Physik Department

Diplomarbeit

A Dynamical Approach To Piezocurrents In Slowly Deformed Crystals

Maximilian Lein

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TECHNISCHE
UNIVERSITÄT
MÜNCHEN
Lehrstuhl M5
Prof. Dr. Herbert Spohn

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Maximilian Lein

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Contents

1 Introduction

In 1880 Pierre and Jacques Curie discovered that some crystals became macroscopically charged when subjected to mechanical strain. Lippmann predicted the converse (inverse) piezoelectric effect from thermodynamic principles one year later; the Curie brothers were able to confirm Lippmann's prediction the same year [Pie05].

Woldemar Voigt was the first to use tensor equations to relate mechanical stress and macroscopic polarization of the sample. His 'Lehrbuch der Kristallphysik' from 1910 remained the standard text up for the study of piezoelectric effects until the middle of the 20th century [Tra03].

Despite numerous applications of piezoelectric effects, gaining insight into the *microscopic* processes that are behind macroscopic effect took much longer. In the 1970s, Martin [Mar74] made a first step by pointing out that previous definitions of polarization in crystals on a microscopic level were ill-defined. But it took until 1993 when King-Smith and Vanderbilt derived polarization from first principles of linear response theory [KSV93]. Their ansatz was an earlier heuristic result by Resta [Res92] whose contributions to the field of polarization deserve mention as well.

1.1 Physics Of Polarization

Phenomenological approaches to piezoelectricity often use the idea of 'fundamental dipoles' that each unit cell contributes to the total polarization. The dipole within a unit cell is in that model attributed to a 'separation of charges'. While this may seem very intuitive, we will show in section 2.1 that this definition is unsuitable to serve as the basis for a microscopic treatment.

There are four different types of piezoelectric effects: direct and indirect piezoelectricity, ferroelectricity and the giant field-induced strain effect. Direct piezoelectricity refers to a strain-induced separation of charges; the converse effect, i. e. when a crystal changes shape after a voltage has been applied, is called indirect piezoelectric effect.

Ferroelectricity is the analog to ferromagnetism: a ferroelectric material remains permanently polarized even if the field, which aligned the 'microscopic dipoles' of the unit cells, is shut off. Like ferromagnetism, this is a mesoscopic effect.

The giant field-induced strain effect is a special case of indirect piezoelectricity. Usually the deformed Bravias lattice is essentially not changed; however some materials undergo a phase transition of crystal structure which allows significantly larger deformations (up to 10^{-3}) [FC00].

Ferroelectricity and the giant field-induced strain effect are more complicated mesoscopic and microscopic phenomena and as such beyond the scope of this thesis.

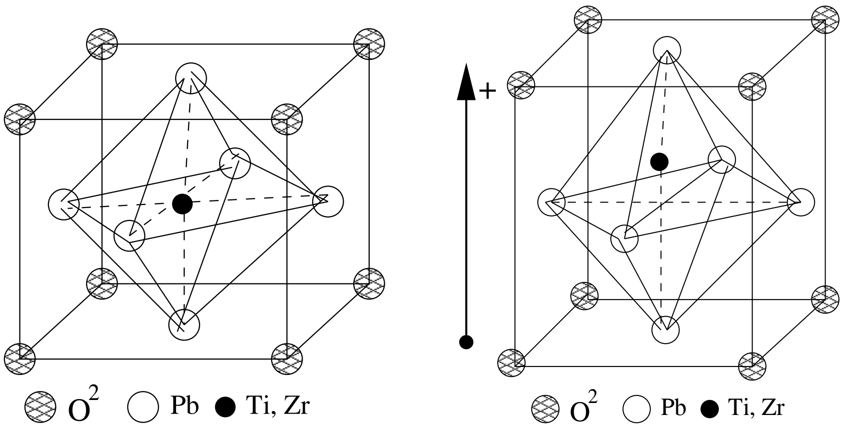

Figure 1.1: The crystal structure of lead zirconium titanate (pzt) [Wot00].

1.1.1 Materials And Applications

In 1917 Langevine developed a piezoelectric transducer for sonar made of quartz, probably the most famous piezoelectric material [Pie05]. Piezoelectric materials are either semiconductors or isolators; the most common are quartz and ceramics with tungsten-bronze crystal structure such as $\mathrm{BaTiO_3}$, $\mathrm{KNbO_3}$, $\mathrm{BiFeO_3}$ and $\mathrm{LiTaO_3}$.

Nowadays there is a large variety of applications for piezoelectric materials, among others sub-micrometer positioning devices (actuators) which are used to control the tips of atomic force microscopes or position mirrors in laser experiments [PI05]. High-end tweeters and small speakers for cell phones use a piezoelectric driver unit to convert the electric signal into sound waves.

The changes in length are rather small, typically ranging from $10^{-8} - 10^{-4}$; even though the relative deformation is small, the potential differences generated by those deformations can be in the 10^3 V range [Tra03].

1.1.2 Symmetries

The role of symmetries in physics cannot be underestimated. From the very beginning, Jacques and Pierre Curie realized that only materials lacking a center of inversion showed piezoelectric effects (21 of the 32 crystal classes are non-centrosymmetric) [Tra03]. Only 20 of the 32 crystal classes show *direct* piezoelectricity, cubic class 432, which has no center of inversion, but the same crystal form at opposite ends, exhibits only indirect piezoelectric effects.

1.1.3 Microscopic Approaches To Polarization

Although the piezoelectric effect is governed by rather simple macroscopic laws, significant progress to gain microscopic understanding was made only much later. In 1974 Martin [Mar74] realized that the prevalent microscopic definition of polarization was ill-defined as it depended on the particular choice of unit cell. To put another way *it is not sufficient* to know what is going on *inside* 'the' unit cell, but the polarization at the boundary has to be specified as well. His paper rendered the intuitive notion of 'dislocated ions' incomplete (see figure 1.1), although it is still used today [Wot00] [Tra03].

However it was only roughly 20 years later that King-Smith and Vanderbilt linked polarization (and thus piezoelectricity) to geometric phases assuming a linear response [KSV93]. They directly applied their concise formula GaAs using electronic structure calculations as input for their forumlas.

Their ansatz was based on an earlier heuristic result by Resta [Res92] who later derived the King-Smith–Vanderbilt formula more rigorously and contributed much to deepen the understanding of the relationship between piezoelectricity and geometric phases. He also proposed ways to go beyond the single-electron approximation and include multi-electron correlations in calculations of polarization effects.

1.2 Intention And Scope

Previous theoretical approaches to a microscopic understanding of piezoelectricity and other polarization effects were focussing on the kinematic aspects; the difference in polarization as a function of the changes in the system was at the end of such efforts.

In this thesis, we will focus on the *dynamics* of an electron in the piezoelectric crystal. We will derive equations of motion which include quantum corrections; as it turns out, those quantum corrections are necessary to understand piezoelectric effects. Before we detail on the scope of this thesis, we will define the model under consideration.

1.2.1 Definition Of The Problem

We consider an electron in the single-electron approximation in a crystalline solid whose Bravais lattice $\Gamma(t)$ is deformed adiabatically by an external force. For simplicity we assume our initial time to be $t = 0$; the Bravais lattice at $t = 0$ is $\Gamma_0 := \Gamma(0)$. By assumption the effective potential $V_{\Gamma(t)}(x)$ is periodic in the lattice at time t for all $\gamma(t) \in \Gamma(t)$ and $t \in \mathbb{R}$; it is generated by the atoms as well as all other electrons.

$$V_{\Gamma(t)}(x + \gamma(t)) = V_{\Gamma(t)}(x) \qquad \gamma(t) \in \Gamma(t) \qquad t \in \mathbb{R} \tag{1.1}$$

$\Gamma(t)$ is the time-dependent Bravais lattice which is spanned by linear combinations of the primitive lattice vectors $\{a_1(t), \ldots, a_d(t)\}$ with integer coefficients. The periodicity lattice $\Gamma(t)$ should not be confused with the sublattices of the crystal (a diamond's periodicity lattice for instance consists of two sublattices).

$$\Gamma(t) := \big\{\gamma(t) \in \mathbb{R}^d \mid \gamma(t) = \textstyle\sum_{j=1}^{d} n_j\, a_j(t),\, n_j \in \mathbb{N}_0\big\} \tag{1.2}$$

Physically we expect a non-trivial time-dependence of the potential *in addition* to the time-dependence due to the deformation, $V_{\Gamma(t)}(x,t)$; this non-trivial time-dependence describes the back-reaction of the system within a unit cell to the forced change of crystal lattice structure. However we do restrict ourselves to cases in which the crystal structure *does not* undergo a phase transition to another crystal structure, i. e. we exclude the giant field-induced strain effect mentioned earlier, a special case of direct polarization where the actual crystal structure changes. We assume this 'reconstruction' of the unit cell is an adiabatic process as well; to put another way the crystal potential $V_{\Gamma(t)}(x,t)$ at time t is always generated by the equilibrium structure within a unit cell.

We introduce a dimensionless parameter $\varepsilon \ll 1$, which is assumed to be small, that describes the separation of timescales between the deformation and the microscopic motion of the electron within a unit cell. We now replace t by εt, where t is the microscopic timescale of the system. This change in variables reflects the separation of microscopic and macroscopic timescales; from an 'electron's perspective' the crystal is deformed very slowly. If on the other hand we are interested in effects from the lattice deformation, we have to consider microscopic times t of order $\mathcal{O}(1/\varepsilon)$.

Thus the potential is given by $V_{\Gamma(\varepsilon t)}(x,\varepsilon t)$ and analogously all quantities derived from the potential such as band energies and eigenfunctions depend on εt as well. Every derivative with respect to microscopic time gives another ε prefactor.

The problem is considered in the one-electron approximation, so we neglect all electron-electron effects which cannot be cast in the form of local potentials (e. g. exchange effects). The single electron moves in a slowly varying potential generated by the atoms and all other electrons. Thus the Hamiltonian of the problem is given by

$$\begin{aligned}\hat{H}(\varepsilon t) &= \tfrac{\hbar^2}{2m_\mathrm{e}}\Delta_x + V_{\Gamma(\varepsilon t)}(x,\varepsilon t)\\ &= -\tfrac{1}{2}\Delta_x + V_{\Gamma(\varepsilon t)}(x,\varepsilon t)\end{aligned} \tag{1.3}$$

in convenient units such that $m_\mathrm{e} = 1$ and $\hbar = 1$. Δ_x is the d-dimensional Laplace operator. For physically relevant problems, we have $d \leq 3$. All spin-related effects such as spin-orbit coupling have been neglected.

