(2\pi)^3} U(\mathbf{q}) \sum_{\mathbf{R}'_1 \mathbf{R}'_2} \mathcal{O}(\mathbf{R}'_1, \mathbf{q}) G^<_{\mathbf{k}-\mathbf{q}, \mathbf{q},t} e^{i(k-q)(\mathbf{R}'_1-\mathbf{R}'_2)} \mathcal{O}^\dagger(\mathbf{R}'_2, \mathbf{q}), \tag{C.27}
\]

where \( \mathcal{O}(\mathbf{R}, \mathbf{q}) \) is a matrix in the band indices with elements

\[
\mathcal{O}_{n_1 n_2}(\mathbf{R}, \mathbf{q}) = \frac{V_{\text{cell}}}{(2\pi)^3} \int_{\text{BZ}} \! d\mathbf{k} \Delta_{n_1 n_2}(\mathbf{k}, \mathbf{k}-\mathbf{q}) e^{-i(k-q)\cdot\mathbf{R}} d\mathbf{k}, \tag{C.28}
\]

which contains the overlap matrix defined in Eq. (5.12); this expression for the self-energy reduces to Eq. (5.10). After these transformations we finally arrive at Eq. (5.8).
Bibliography


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