We are interested in solutions of the *time-dependent* Schrödinger equation

$$i\frac{\mathrm{d}}{\mathrm{d}t}\Psi = \hat{H}(\varepsilon t)\Psi \qquad\qquad \Psi \in L^2(\mathbb{R}^d) \tag{1.4}$$

As the potential is periodic with respect to the instantaneous lattice $\Gamma(\varepsilon t)$ at all times, the Bloch theorem holds for the solutions to the Schrödinger equation $\psi_n(\cdot,\varepsilon t)$ at time $t \in \mathbb{R}$ [AM01, p. 166]. In other words, an eigenfunction ψ_n of the nth energy band is quasi-periodic in x.

$$\psi_n(x+\gamma(\varepsilon t),\varepsilon t) = c_n(\gamma(\varepsilon t))\,\psi_n(x,\varepsilon t) \qquad\qquad |c_n| = 1 \quad \forall t \in \mathbb{R}$$

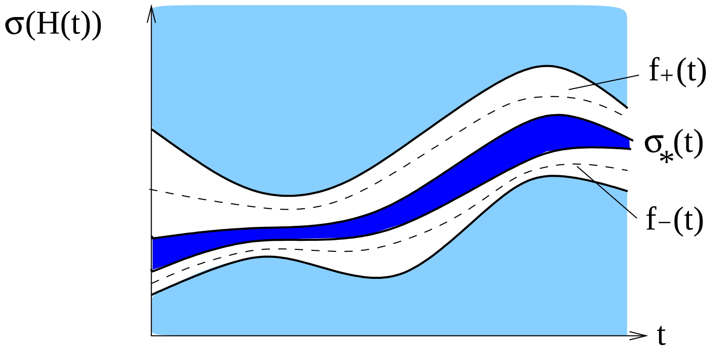

Figure 1.2: The spectral gap in the spectrum, with kind permission from the author [Teu03, p. 8].

Commutativity of translations yields that the unimodular prefactor is of the form $c_n(\gamma) = e^{ik\cdot\gamma}$ which means eigenfunctions are also characterized by the crystal momentum k, $\psi_n \equiv \psi_n(k, x, \varepsilon t) = e^{ik\cdot x}\, u_n(k, x, \varepsilon t)$ in addition to the band index n (in the crystal momentum representation). The Bloch functions $u_n(k, x, \varepsilon t)$ are periodic in the instantaneous crystal lattice $\Gamma(\varepsilon t)$, $u_n(k, x + \gamma(\varepsilon t), \varepsilon t) = u_n(k, x, \varepsilon t)$ for all times $t \in \mathbb{R}$.

We also assume we have solved the problem of calculating the Hamiltonian's spectrum for all times εt and that we have obtained the corresponding instantaneous Bloch functions by other means.

To apply our technique of choice, space-adiabatic perturbation theory, we need to assume that the band whose dynamics we are interested in, the nth band, is separated from the rest of the spectrum by a gap (see figure 1.2). A wavefunction which starts in that band cannot 'flow out' of the band of interest to others (at points where two bands intersect for instance) and transitions to neighboring bands are strongly suppressed.

1.2.2 Scope Of This Thesis

We want to understand the semiclassical motion of an electron in a crystal whose periodicity lattice is deformed slowly. In other words, we want to deepen the understanding of the piezoelectric effect on a microscopical level.

To zeroth order the semiclassical equations of motion of an electron in the nth band are given by [AM01, p. 276]

$$\begin{aligned} \dot{r} &= +\nabla_k E_n(k) \\ \dot{k} &= 0 \end{aligned} \tag{1.5}$$

Our goal is to compute first-order corrections to these equations in the adiabatic parameter ε to these semiclassical equations of motion and to explore their physical ramifications. We will proceed by finding corrections to the effective Hamiltonian $E_n(k)$ first and to explore their meaning and to obtain the proper semiclassical equations of motion from this corrected effective Hamiltonian.

1.2.3 Structure Of This Thesis

In chapter 2 we will briefly present a few important contributions to the understanding of piezoelectric effects and polarization. We include three different approaches: a pragmatic treatment by King-Smith–Vanderbilt who derive a concise formula for the difference in polarization, Resta's position operator which is used for 'real-world' calculations and a mathematically rigorous approach based on space-adiabatic perturbation theory by Panati et al [PST].

Chapter 3 provides the necessary background of the mathematical methods used in this thesis; it is to be understood as a pedagogical introduction by example to space-adiabatic perturbation theory at the expense of mathematical rigor.

The formulas which will be be derived in chapter 3 will be put to use in chapter 4, the central part of this thesis. We will derive an effective Hamiltonian for an electron which moves in an adiabatically deformed crystal and obtain first-order corrections in a systematical manner. This effective Hamiltonian is the basis for the derivation of semiclassical equations of motion of an electron in a certain band and we eventually recover the kinematic equation for the piezocurrent.

Chapter 5 illustrates the results of chapter 4 with toy models.

The last chapter proposes experiments to test the equations derived in section 4 and give a brief outlook on what questions might be of interest for further investigation.

For the convenience of the reader, we have included an appendix which contains a brief introduction to geometric phases.

1.2.4 Conclusions

We have derived equations for an electron in a crystal which is slowly deformed (see section 4.2), i. e. we focused on the dynamical aspects of piezoelectricity. For the first time deformations of the unit cell have been taken into account properly using a technique which is – in principle – mathematically exact. We have given error estimates on both, the unitary evolution and the semiclassical flow generated by the effective Hamiltonian. These error estimates give for the first time a range of validity for the linear response ansatz.

Based on the dynamical equation we recover a concise equation for the piezocurrent. We get two new terms which can be attributed to the deformation; the first one accounts for the adiabatically induced motion of the electrons which follow the nuclei. The second term is another geometric phase correction. In the limiting case of vanishing deformation we recover the King-Smith–Vanderbilt formula. We close the discussion by proposing an experiment on ultra-cold gases to detect the corrections to King-Smith–Vanderbilt derived in this thesis.

2 Previous Approaches To Piezoelectricity

We would like to summarize some of the previous approaches to obtain a (piezoelectric) current from a time-dependent Hamiltonian. Two of them are motivated by finding a solution to a practical problem whereas the last approach puts a linear response ansatz on a solid theoretical foundation.

However we will start with some comments on the proper (microscopic) definition of polarization.

2.1 Problem Of Defining Polarization

For a long time, the subtleties of a precise microscopic definition of polarization *in infinite systems* were not recognized as such. Martin [Mar74] was one of the first to recognize that in previous treatments of polarization, a surface term has been neglected, or equivalently, an attempt to define polarization in periodic media by means of a volume integral *only* is bound to fail, because the field does not vanish at the boundaries and a different choice of unit cell seemingly gives rise to a different polarization.

Bennett et al [BM72] used the simple guess

$$P = \frac{1}{|M|} \int_M \mathrm{d}r \, r \, \rho(r)$$

to obtain the polarization P of the unit cell in terms of the electron density ρ. M is the unit cell of choice and $|M|$ its volume. Martin realized that the value depends on the choice of the unit cell and even results in a net polarization for materials which exhibit no polarization effects whatsoever due to symmetry (point symmetry of the unit cell is a sufficient condition for a vanishing of polarization currents).

The polarization per unit cell can now be defined as the average polarization in a unit cell.

$$P = \frac{1}{|M|} \int_M \mathrm{d}r \, P(r) \tag{2.1}$$

$P(r)$ and P are the local and the total polarization, M is the unit cell and $|M|$ the volume of the unit cell. From electrodynamics we know that polarization can be attributed to the *localized* charges whose charge density is given[1] by ρ. Maxwell's equations relate the local polarization $P(r)$ with the local charge density ρ.

$$\nabla \cdot P(r) = -\rho(r)$$

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[1] In the standard textbooks for electrodynamics, [Jac98] for instance, the charges are classified as free and localized charges.

We integrate equation 2.1 by parts and use Maxwell's equation to relate P with the local charge density $\rho(r)$.

$$P = \frac{1}{|M|} \int_M \mathrm{d}r \, r \, \rho(r) + \frac{1}{|M|} \int_{\partial M} \mathrm{d}r \, r \, \hat{n} \cdot P(r) \tag{2.2}$$

Bennet et al used the first term to obtain the polarization per unit cell, neglecting the second term. However the second term is essential, it is the charge transferred across the surface of the unit cell ∂M. If we choose a different unit cell M', the first and second integral will in general be different, only their sum remains unchanged.

For finite system, the charge density, which is an integrable function, $\rho \in L^1(\mathbb{R}^d)$, vanishes at infinity, and so does the surface term.

If the crystal does not have inversion symmetry, we cannot choose a unit cell such that the surface term *a priori* vanishes. Thus only the sum of volume term *and* surface are independent of the choice of the unit cell; in the case of a crystal whose unit cell has a center of inversion, the flux across the surface exactly cancels the volume term [Mar74].

In addition to the independence of the choice of unit cell, a well-defined notion of polarization should also include the fact that experimentally, only *differences in polarizations* are measured; absolute polarizations are in principle inaccessible to measurement [Res94].

The similarity to electric fields and electric potentials might seem conincidental, but it is not. As we shall see later on in section 2.3, the local change in polarization $\dot{P}(k,t)$ satisfies equations which are formally the same as the kinematic Maxwell equations for an electric field (equation 2.4).

Equation 2.2 suggests that we have to specify the polarization as a boundary condition; indeed as it turns out, the method of choice for most electronic structure calculations, density functional theory [VAS05], proved to be unable to reproduce polarization effects accurately. Instead Gonze, Ghosez and Godby [GGG95] were able to show that conventional density functional theory had to be modified to encompass polarization effects as well. The key idea is that the energy functional depends on both, the electron density *and* polarization at the boundary [MO97].

2.2 The King-Smith-Vanderbilt Formula

A short, but nevertheless very important paper by King-Smith and Vanderbilt [KSV93] derived polarization from first principles in the linear-response approximation and related the piezocurrent to Berry phases (see appendix A for a brief introduction to Berry phases).

Instead of postulating an expression similar to $C \int_M \mathrm{d}r \, r \, \rho(r)$, they derived a concise formula from a perturbative ansatz which was derived by Resta [Res92]. From the very beginning King-Smith and Vanderbilt had real-world (dft) calculations in mind and they applied their result to a GaAs crystal.

Their focus lied on the *kinematic aspects* of polarization, all that is needed are initial and final state of the solid to compute the difference in polarization. Nevertheless, they make several crucial observations, for instance polarization is defined only up to a constant times a lattice vector $\gamma \in \Gamma$, $c\gamma$.[2]

King-Smith and Vanderbilt consider a crystalline solid with *fixed* periodicity lattice Γ. The changes in structure are contained in the time-dependence of the effective potential $V_\Gamma \equiv V_\Gamma(x,t)$.[3] For convenience we choose units such that $m_\mathrm{e} = 1$, electronic charge $e = 1$ and $\hbar = 1$. In crystal momentum representation the Hamiltonian reads

$$\begin{aligned} H(k,t) &= \tfrac{1}{2m_\mathrm{e}}(-i\hbar\nabla_x + \hbar k)^2 + V_\Gamma(x,t) \\ &= \tfrac{1}{2}(-i\nabla_x + k)^2 + V_\Gamma(x,t) \end{aligned} \tag{2.3}$$

The material in question is assumed to be an insulator which means that the highest filled band is fully occupied and (far) away from the Fermi energy. $\psi_n(k,x,t)$ are the Bloch functions of the nth band $E_n(k,t)$.

$$H(k,t)\,\psi_n(k,x,t) = E_n(k,t)\,\psi_n(k,x,t)$$

They use an earlier result by Resta [Res92] as their ansatz and obtain a formula which relates the relative polarization to an integral of the pseudo-electric field Θ_n over the first Brillouin zone M^*. Like the pseudo-magnetic field (equation A.10) it is an inherently gauge-invariant quantity defined by

$$\begin{aligned} \Theta_n(k,t) &:= -\,\partial_t \mathcal{A}_n(k,t) - \nabla_k \Phi_n(k,t) \qquad (2.4) \\ \mathbf{E}(x,t) &= -\,\partial_t A(x,t) - \nabla_x \Phi(x,t) \end{aligned}$$

where $\mathcal{A}_n$ and Φ_n are the geometric vector potential (Berry connection) and the geometric scalar potential, respectively. In terms of Bloch functions ψ_n they are defined as

$$\begin{aligned} \mathcal{A}_n(k,t) &:= +i\,\langle \psi_n, \nabla_k \psi_n \rangle \\ \Phi_n(k,t) &:= -i\,\langle \psi_n, \partial_t \psi_n \rangle \end{aligned}$$

A Bloch function is only defined up to a k-dependent phase factor which satisfies the same periodicity condition at the boundary of the first Brillouin zone M^*. This property is sometimes referred to as *Bloch-gauge freedom*. A change in gauge is equivalent to multiplying ψ_n by a phase factor $e^{-i\varphi_n(k,t)}$. Thus the Berry connection and the geometric scalar potential in the changed gauge are

$$\begin{aligned} \mathcal{A}_n(k,t) &\mapsto \mathcal{A}'_n(k,t) = \mathcal{A}_n(k,t) + \nabla_k \varphi_n(k,t) \\ \Phi_n(k,t) &\mapsto \Phi'_n(k,t) = \Phi_n(k,t) - \partial_t \varphi_n(k,t) \end{aligned}$$

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[2] The momentum of an electron in a periodic potential is also defined only up to reciprocal lattice vectors.

[3] King-Smith and Vanderbilt assumed a general dependence on a parameter λ and that the potential under consideration is the Kohn-Sham potential.

Now we can express King-Smith and Vanderbilt's result in language of geometric phases: the polarization current is the 'averaged' pseudo-electric field (over the first Brillouin zone M^*) at a given time t. If the l filled bands are separated from each other and do not cross, the total change in polarization ΔP is the sum of the contributions of each band. The piezocurrent is *per definitionem* given by the change of polarization in time $\dot{P}(t) \equiv \partial_t P(t)$.

$$\begin{aligned} \Delta P &= \int_{t_0}^{t_1} \mathrm{d}t \, \dot{P}(t) \\ j(t) := \dot{P}(t) &= -\frac{f}{8\pi^3 \, |M|} \sum_{n=1}^{l} \int_{M^*} \mathrm{d}k \, \Theta_n(k,t) \end{aligned} \tag{2.5}$$

f is the occupation number of states in the system; for spin-degenerate systems, $f = 2$, otherwise $f = 1$.

Now we will briefly sketch the derivation. Following King-Smith and Vanderbilt [KSV93] we start with the result of a phenomenological computation obtained by Resta [Res92].

$$\dot{P} = -i \, \frac{f}{(2\pi)^3 \, |M|} \sum_{n=1}^{l} \sum_{c=l+1}^{\infty} \int_{M^*} \mathrm{d}k \, \frac{\langle \chi_n(k,t), p \, \chi_c(k,t) \rangle \, \langle \chi_c(k,t), \partial_t V(\cdot,t) \, \chi_n(k,t) \rangle}{(E_n(t) - E_c(t))^2} - \text{c. c.} \tag{2.6}$$

where c. c. denotes the complex conjugate of the term to the left. χ_n are the eigenfunctions to the Hamiltonian and are related to Bloch functions via a phase factor.

$$\chi_n(k,x,t) = e^{ik \cdot x} \psi_n(k,x,t)$$

We use commutation relations to calculate the numerator of equation 2.6. Inserting

$$\begin{aligned} \langle \chi_c(k,t), p \, \chi_n(k,t) \rangle &= \langle \psi_c(k,t), [\nabla_k, H(k,t)] \, \psi_n(k,t) \rangle \\ &= -(E_c - E_n) \, \langle \psi_c(k,t), \nabla_k \psi_n(k,t) \rangle \end{aligned}$$

for the first inner product and

$$\begin{aligned} \langle \chi_n(k,t), \partial_t V(\cdot,t) \, \chi_c(k,t) \rangle &= \langle \psi_n(k,t), [\partial_t, H(k,t)] \, \psi_c(k,t) \rangle \\ &= (E_c - E_n) \, \langle \psi_n(k,t), \partial_t \psi_c(k,t) \rangle \end{aligned}$$

for the second, we get

$$\Delta P = -i \frac{f}{8\pi^3 \, |M|} \sum_{n=1}^{l} \int_{t_0}^{t_1} \mathrm{d}t \int_{M^*} \mathrm{d}k \, \big(\langle \nabla_k \psi_n(k,t), \partial_t \psi_n(k,t) \rangle - \langle \partial_t \psi_n(k,t), \nabla_k \psi_n(k,t) \rangle \big) \tag{2.7}$$

If we compare this with the explicit expression for Θ_n in terms of the Bloch functions, we see that they agree.

$$\begin{aligned} \Theta_n(k,t) &= -\partial_t \mathcal{A}_n(k,t) - \nabla_k \Phi_n(k,t) \\ &= i \big(\langle \nabla_k \psi_n(k,t), \partial_t \psi_n(k,t) \rangle - \langle \partial_t \psi_n(k,t), \nabla_k \psi_n(k,t) \rangle \big) \end{aligned}$$

If we assume a time-independent Brillouin zone, we can interchange the integration with respect to time and momentum and integrate by parts. This yields a volume term and a surface term and brings us right back to Martin's comment.

$$\Delta P = i\frac{f}{8\pi^3\,|M|}\sum_{n=1}^{l}\int_{M^*}\mathrm{d}k\,\Big(\big[\langle\psi_n(k,t),\partial_{k_j}\psi_n(k,t)\rangle\big]_{t_0}^{t_1} - \int_{t_0}^{t_1}\mathrm{d}t\,\partial_{k_j}\,\langle\psi_n(k,t),\partial_t\psi_n(k,t)\rangle\Big) \tag{2.8}$$

$$\begin{aligned}
&= \frac{f}{8\pi^3\,|M|}\sum_{n=1}^{l}\int_{M^*}\mathrm{d}k\,\Big(\big[\mathcal{A}_n\big]_{t_0}^{t_1} + \int_{t_0}^{t_1}\mathrm{d}t\,\partial_{k_j}\Phi\Big)\\
&= \frac{f}{8\pi^3\,|M|}\sum_{n=1}^{l}\int_{M^*}\mathrm{d}k\int_{t_0}^{t_1}\mathrm{d}t\,\Big(+\partial_t\mathcal{A}_n(k,t) + \partial_{k_j}\Phi_n(k,t)\Big)\\
&= -\frac{f}{8\pi^3\,|M|}\sum_{n=1}^{l}\int_{M^*}\mathrm{d}k\int_{t_0}^{t_1}\mathrm{d}t\,\Theta_{n\,j}(k,t)
\end{aligned} \tag{2.9}$$

The piezocurrent is the pseudo-electric field averaged over the Brillouin zone. The geometric scalar potential does not have a meaning as a bare number, only differences do result in physical effects. Martin's idea was basically to use a gauge which sets $\Phi_n = 0$ to zero; we will refer to this gauge *parallel transport gauge*.

Now we can rephrase Martin's comment in terms of gauges: a change in gauge changes both terms individually, but the sum is still gauge-invariant. Φ_n is periodic in k (because Bloch functions are), the integral of the second term vanishes and we get

$$\dot{P}(t) = \frac{f}{8\pi^3\,|M|}\sum_{n=1}^{l}\int_{M^*}\mathrm{d}k\,\mathcal{A}_n(k,t) \tag{2.10}$$

Here, the 'gauge-invariance' is no longer explicit and (obviously) the integrand is not pointwise gauge-invariant.

2.3 An Approach Based On Adiabatic Perturbation Theory

In a paper by Panati, Sparber and Teufel [PST] the technique which will be used in this thesis as well, space-adiabatic perturbation theory (see section 3.2), has been applied to a simplified model of piezoelectricity.

We will not detail how these equations are obtained, but only state and interpret the final results. For the special case of vanishing deformation of the lattice our general result in chapter 4 reduces to their result.

2.3.1 Statement Of The Problem

The situation is the same as in the paper by King-Smith and Vanderbilt: the result of the stress applied to the crystal are rearrangements within the unit cell and deformations of an insulator's translational lattice are neglected as they are small (at most 10^{-3}). In other words, the effective crystal potential depends on time, $V_\Gamma \equiv V_\Gamma(x,t)$, but is periodic in the periodicity lattice at time $t = 0$, $V_\Gamma(x+\gamma,t) = V_\Gamma(x,t)$ for all lattice vectors $\gamma \in \Gamma$.

The Hamiltonian is thus given by

$$\hat{H}(t) = \tfrac{1}{2}(-i\nabla_x)^2 + V_\Gamma(\hat{x},t)$$

King-Smith and Vanderbilt's ansatz is linear response theory. Although physically we expect that to be a good approximation, there was no attempt to show that the error is and remains small over *macroscopic* time intervals. The King-Smith–Vanderbilt formula just gives the kinematics of the polarization current density, i. e. if we know initial and final state of our system with Hamiltonian $\hat{H}(t)$, we can obtain the difference in polarization.

Panati et al use space-adiabatic perturbation theory (see section 3.2) to clarify the range of validity and to deepen the understanding. There are two different intrinsic timescales of the problem: the macroscopic timescale t of the deformation and the microscopic timescale t_μ of the electronic dynamics. The difference in timescales is quantified with a dimensionless parameter $\varepsilon \ll 1$, $t = \varepsilon t_\mu$.

In a first step, they obtain an effective Hamiltonian h which governs the dynamics of the bands below the Fermi energy, estimating all transitions to bands above the Fermi energy to be small. The band gap for band insulators is rather large, of the order of a few electron volts; the probabilities of transitions to bands above the Fermi energy are negligible (10^{-40} or smaller) [AM01, p. 714].

This effective Hamiltonian gives rise to semiclassical equations of motion which contain quantum mechanical first-order corrections. These first-order corrections are responsible for the piezocurrent. It can be shown that these equations of motion yield the correct form of the difference in polarization and the piezocurrent itself. Thus the King-Smith–Vanderbilt formula is derived in a mathematically rigorous fashion.

Their paper closes with some important observations concerning the symmetries of the crystal and the vanishing of the piezocurrent.

2.3.2 Semiclassical Results

After a lengthy derivation, Panati et al [PST] find that effective Hamiltonian is given by the following function (up to second order in ε): if ψ_α and ψ_β are two Bloch functions of the band α and β, then the matrix element $h_{\alpha\beta}$ is given by

$$h_{\alpha\beta}(k,t) = \left\langle \psi_\alpha, \hat{H}\,\psi_\beta \right\rangle = E_\alpha(k,t)\,\delta_{\alpha\beta}$$

k is the crystal momentum of the electron.

The equations of motion which are derived from this effective Hamiltonian have to be corrected to first order in ε (see section 3.2.4 for details). For an electron in a single band (the nth band) which is separated from the other bands by a gap, the equations of motion are

$$\begin{aligned}\dot{q} &= \nabla_k E_n(k,t) - \varepsilon \Theta_n(k,t) \\ \dot{k} &= 0\end{aligned} \tag{2.11}$$

The pseudo-electric field Θ_n is defined as in equation 2.4. If we integrate $\dot{q}$ over the first Brillouin zone M^*, we get the total piezocurrent carried by the nth band. Since the material under investigation is an insulator, the bands below the Fermi energy are completely filled, the wavefunction in momentum representation is constant, $(\mathcal{F}\psi)(k) = 1$, the ones above the Fermi energy are unoccupied.

$$j(t) := \int_{M^*} \mathrm{d}k \, \dot{q}(k,t) = -\varepsilon \int_{M^*} \mathrm{d}k \, \Theta_n(k,t) \tag{2.12}$$

The integral over $\nabla_k E_n(k,t)$ vanishes as $E_n(k,t)$ is periodic in k and thus its gradient is an odd function with respect to inversion.

2.3.3 Interpretation

Gauge Invariance The equations of motion for an electron in the nth band, equation 2.11, are inherently gauge-invariant since Θ_n is gauge-invariant (with respect to the gauge of the Berry connection). The physics of a problem must not depend on the gauge of choice, the (explicit) gauge-invariance of equation 2.11 is a most-welcome feature.

$$\Theta'_n = \Theta_n$$

Role Of Symmetries It is (experimentally) well-known that crystals with inversion symmetry do not show any piezoelectric effects [Tra03]. We are able to reproduce this characteristic within the theoretical framework of geometric phases.

We have two quantities which have a pendant in electrodynamics, the Berry curvature Ω_n and the pseudo-electric field Θ_n. They are defined as

$$\begin{aligned}\Omega_n(k,t) &= \nabla_k \wedge \mathcal{A}_n(k,t) & \mathbf{B}(x,t) &= \nabla_x \wedge A(x,t) \\ \Theta_n(k,t) &= -\partial_t \mathcal{A}_n(k,t) - \nabla_k \Phi_n(k,t) & \mathbf{E}(x,t) &= -\partial_t A(x,t) - \nabla_x \Phi(x,t)\end{aligned}$$

with $\mathcal{A}_n := +i \langle \psi_n, \nabla_k \psi_n \rangle$ and $\Phi_n := -i \langle \psi_n, \partial_t \psi_n \rangle$ being the Berry connection and the geometric scalar potential (ψ_n is the Bloch function of the nth band, see appendix A for a brief introduction). Both sets of quantities fulfill formally the same set of kinematic Maxwell equations, because the two share the same symmetry group, $U(1)$.

In electrodynamics, we know that the electric field $\mathbf{E}$ is a vector and the magnetic field $\mathbf{B}$ is an axial vector, i. e. if we invert space, $x \mapsto -x$, the electric field changes sign, the magnetic field does not [Jac98].

$$\begin{aligned}\mathbf{E}(x) &\mapsto \mathbf{E}(-x) = -\mathbf{E}(x) \\ \mathbf{B}(x) &\mapsto \mathbf{B}(-x) = +\mathbf{B}(x)\end{aligned}$$

In a similar fashion, we can show that the analogous geometric quantities, the pseudo-magnetic field Ω_n (or Berry curvature as defined in equation A.10) and the pseudo-electric field Θ_n have the same symmetry properties (in k space) with respect to inversion.

$$\begin{aligned}\Theta_n(k,t) &\mapsto \Theta_n(-k,t) = -\Theta_n(k,t)\\ \Omega_n(k,t) &\mapsto \Omega_n(-k,t) = +\Omega_n(k,t)\end{aligned}$$

Similarly they have opposite behavior with respect to time-reversal symmetry. Again, the analogy to electromagnetism holds.

$$\begin{aligned}\Theta_n(k,t) &\mapsto \Theta_n(-k,t) = +\Theta_n(k,t)\\ \Omega_n(k,t) &\mapsto \Omega_n(-k,t) = -\Omega_n(k,t)\end{aligned}$$

Time-reversal also reflects the momentum, classically this means the trajectories are traversed in opposite direction.

In quantum mechanics the time-reversal operator is *essentially* given by complex conjugation (up to a unitary phase factor). The Hamiltonian of the current problem *has* time-reversal symmetry (since we have not applied a magnetic field which would break time-reversal symmetry) [Sak94].

This means if our Hamiltonian at fixed time t commutes with the time-reversal operator T *and* the space-inversion operator R,

$$[T,\hat{H}] = 0 \qquad\qquad [R,\hat{H}] = 0$$

then we can conclude the pseudo-electric field vanishes, because

$$\begin{aligned}\Theta_n(-k,t) &= -\Theta_n(k,t)\\ &= -\Theta_n(-k,t)\end{aligned}$$

must hold. This means Θ_n must vanish pointwise. Similarly Ω_n *must vanish pointwise as well* for the same reason. Since the pseudo-electric field vanishes pointwise, the piezocurrent vanishes as well.

Hence materials whose crystal has inversion symmetry show no piezoelectric effects.

2.4 Position Operator In Periodic Potentials

The expectation value of the position operator may be used to *define* polarization (in periodic media) as well, so we will have to expand on this appraoch. There are two aspects that come into play here: one fundamental aspect (which is related to problems beyond the one-electron approximation) and a practical issue concerning the expectation value of non-continuous functions.

Resta was among the first to clearly define polarization and relate it to Berry phases. We will only outline a few of his major results and ideas as his work in that field is quite extensive [Res98] [Zak00] [Res99] [Res00b] [Res94] [Res00a].

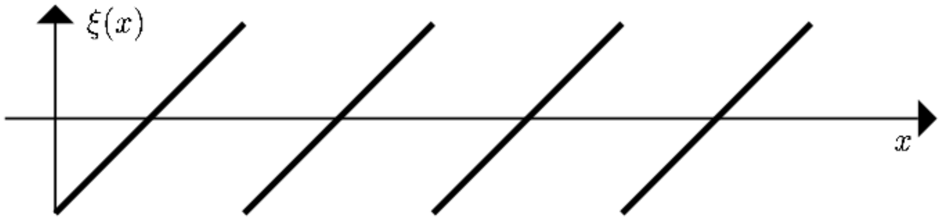

Figure 2.1: The $x \bmod L$ operator as a simple guess to replace the non-periodic multiplication operator x [Res00a, p. 71].

2.4.1 Resta's Position Operator

An important tool for practical calculations is Resta's position operator. He noticed that the usual position operator is ill-defined for problems with periodic boundary conditions, as the regular multiplication operator by x is not periodic. The question of finding a suitable position operator deserves some more elaboration.

Resta expanded on the work of a group of theoretical chemists [FSPC88] which proposed a non-trivial position operator. Despite its rather peculiar definition, it was intended for direct application to calculations. Resta derived the King-Smith–Vanderbilt formula from this non-trivial position operator; he also generalized this position operator to several particles to include multi-particle correlations.

A modified position operator will be useful for both, theoretical arguments and limits as well as applications in (density functional theory) computations.

In principle every periodic function in x is a candidate to be the position operator in a periodic potential. The 'sawtooth operator', $x \bmod L$, for instance was used as a replacement in many papers [Gou02] [Har87] [Sch00] [Mar74]. Resta claims one *cannot* 'fix' the position operator in this way [Res00a, p. 70] [Res00c, p. 4].

Instead, Fois et al [FSPC88] proposed an operator $\hat{z}$, which was adapted by Resta later on. This operator acts on the space of Bloch functions, $L^2(M)$ where M is the unit cell (typically the Wigner-Seitz cell) with periodic boundary conditions.

$$\hat{z} := e^{i\frac{2\pi}{L}\hat{x}} \tag{2.13}$$

$\hat{x}$ is the position operator of the particle [Res98]; generalizations to d dimensions are straight forward, one defines z component-wise, using a suitable dimension L for each direction.

Now the expectation value of Resta's position operator with respect to the Bloch function of the nth band ψ_n is defined as

$$x_{\mathrm{R}}[\psi_n] := \tfrac{L}{2\pi}\,\mathrm{Im}\ \ln\langle\psi_n, \hat{z}\,\psi_n\rangle \tag{2.14}$$

First of all this is well-defined: z is a periodic function of x. The function $e^{i\frac{2\pi}{L}x}$ (where x is a *parameter* as indicated by the lack of a hat ˆ) is periodic and even continuous at the boundary whereas $x \bmod L$ is not continuous at the boundary (as a function of the variable x).

The expectation value $\langle \psi_n, \hat{z}\, \psi_n \rangle$ is a complex number; the imaginary part of the natural logarithm of that number gives the phase of that expectation value. As suggested by the form of the $\hat{z}$ operator, the center of the wavefunction ψ_n is defined as this phase.

The initial motivation for Fois et al to use the $\hat{z}$ operator in the first place, as expectation values are numerically more stable [Res05]. The function $z(x)$ is smooth and continuous whereas the sawtooth operator has a discontinuity as the border of the unit cell. As many calculations are done in momentum space, we have to consider the Fourier transform of the $\hat{z}$ operator and the sawtooth operator. If the wavefunction in question approaches the border of the unit cell, a lot of Fourier modes contribute to the expectation value of the sawtooth operator which makes it computationally expensive and instable. The function $z(x)$ has only one Fourier component and is very smooth so that it is numerically more stable and less costly.

Essentially, the non-continuous part of the operation was postponed until after an expectation value with respect to a specific state was taken. Alternatively the edge of the sawtooth could be smeared out to avoid high-frequency contributions [SP01].[4]

So in essence, the phase gives the position, but the $\hat{z}$ operator contains even more information – the modulus gives a natural measure of the localization of the wavefunction [Res99].

2.4.2 Polarization In Multi-Electron Systems

Let us define the multi-electron generalization of the $\hat{z}$ operator; assume N electrons, the usual position operator of the jth particle is given by $\hat{x}_j$. The collective position operator, the sum of all single-particle position operators is denoted by $\hat{x} = \sum_{j=1}^{N} \hat{x}_j$.

$$\hat{z}_N := e^{i\frac{2\pi}{L}\hat{x}} = e^{i\frac{2\pi}{L}\sum_{j=1}^{N}\hat{x}_j} \tag{2.15}$$

The $\hat{z}_N$ operator now acts on the fermionic N-particle space, as does the position functional x_{R}. To avoid confusion, we will denote multi-particle wavefunctions with a capital Ψ (as opposed to ψ for single-particle wavefunctions).

Eventually we are interested in the limit of an infinite-sized system, whose average electron density remains constant, $N \longrightarrow \infty$, $L \longrightarrow \infty$ and ${}^{N}\!/_{L} = \rho_0 = \text{constant}$.

Resta defines a dimensionless quantity D which he relates to the localization length of a (N-electron) state ψ.

$$D := \lim_{\substack{N \longrightarrow \infty \\ L \longrightarrow \infty \\ N/L = \text{const.}}} \left(-N \ln |\langle \hat{z}_N \rangle_\Psi|^2 \right) \tag{2.16}$$

---

[4] According to Resta, the situation is different for multi-electron theories, as there is no analog of the ‘sawtooth operator’.

2.4.3 Definition Of Polarization

From Resta's position operator, we can define polarization in a straight-forward manner. We now consider a problem whose potential V_Γ depends (slowly) on time. Hence, the Bloch functions also depend on time and we assume that the change in potential is slow enough so that no transitions are induced.

The dipole per unit length for the multi-electron ground state[5] ψ_0 at time $t = 0$ in a cubic box is given by

$$P_{\mathrm{el}} := \frac{1}{2\pi} \mathrm{Im}\, \ln \langle \Psi_0, e^{i\frac{2\pi}{L}\hat{x}} \Psi_0 \rangle \equiv \frac{1}{L} x_{\mathrm{R}}[\Psi_0] \tag{2.17}$$

where $\hat{x} = \sum_{j=1}^{N} \hat{x}_j$ is the total position operator of the N particles. Then the polarization current is the time-derivative of (the multi-particle generalization of) equation 2.14.

$$j_{\mathrm{pol}} = \frac{1}{L} \frac{\mathrm{d}}{\mathrm{d}t} x_{\mathrm{R}}[\Psi_0] \equiv \frac{\mathrm{d}}{\mathrm{d}t} P_{\mathrm{el}} \tag{2.18}$$

In general, use of perturbation theory would not be applicable as the phases change erratically. However in this case, the 'random' phases cancel each other exactly and we can expand to first order, i. e. we assume a *linear response*. This formula is the precursor to the celebrated King-Smith–Vanderbilt formula (equation 2.5). $\gamma_L := \frac{2\pi}{L} x_{\mathrm{R}}[\psi_n]$ is the imaginary part of the phase of the expectation value of $\hat{z}$ with respect to the state ψ_n; it cannot be calculated from perturbation theory.

$$\hat{z}\, |\Psi_0\rangle = e^{i\gamma_L} \Big(|\Psi_0\rangle - \frac{2\pi}{L} \sum_{j\, \in \mathbb{N}} |\Psi_j\rangle \frac{\langle \Psi_j, \hat{p}\, \Psi_0 \rangle}{E_0 - E_j} \Big) + \mathcal{O}(1/L^2) \tag{2.19}$$

If we sandwich equation 2.19, the phase factor $e^{i\gamma_L}$ cancels. Plugging equation 2.19 into equation 2.18, we get

$$j_{\mathrm{pol}} = \frac{1}{2\pi} \mathrm{Im} \left(\frac{\langle \dot{\Psi}_0, e^{i\frac{2\pi}{L}\hat{x}} \Psi_0 \rangle}{\langle \Psi_0, e^{i\frac{2\pi}{L}\hat{x}} \Psi_0 \rangle} + \frac{\langle \Psi_0, e^{i\frac{2\pi}{L}\hat{x}} \dot{\Psi}_0 \rangle}{\langle \Psi_0, e^{i\frac{2\pi}{L}\hat{x}} \Psi_0 \rangle} \right) \tag{2.20}$$

A Taylor expansion yields the formula which King-Smith and Vanderbilt used to obtain their famous result on polarization.

$$\frac{1}{L} \frac{\mathrm{d}}{\mathrm{d}t} x_{\mathrm{R}}[\Psi_0] = i \frac{1}{L} \sum_{j\, \in \mathbb{N}} \langle \dot{\Psi}_0, \Psi_j \rangle \frac{\langle \Psi_j, \hat{p}\, \Psi_0 \rangle}{E_0 - E_j} - \text{c. c.} \tag{2.21}$$

---

[5] We would like to remind the reader that in this context the ground state is not the lowest-lying energy state of a single electron, but the lowest N filled bands. If an electron is excited, it occupies a higher energy band and leaves a hole in the band it originated from.

2.4.4 Polarization And Localization

As the limit of a system of infinite size is taken, $\hat{z}_N$ tends to the identity operator, $\hat{z}_N \longrightarrow \mathrm{id}$, but the number of electrons is increased at the same rate [Res00c].

If the N electrons are in a delocalized state Ψ, they are spread out equally over a unit cell,

$$\rho(x_1, \ldots, x_N) = |\Psi|^2 \sim {}^1\!/\!_L,$$

and hence the modulus of the expectation value of $\hat{z}_N$ with respect to the delocalized state Ψ tends to zero,

$$\left|\langle \hat{z}_N \rangle_\Psi\right| \longrightarrow 0$$

and so the contribution to the changes in phase will vanish as well. As we can see from the definition of D, D diverges for such a state.

On the other hand, if $\tilde{\Psi}$ is a *localized* state, the modulus is different from zero and D is finite even for the limit of large N,

$$0 < \left|\langle \hat{z}_N \rangle_{\tilde{\Psi}}\right| \leq 1$$

D and a related quantity, the localization length λ, can now be used to classify crystalline materials into insulators ($\lambda < \infty$) and metals ($\lambda = \infty$).

$$\lambda := \frac{\sqrt{D}}{2\pi\, \rho_0}$$

This implies that *only localized charges contribute to piezoelectric effects!* Physically, this fact is intuitively sensible as ‘mobile’ charge carriers, i. e. delocalized ones, would immediately neutralize any charge accumulation. Or to put another way, the electrons would be in a metallic state.

2.5 Conclusion

We have presented a selected few approaches to piezoelectricity. King-Smith and Vanderbilt (see section 2.2), Resta et al (see section 2.4), and Panati et al (see section 2.3) have treated crystals with time-dependent potential but fixed crystal lattice. The first three have derived a relation between the pseudo-electric field and polarization from a heuristic linear-response ansatz. Both groups had direct applications of their methods in mind.

The method used by Panati, Sparber and Teufel is in principle mathematically exact and gives estimates on the errors in the dynamics. The results obtained with their technique also includes the dynamical aspects, i. e. equations of motion for electrons which belong to a certain band. Although their efforts were focussed on deepening the theoretical understanding, their results agree with that of King-Smith and Vanderbilt and put their formula on a more solid theoretical footing.

All of these approaches neglected the deformation of the periodicity lattice which cannot *a priori* be neglected. In this thesis, we will expand on the work of Panati et al and include corrections due to the deformation in both, the equations of motion and the piezocurrent.

3 Mathematical Tools

3.1 Symbols And Weyl Quantization

We will introduce the concept of symbols as it is central to the discussion and in important piece of the machinery of space-adiabatic perturbation theory.

3.1.1 Common Structure Of Adiabatic Problems

Before we introduce the concept of symbols, we will elaborate on what adiabatic problems do have in common with each other. We will start with a familiar example, the Born Oppenheimer approximation (the brief presentation given here is based on a book by Bohm [Boh93, p. 623]).

Let us consider a molecule consisting of identical nuclei and electrons in the Born-Oppenheimer approximation. Let $P \equiv (P_1, \ldots, P_N)$ be the (collective) momentum of the N heavy nuclei, $Q \equiv (Q_1, \ldots, Q_N)$ their respective positions. Similarly $p \equiv (p_1, \ldots, p_n)$ and $q \equiv (q_1, \ldots, q_n)$ denote the momentum and positions of the n electrons. Thus the Hamiltonian is of the form

$$\hat{H} = \frac{1}{2m_{\mathrm{nuc}}}\hat{P}^2 + \frac{1}{2m_{\mathrm{e}}}\hat{p}^2 + V_{\mathrm{e-e}}(\hat{q}) + V_{\mathrm{e-nuc}}(\hat{q}, \hat{Q}) + V_{\mathrm{nuc}}(\hat{Q}) =: \frac{1}{2m_{\mathrm{e}}}\hat{P}^2 + \hat{H}_{\mathrm{e}}(\hat{Q}) \tag{3.1}$$

This Hamiltonian acts on the space of nuclei and electrons $L^2(\mathbb{R}^{3N}) \otimes L^2(\mathbb{R}^{3n})$. The first two terms are the kinetic energies of nuclei and electrons. $V_{\mathrm{e-e}}$ is the potential energy due to the interactions among the electrons, $V_{\mathrm{nuc-nuc}}$ is the corresponding potential due to the nuclei-nuclei interaction. The last term $V_{\mathrm{e-nuc}}$ arises from the interaction between nuclei and electrons. We have also defined $\hat{H}_{\mathrm{e}}$ which includes all potentials and the electronic kinetic energy term.

Instead of solving this problem in full generality, i. e. find solutions Ψ to the full Schrödinger equation

$$i\frac{\mathrm{d}}{\mathrm{d}t}\Psi(Q, q) = \hat{H}\,\Psi(Q, q) \tag{3.2}$$

we will reduce the problem to two simpler problems: we will consider the dynamics of electrons and nuclei separately.

Physically the typical mass of the nuclei is $10^4 - 10^5$ times heavier than one of the electrons, $m_{\mathrm{nuc}} \gg m_{\mathrm{e}}$, so we expect the electrons to adjust ‘instantaneously’ to a new configuration of the nuclei. Switching the point of view from the nucleons to the electrons, the larger the mass of the nuclei, the more they seem ‘frozen’ on the electrons' typical timescale. The adiabaticity assumption means that the motion of the nuclei will not induce any electronic transitions *and* that the electrons will always be in the equilibrium configuration corresponding to the positions of the nuclei; due to the large difference in typical velocities, we can safely make this approximation. We will dub the nucleonic degrees of freedom slow and the electronic ones fast.

$$L^2(\mathbb{R}^{3N}) \otimes L^2(\mathbb{R}^{3n}) =: \mathcal{H}_{\mathrm{slow}} \otimes \mathcal{H}_{\mathrm{fast}} \tag{3.3}$$

To rephrase this mathematically, we introduce the dimensionless parameter ε which is defined as the square root of the mass ratio of electron and nucleus; it quantifies the difference in velocities.

$$\varepsilon := \sqrt{m_{\mathrm{e}}/m_{\mathrm{nuc}}} \sim 10^{-2} \ll 1$$

We choose units such that $m_{\mathrm{e}} = 1$, $\hbar = 1$; the Hamiltonian simplifies to

$$\begin{aligned} H &= \tfrac{1}{2}\hat{p}^2 + \tfrac{\varepsilon^2}{2}\hat{P}^2 + V_{\mathrm{e-e}}(\hat{q}) + V_{\mathrm{e-nuc}}(\hat{q},\hat{Q}) + V_{\mathrm{nuc}}(\hat{Q}) = \tfrac{\varepsilon^2}{2}\hat{P}^2 + \hat{H}_{\mathrm{e}}(\hat{Q}) \\ &= \big(\tfrac{\varepsilon^2}{2}\hat{P}^2 + V_{\mathrm{nuc}}(\hat{Q})\big) \otimes \mathrm{id}_{\mathcal{H}_{\mathrm{fast}}} + \mathrm{id}_{\mathcal{H}_{\mathrm{slow}}} \otimes \big(\tfrac{1}{2}\hat{p}^2 + V_{\mathrm{e-e}}(\hat{q})\big) + V_{\mathrm{e-nuc}}(\hat{Q},\hat{q}) \end{aligned} \tag{3.4}$$

We have chosen this somewhat cumbersome notation to clarify what part of the Hamiltonian acts on what factor of the Hilbert space $\mathcal{H}_{\mathrm{slow}} \otimes \mathcal{H}_{\mathrm{fast}}$. Mathematically if we let $\varepsilon \longrightarrow 0$, we 'freeze out' the nuclei, the electrons have no influence on the nucleons' dynamics anymore.

So if we neglect the kinetic energy term of the nucleons, we have $\hat{H} \equiv \hat{H}_{\mathrm{e}}$. Obviously the nucleonic position operator $\hat{Q}$ commutes with $\hat{H}_{\mathrm{e}}$, $[\hat{Q}, \hat{H}_{\mathrm{e}}] = 0$, so that we can label states with the nuclei's positions *Q even though $\hat{H}_{\mathrm{e}}$ acts on the full Hilbert space* $\mathcal{H}_{\mathrm{slow}} \otimes \mathcal{H}_{\mathrm{fast}}$. In braket notation this implies we can write the state ket $|Q, E_n\rangle$, which describes the eigenfunction of the nth electronic energy band with the nuclei being located (sharply) at Q, $[\hat{Q}, \hat{H}_{\mathrm{e}}(\hat{Q})] = 0$ implies

$$\begin{aligned} \hat{H}_{\mathrm{e}}(\hat{Q})\,|Q, E_n\rangle &= \hat{H}_{\mathrm{e}}(\hat{Q})\,|Q\rangle \otimes |E_n(Q)\rangle \\ &= |Q\rangle \otimes H_{\mathrm{e}}(Q)\,|E_n(Q)\rangle = |Q\rangle \otimes E_n(Q)\,|E_n(Q)\rangle \end{aligned} \tag{3.5}$$

where $|Q\rangle \otimes |E_n(Q)\rangle \in \mathcal{H}_{\mathrm{slow}} \otimes \mathcal{H}_{\mathrm{fast}}$. In other words, if we apply $\hat{Q}$ on $|Q, E_n\rangle$, we get

$$\hat{Q}\,|Q, E_n\rangle = Q\,|Q, E_n\rangle$$

It is not a physical state, but we can expand physical states in terms of this basis.

$$\chi(Q)\,\psi_n(Q,q) \equiv \big(\langle\chi| \otimes \langle q|\big)\big(|Q\rangle \otimes |E_n(Q)\rangle\big) = \langle\chi|Q\rangle \otimes \langle q|E_n(Q)\rangle \in \mathcal{H}_{\mathrm{slow}} \otimes \mathcal{H}_{\mathrm{fast}}$$

$\chi(Q)$ is the nucleonic wavefunction; $\psi_n(Q,q)$ depends *parametrically* on the nucleons' positions Q.

The difference between $\hat{H}_{\mathrm{e}}(\hat{Q})$ in the first line of equation 3.5 and $H_{\mathrm{e}}(Q)$ in the last line is essential, only the last term is a *function* of Q which acts as an operator on $\mathcal{H}_{\mathrm{fast}}$, the other two are operators which act on the *full* Hilbert space $\mathcal{H}_{\mathrm{slow}} \otimes \mathcal{H}_{\mathrm{fast}}$. For every value of Q we have an associated operator $H_{\mathrm{e}}(Q)$ on $\mathcal{H}_{\text{fast}}$, in more mathematical terms, H_{e} is an operator-valued funciton.

$|Q\rangle$ is the state ket which corresponds to the N nuclei being located at positions $Q \equiv (Q_1, \ldots, Q_N)$. We can identify the ket $|E_n(Q)\rangle$ with a wavefunction by setting

$$\langle q|E_n(Q)\rangle \equiv \psi_n(Q,q) \qquad\qquad \psi_n \in \mathcal{H}_{\text{fast}}$$

which is the eigenfunction to the electronic eigenvalue problem

$$H_{\mathrm{e}}(Q)\psi_n(Q,q) = E_n(Q)\psi_n(Q,q) \tag{3.6}$$

Hence we solve the *electronic* problem for all nucleonic positions Q and obtain a set of eigenfunctions $\{\psi_n(Q,\cdot)\}_n$ which are solutions of the corresponding eigenvalue equation 3.6 with eigenvalues $\sigma(H_{\mathrm{e}}(Q)) = \{E_n(Q)\}_n$.

For $0 < \varepsilon \ll 1$ the nuclei's dynamics is weakly coupled to the dynamics of the fast (electronic) degrees of freedom. The 'back reaction' of the dynamics of the slow (nucleonic) degrees of freedom is small so that we can make a similar approximation to that of spin-orbit coupling: the quantum numbers Q and n are 'almost good' quantum numbers [Sak94, p. 311]. To put another way, the commutator $[\hat{Q}, \hat{H}]$ is of order $\mathcal{O}(\varepsilon^2)$.

$$\big[\hat{Q}, \hat{H}\big] = \big[\hat{Q}, \tfrac{\varepsilon^2}{2}\hat{P}^2\big] = \mathcal{O}(\varepsilon^2) \tag{3.7}$$

If we are interested in the contribution of the nth electronic band to the approximate dynamics, the initial Hamiltonian

$$\hat{H} \equiv \hat{H}(\hat{P}, \hat{Q}) = \tfrac{\varepsilon^2}{2}\hat{P}^2 + \hat{H}_{\mathrm{e}}(\hat{Q})$$

gives rise to an effective Hamiltonian

$$\big(\tfrac{\varepsilon^2}{2}\hat{P}^2 + E_n(\hat{Q})\big)\chi(Q) =: \hat{E}_{\mathrm{nuc}\,n}(\hat{P}, \hat{Q})\chi(Q) \tag{3.8}$$

The dynamics of the effective Hamiltonian remains close to the full dynamics in the following sense: let $t = \varepsilon t_\mu$ be the microscopic time and $P_n := \mathrm{id}_{\mathcal{H}_{\text{slow}}} \otimes \pi_{\psi_n}$ be the projector onto the nth band subspace. π_{ψ_n} is the projector on the state ψ_n which belongs to the nth energy band $E_n(Q)$. If $\psi \in \mathcal{H}_{\text{fast}}$ is a wavefunction in the space of the fast degrees of freedom, the projector acts as

$$\big(\pi_{\psi_n}\psi\big)(Q,q) = \langle\psi_n(Q,\cdot), \psi\rangle_{\mathcal{H}_{\text{fast}}}\psi_n(Q,q)$$

Then if we compare the dynamics generated by the effective Hamiltonian $\hat{E}_{\mathrm{nuc}\,n} \otimes \mathrm{id}_{\text{fast}}$ to the full dynamics whose generator is the initial Hamiltonian $\hat{H}$, it was shown in [PST03b] that both agree up to order $\mathcal{O}(\varepsilon^2)$ for microscopic times.

$$\Big\|P_n\big(e^{i\hat{H}t_\mu} - e^{i(\hat{E}_{\mathrm{nuc}\,n}\otimes\mathrm{id}_{\mathcal{H}_{\text{fast}}})t_\mu}\big)\,P_n\,\pi(\hat{H} < E_{\max})\Big\| = \mathcal{O}(\varepsilon^2\,(1 + |t_\mu|)) \tag{3.9}$$

$\pi(\hat{H} < E_{\max})$ projects onto all states with energy less than $E_{\max}$, it is an energy cut-off. The cut-off is needed only so that we can compare the two evolution operators (whose difference of generators is in general unbounded).

We can conclude from equation 3.9 that even for times on the nucleonic timescale, $\mathcal{O}(1/\varepsilon)$, the error does not exceed $\mathcal{O}(\varepsilon)$. If we start with a wavefunction in the nth band, it will not 'flow out' of the nth band even if we consider macroscopic times[1].

In other words the *approximate solutions* to Born Oppenheimer-type problems are product wavefunctions of the form

$$\Psi_n(Q,q) = \chi(Q)\,\psi_n(Q,q) \in \mathcal{H}_{\text{slow}} \otimes \mathcal{H}_{\text{fast}} \tag{3.10}$$

The wavefunction factors into a q-independent factor – the nucleonic factor $\chi(Q)$ – and a factor that depends parametrically on the nucleonic and (as variables) on the electronic coordinates – the electronic factor $\psi_n(Q,q)$. If the nucleonic momenta are not too large and times are not too long, this approximation is valid.

If we assume that the nucleonic wavefunction has the form of wavepackets whose center essentially follows its classical trajectory, we can assume the nuclei are now classical particles whose dynamics are generated by

$$H(P,Q) = \tfrac{\varepsilon^2}{2}P^2 + \langle \psi_n(Q,\cdot), H_{\text{e}}(Q)\psi_n(Q,\cdot)\rangle =: \tfrac{\varepsilon^2}{2}P^2 + E_n(Q) \tag{3.11}$$

at least in an approximate sense as stated in equation 3.9. The equation above takes only the contribution of the nth band into account, provided that it is separated from all other bands by a gap. The adiabaticity assumption is now equivalent to the statement that the wavefunction $\psi_n(Q,\cdot)$ adjusts 'instantaneously' (adiabatically) to new configurations of nuclei. It is essential that a state is not just 'labelled' by initial conditions in phase space (P_0, Q_0), but also by an electronic wavefunction $\psi_n \in \mathcal{H}_{\text{fast}}$. The forces acting on a classical nucleus are given by the gradient of the Born-Oppenheimer potential E_n.

$$F = -\nabla_Q \left\langle \psi_n(Q,\cdot), H_{\text{e}}(Q)\psi_n(Q,\cdot)\right\rangle_{\mathcal{H}_{\text{fast}}} \equiv -\nabla_Q E_n(Q)$$

where $\psi_n(Q,\cdot)$ is the electronic state if the nuclei are located at the position $Q = (Q_1, \ldots, Q_N)$. It is nothing but the derivative of the expectation value of the electronic Hamiltonian with respect to the eigenstate ψ_n.

In the Born-Oppenheimer case, the identification of slow and fast degrees of freedom was conceptually and mathematically obvious; however there are many interesting cases where such a distinction is more subtle.

Consider a crystalline solid with translation lattice Γ in a slowly vaying electromagnetic field; the dimensionless parameter ε quantifies the separation of scales in space. We are interested in the motion of a single electron in the Γ-periodic effective potential

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[1] If we consider a single band, this is only true if for all Q the nth band $E_n(Q)$ is separated by a gap from the rest. However we can apply the same theory for a group of neighboring bands which are separated from the remainder of the spectrum by a gap; band crossings *within* the relevant part of the spectrum are admissible, but require a more careful treatment.

V_Γ created by the nuclei and all band electrons, i. e. we will work in the one-elekctorn approximation,

$$\hat{H} = \tfrac{1}{2}\big(\hat{p} - A(\varepsilon\hat{x})\big)^2 + V_\Gamma(\hat{x}) + \Phi(\varepsilon\hat{x})$$

Φ and A are the slowly varying electromagnetic scalar and vector potential, which are functions of εx and not just x.

Before we continue with our analysis, we need to identify the fast and slow degrees of freedom. If we think of the electron as a particle for a moment, the macroscopic motion would be dominated by the slowly varying electromagnetic field, e. g. we would expect a cyclotron motion perpendicular to the magnetic field which is spread out over many lattice spacings. Within a unit cell, the electromagnetic field is approximately constant, so we expect that the electron's motion is dominated by the band structure of the solid for vanishing external fields. This is analogous to the motion of a fast spinning top which precesses slowly around an axis – two motions on different timescales are superposed to yield (approximately) the total motion.

Mathematically we will decompose $\mathbb{R}^d$ in a small space, the Wigner-Seitz cell M, and a large space which is related to the lattice Γ. We can write every vector $x \in \mathbb{R}^d$ as lattice vector $\gamma \in \Gamma$ which points to the right unit cell and a position $y \in M$ within the Wigner-Seitz cell. In this spirit, we decompose $\mathbb{R}^d$ into

$$\mathbb{R}^d \cong \Gamma \times M$$

The Hamiltonian $\hat{H}$ acts on the space $L^2(\mathbb{R}^d)$, so if we decompose $\mathbb{R}^d$ to $\Gamma \times M$, the Hilbert space factors into

$$L^2(\mathbb{R}^d) \cong L^2(\Gamma \times M) \cong L^2(\Gamma) \otimes L^2(M)$$

We will change representation to make the first factor $L^2(\Gamma)$ (which is the space of square-summable sequences) a regular function space of square-integrable functions. To do that we introduce the Zak transform and rewrite the Hamiltonian as well as the spaces involved in Zak representation (which is closely related to the crystal momentum representation).

For a quickly-decaying function $\psi \in \mathcal{S}(\mathbb{R}^d)$ we define its Zak transform to be

$$\big(\mathcal{F}\psi\big)(k,y) := \sum_{\gamma\in\Gamma} e^{-ik\cdot(y+\gamma)}\psi(y+\gamma) \tag{3.12}$$

It is easy to show that $\mathcal{F}$ is indeed a unitary transformation and that a Zak transformed function has the following periodicity properties:

$$\begin{aligned} \big(\mathcal{F}\psi\big)(k+\gamma^*,y) &= e^{-i\gamma^*\cdot y}\,\big(\mathcal{F}\psi\big)(k,y) \\ \big(\mathcal{F}\psi\big)(k,y+\gamma) &= \big(\mathcal{F}\psi\big)(k,y) \end{aligned} \tag{3.13}$$

Here $\gamma \in \Gamma$ is a (real) lattice vector, $\gamma^* \in \Gamma^*$ a reciprocal lattice vector. So its periodicity properties compared to those of the Fourier transform are reversed, a Zak transformed function is *quasi*periodic in k and periodic in y. $k \in M^* \cong \mathbb{T}^d$ takes values in the first Brillouin zone, $y \in M \cong \mathbb{T}^d$ takes values in the Wigner-Seitz cell. The exponential factor $e^{-i\gamma^* \cdot y}$ tells us how to 'glue' wavefunctions at the boundaries. The Zak transform maps $L^2(\Gamma) \otimes L^2(M)$ to

$$L^2(\Gamma) \otimes L^2(M) \xrightarrow{\mathcal{F}} L^2(M^*) \otimes L^2(M)$$

M^* is the first Brillouin zone which is the unit cell in reciprocal space; like in the usual crystal momentum representation, the translation invariance of the Bloch functions translate to labelling states by band index *and* crystal momentum k.

Now we can identify slow and fast degrees of freedom:

$$L^2(M^*) \otimes L^2(M) =: \mathcal{H}_{\text{slow}} \otimes \mathcal{H}_{\text{fast}} \tag{3.14}$$

Before we calculate the Zak transform of the Hamiltonian $\mathcal{F}\hat{H}\mathcal{F}^{-1}$, we give the Zak transform of $\hat{p}$, $\hat{x}$ and $V_\Gamma(\hat{x})$ where the potential is obviously periodic in the crystal's translation lattice Γ, $V_\Gamma(x+\gamma) = V_\Gamma(x)$,

$$\begin{aligned} \mathcal{F}\hat{p}\mathcal{F}^{-1} &= \mathrm{id}_{\mathcal{H}_{\text{slow}}} \otimes -i\nabla_y + \hat{k} \otimes \mathrm{id}_{\mathcal{H}_{\text{fast}}} \\ \mathcal{F}\hat{x}\mathcal{F}^{-1} &= i\nabla_k \\ \mathcal{F}V_\Gamma(\hat{x})\mathcal{F}^{-1} &= V_\Gamma(\hat{y}) \end{aligned}$$

Since we are dealing with gradients on tori, we would have to specify the proper boundary conditions, but we will omit these technical details, see [Teu03, p. 146 ff.].

Now we can explicitly calculate the Zak transformed Hamiltonian (in short-hand notation, omitting the tensor product for the Zak transform of $\hat{p}$).

$$\begin{aligned} \hat{H}_{\mathrm{Z}} := \mathcal{F}\hat{H}\mathcal{F}^{-1} &= \tfrac{1}{2}\big(-i\nabla_y + \hat{k} - A(i\varepsilon\nabla_k)\big)^2 + V_\Gamma(\hat{y}) + \Phi(i\varepsilon\nabla_k) \\ &= \tfrac{1}{2}\big(-i\nabla_y + \hat{k} - A(\hat{r})\big)^2 + V_\Gamma(\hat{y}) + \Phi(\hat{r}) \end{aligned} \tag{3.15}$$

The similarities to the Born-Oppenheimer Hamiltonian are clear: we have two sets of conjugate variables, $-i\nabla_y$ and $\hat{y}$ as well as $i\varepsilon\nabla_k =: \hat{r}$ and $\hat{k}$ whose typical timescales are separated by ε.

The situation here is more intricate than in the Born-Oppenheimer case; we were able to split the Born-Oppenheimer Hamiltonian into $H_{\mathrm{BO}} = f(P) + g(Q)$. The Zak-transformed Hamiltonian $\hat{H}_{\mathrm{Z}}$ does not allow for such a decomposition.

As we will see, we need both, k and r to label states. Instead if we decompose the Zak transformed Hamiltonian into periodic part whose momentum is shifted by $-A(\hat{r})$ and electric scalar potential $\Phi(\hat{r})$ and use the Bloch functions of the periodic Hamiltonian to construct our approximate solutions.

$$\hat{H}_{\mathrm{Z}} \equiv \hat{H}_{\mathrm{Z}}(\hat{k}, \hat{r}) = \hat{H}_{\mathrm{per}}(\hat{k} - A(\hat{r})) + \Phi(\hat{r}) \tag{3.16}$$

The periodic Hamiltonian $\hat{H}_{\mathrm{per}}(\hat{k})$ describes the system for vanishing external fields.

$$\hat{H}_{\mathrm{per}}(\hat{k}) := \tfrac{1}{2}\big(-i\nabla_y + \hat{k}\big)^2 + V_\Gamma(\hat{y})$$

The Bloch functions to the periodic Hamiltonian depend on k *and* y; again we will denote the Bloch function to the nth band ${E_\mathrm{b}}^2$ with ψ_n.

$$H_\mathrm{per}(k)\,\psi_n(k,y) = E_\mathrm{b}(k)\,\psi_n(k,y)$$

Now that we have identified slow and fast degrees of freedom, we have to clarify the notion of 'approximate eigenvalues' as in equation 3.5. Let us assume for a moment that the magnetic field vanishes, i. e. $A(r) \equiv 0$. Then we have no shift in momentum k and our Hamiltonian is given by

$$\hat{H}_\mathrm{Z} = \hat{H}_\mathrm{per}(\hat{k}) + \Phi(\hat{r})$$

Although Φ need not be small, it is locally (on the microscopic scale) approximately constant. If we let $\varepsilon \longrightarrow 0$ formally, the scalar potential becomes a mere shift in zero point of the energy, $\Phi(r) \longrightarrow \Phi(0) = \text{constant}$. Hence we neglect the electrostatic potential to obtain approximate eigenfunctions. In the spirit of equation 3.5, we see that $\hat{k}$ commutes with $\hat{H}_\mathrm{per}$, $[\hat{k}, \hat{H}_\mathrm{per}] = 0$. We can use k and E_n to label eigenstates $|k, E_n\rangle = |k\rangle \otimes |E_n(k)\rangle \in \mathcal{H}_\mathrm{slow} \otimes \mathcal{H}_\mathrm{fast}$.

$$\hat{H}_\mathrm{per}(\hat{k})\,|k, E_n\rangle = \hat{H}_\mathrm{per}(\hat{k})\,|k\rangle \otimes |E_n(k)\rangle = |k\rangle \otimes H_\mathrm{per}(k)\,|E_n(k)\rangle$$

So far the situation is completely analogous to the Born-Oppenheimer case: the commutator of the actual Hamiltonian $\hat{H}_\mathrm{Z}$ is of order $\mathcal{O}(\varepsilon)$,

$$[\hat{k}, \hat{H}_\mathrm{Z}] = \varepsilon\,\nabla_r \Phi = \mathcal{O}(\varepsilon)$$

so the eigenvalues $|k\rangle \otimes |E_n\rangle$ are *approximate eigenvalues* we can use to approximate solutions to the full equation.

However if we consider the general case with non-vanishing magnetic vector potential, the situation is more intricate. We will (naively) use the same braket notation as before to illustrate the expansion; assume the state ket $|k, r, E_n\rangle$ decomposes as

$$|k, r, E_n\rangle = |k, r\rangle \otimes |E_n(k, r)\rangle \in \mathcal{H}_\mathrm{slow} \otimes \mathcal{H}_\mathrm{fast}$$

As in the Born-Oppenheimer case, we would naturally get a function $H_\mathrm{Z}(k, r)$ which associates an operator acting on $\mathcal{H}_\mathrm{fast}$ to each pair (k, r). Again, $H_\mathrm{Z}(k, r)$ acts only on the Hilbert space of the fast degrees of freedom whereas $\hat{H}_\mathrm{Z}(\hat{k}, \hat{r})$ acts on the *full Hilbert space* $\mathcal{H}_\mathrm{slow} \otimes \mathcal{H}_\mathrm{fast}$.

$$\begin{aligned} \hat{H}_\mathrm{Z}(\hat{k}, \hat{r})\,|k, r, E_n\rangle &= \hat{H}_\mathrm{Z}(\hat{k}, \hat{r})\,|k, r\rangle \otimes |E_n(k, r)\rangle \\ &= |k, r\rangle \otimes H_\mathrm{Z}(k, r)\,|E_n(k, r)\rangle \end{aligned}$$

Unfortunately *there is no state ket* $|k, r\rangle$ which localizes in both variables at the same time. This does not mean we are at an impasse, it just means that a simple product ansatz for the wavefunctions fails.

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[2] As we will only consider one single band, the 'nth band', the potential risk to confuse two bands is minimal.

The product ansatz is not the key point of the adiabatic approximation, but the idea of 'almost good quantum numbers' is. Our full Hamiltonian $\hat{H}_{\mathrm{Z}}(\hat{k},\hat{r})$ *does* almost-commutes with $\hat{k}$ and $\hat{r}$, because $\hat{k}$ and $\hat{r}$ almost-commute with each other, i. e. they commute up to an error of order $\mathcal{O}(\varepsilon)$.

$$[\hat{k},\hat{r}] = i\varepsilon\,\mathrm{id} = \mathcal{O}(\varepsilon) \implies [\hat{r},\hat{H}_{\mathrm{Z}}] = \mathcal{O}(\varepsilon),\ [\hat{k},\hat{H}_{\mathrm{Z}}] = \mathcal{O}(\varepsilon)$$

The idea is to 'postulate' a Hamiltonian on the fast degrees of freedom which depends parametrically on the slow variables *and then* quantize it. We will postpone the discussion of defining a quantization rule for operator-valued functions to section 3.1.3. In our case, we set

$$H(k,r) := \tfrac{1}{2}\big(-i\nabla_y + k - A(r)\big)^2 + V_\Gamma(\hat{y}) + \Phi(r)$$

which we will quantize later on to an operator $\hat{H}_{\mathrm{Z}}(\hat{k},\hat{r})$ on the total space $\mathcal{H}_{\mathrm{slow}}\otimes\mathcal{H}_{\mathrm{fast}}$.

With this in mind, we start by solving

$$H_{\mathrm{per}}(k-A(r))\,\psi_n(k-A(r)) = E_{\mathrm{b}}(k-A(r))\,\psi_n(k-A(r))$$

for the fast degrees of freedom. Assume we are interested in the contribution of the nth band. The strategy is now the same as in the Born-Oppenheimer case: we solve the eigenvalue equation for all parameters k and r and use the corresponding Bloch functions as approximate solutions for perturbed dynamics generated by $\hat{H}_{\mathrm{Z}}$. Band energy and Bloch function are now functions of both, k and r.

$$\begin{aligned} E_n(k,r) &:= E_{\mathrm{b}}(k-A(r)) + \Phi(r) \\ \psi_n(k,r) &\equiv \psi_n(k-A(r)) \end{aligned}$$

$E_n(k,r)$ is the *total band energy* which also includes the electromagnetic scalar potential. We use the proper boundary conditions (equations 3.13) to 'glue' Bloch functions at the border of neighboring unit cells together.

It is important not to confuse $\psi_n(k-A(r),y) \equiv \psi_n(k,r,y) \in \mathcal{H}_{\mathrm{fast}}$ with a wavefunction on the full Hilbert space which depend only on k and y or r and y, but not k, r and y since k and r are conjugate to each other. We will discuss in section 3.2 in detail how to use solutions to the problem in the fast degrees of freedom to construct approximate solutions to the full problem.

We expect that $\hat{E}_n(\hat{k},\hat{r})$ is an effective Hamiltonian at least to zeroth order; we will show later on that this *is* the lowest order of the effective Hamiltonian, but since the Hamiltonian commutes only to zeroth order in ε, $[\hat{k},\hat{H}_{\mathrm{Z}}] = \mathcal{O}(\varepsilon)$, we cannot expect $\hat{E}_n(\hat{k},\hat{r})$ to be suitable to describe the dynamics for *macroscopic times* of order $\mathcal{O}(1/\varepsilon)$. As it turns out, we need the more sophisticated machinery of space-adiabatic perturbation theory to rigorously justify our zeroth-order guess and systematically derive higher-order corrections.

Apparently there still seems some confusion as to *what the adiabatic approximation really is* [DMN05]. The adiabatic approximation is the assumption that we can neglect transitions to other bands induced by the change in the Hamiltonian. To put another way, in the case of the Born-Oppenheimer Hamiltonian the motion of the nuclei does not induce transitions from one electronic band to another if they are *separated by a gap*. If $\psi_n(Q, q, t)$ solves the Schrödinger equation $H(P(t), Q(t))\,\psi_n(Q(t), q, t) = E_n(Q(t))\,\psi_n(Q(t), q, t)$, then in the adiabatic approximation, the wavefunction at time t, which solves the Schrödinger equation, is given by

$$\psi(Q(t), q, t) \overset{\text{adiabatic}}{=} c(t)\,\psi_n(Q(t), q, t)$$

where $c(t)$ is a prefactor with initial condition $c(0) = 1$ [BMK$^+$03, p. 13]. The validity of the adiabatic approximation rests on a separation of scales into slow and fast degrees of freedom.

Although physically the distinction between slow and fast degrees of freedom might be easy, to identify them mathematically might require more effort. A dimensionless parameter ε quantifies the difference in scales.

We then solve the problem in 'frozen form', e. g. we solve

$$H_{\mathrm{Z}}(k, r)\,\psi_n(k, r, y) = E_n(k, r)\,\psi_n(k, r, y)$$

in the case of a Bloch electron in a slowly varying electromagnetic potential. We then construct approximate solutions to the full problem using those solutions of the fast degrees of freedom which parametrically depend on the slow variables.

The validity of the adiabatic approximation can be rephrased in the following way: the adiabatic approximation holds if Hamiltonian and the operators of the slow degrees of freedom 'almost commute', i. e. $[\hat{H}_{\mathrm{Z}}, \hat{k}] = \mathcal{O}(\varepsilon)$ in our second example. This implies k, r and n are *almost good* quantum numbers which can be used to label states. In this sense, we have split one difficult problems into two easier ones, as the parameter-dependent Hamiltonian $H_{\mathrm{Z}}(k, r)$ acts only on the space of the fast degrees of freedom, $\mathcal{H}_{\mathrm{fast}}$.

In more sophisticated cases than the Born-Oppenheimer approximation, we need to include first-order corrections to guarantee that the effective dynamics agrees with the full dynamics for macroscopic times $t = \varepsilon t_\mu$ up to order $\mathcal{O}(1)$. The inclusion of higher-order corrections either allows for increased precision or longer timescales.

3.1.2 Symbols

In both procedures we obtained *functions* of the phase space variables of the slow degrees of freedom, $H_{\mathrm{e}}(Q)$ for the Born-Oppenheimer Hamiltonian, $H_{\mathrm{Z}}(k, r)$ for the Bloch electron in the slowly varying electromagnetic field, with values in the space of *operators on the fast degrees of freedom* $\mathcal{H}_{\mathrm{fast}}$; those functions emerged naturally from the adiabatic approximation, for instance in the case of the Born-Oppenheimer approximation the wavefunction factors into nucleonic and electronic part (see equation 3.5).

$$\hat{H}_{\mathrm{e}}(\hat{Q})\big(|Q\rangle \otimes |E_n\rangle\big) = |Q\rangle \otimes H_{\mathrm{e}}(Q)\,|E_n(Q)\rangle$$

The notation suggests that we can reduce an operator on the full Hilbert space $\mathcal{H}_{\mathrm{slow}} \otimes \mathcal{H}_{\mathrm{fast}}$ to an operator-valued function on the Hilbert space of the *fast* degrees of freedom $\mathcal{H}_{\mathrm{fast}}$.

These operator-valued functions, i. e. maps which associate an operator (acting on $\mathcal{H}_{\mathrm{fast}}$) to each point in phase space of the slow degrees of freedom, are called *symbols*. Let $\mathbb{R}^d \times \mathbb{R}^d$ be the phase space of the slow degrees of freedom and $B(\mathcal{H}_{\mathrm{fast}})$ the space of bounded operators on $\mathcal{H}_{\mathrm{fast}}$.

$$H : \mathbb{R}^d \times \mathbb{R}^d \longrightarrow B(\mathcal{H}_{\mathrm{fast}}) \tag{3.17}$$

Of particular significance are *semiclassical symbols* H^ε which are symbols with an asymptotic expansion in ε.

$$H^\varepsilon \asymp \sum_{n \in \mathbb{N}_0} \varepsilon^n \, H_n \tag{3.18}$$

Asymptotic expansions are a familiar concept in physics, in scattering theory for instance the scattering matrix is expanded in terms of the (small) coupling constant α (which corresponds to ε here). Graphically, the different terms of the expansion of the scattering matrix can be cast into the form of Feynman diagrams. The convergence of this expansion is also not guaranteed [PS95, p. 90 ff.].

The availability of the expansion in ε is the very reason why symbols are introduced in space-adiabatic perturbation theory. Operators (as they may be quantizations of symbols which do not admit an expansion in ε) do not possess this property and hence the extraction of explicit formulas will be more intricate.

Because of their special significance, the zeroth term H_0 is called principal symbol, the first correction H_1 is dubbed sub-principal symbol.

$$H^\varepsilon \asymp H_0 + \varepsilon \, H_1 + \mathcal{O}(\varepsilon^2)$$

3.1.3 Weyl Quantization

Now it is time to promote the symbols back to full-fledged operators. Since either $\hat{q} \cdot \hat{p}$ and $\hat{p} \cdot \hat{q}$ yield the symbol $q \cdot p = p \cdot q$, there is an ambiguity if we want to go back from the level of symbols to the level of operators. For symbols which decompose as the sum of functions of each variable separately, $H(p, q) = f(p) + g(q)$, there is no ambiguity. If we cannot separate the symbol, we have to *prescribe* an operator ordering, i. e. we *define* the quantization of $q \cdot p$ to be $\hat{q} \cdot \hat{p}$ for instance (Kohn-Nierenberg quantization rule). This choice is not unique. We will use a different kind of quantization, namely Weyl quantization.

The fundamental definition of a Weyl quantized symbol is given in terms of the inverse Fourier transform of a symbol which will be denoted as $\mathcal{U}_{\mathrm{F}}$ here to set it apart from the Zak transform $\mathcal{F}$. Let $H \in \mathcal{S}(\mathbb{R}^{2d}, \mathcal{L}(\mathcal{H}_{\mathrm{fast}}))$ be an operator-valued symbol; then the Weyl quantization is defined as

$$\hat{H} := \frac{1}{(2\pi)^d} \int_{\mathbb{R}^d} \int_{\mathbb{R}^d} \mathrm{d}\eta \, \mathrm{d}\xi \, e^{i(\eta \cdot \hat{q} + \xi \cdot \hat{p})} \otimes \big(\mathcal{U}_{\mathrm{F}} H\big)(\eta, \xi) \tag{3.19}$$

There are more concise formulas, but we will omit them for two reasons: for one, they do not offer additional insight as to what is really going on. Also, they aren't really shorter and unnecessary for most explicit computations. To relate this formula to the problem of the dynamics of a Bloch electron in a slowly varying potential, we set $\hat{q} := \hat{k}$ and $\hat{p} := \hat{r} = i\varepsilon\nabla_k$. Adapting the notation accordingly, we now get

$$\hat{H} := \frac{1}{(2\pi)^d} \int_{\mathbb{R}^d} \int_{\mathbb{R}^d} \mathrm{d}\eta \, \mathrm{d}\xi \, e^{i(\eta\cdot\hat{k} + \xi\cdot i\varepsilon\nabla_k)} \otimes \big(\mathcal{U}_{\mathrm{F}} H\big)(\eta,\xi) \tag{3.20}$$

The symbol H is a mapping from phase space (k,r) to the space of bounded linear operators, i. e. for each (k,r), we have a linear operator $H(k,r)$ acting on the Hilbert space of the fast degrees of freedom $\mathcal{H}_{\mathrm{fast}}$. This means the Schrödinger equation for electronic wavefunctions for the nth band is given by

$$i\frac{\mathrm{d}}{\mathrm{d}t}\chi_n(k_0,r_0;x) = H(k_0,r_0)\,\chi_n(k_0,r_0;x) \tag{3.21}$$

The Weyl quantized operator $\hat{H}$ on the other hand *should* map functions onto functions as Schrödinger operators are supposed to,

$$\hat{H} : \mathcal{H}_{\mathrm{slow}} \otimes \mathcal{H}_{\mathrm{fast}} \longrightarrow \mathcal{H}_{\mathrm{slow}} \otimes \mathcal{H}_{\mathrm{fast}} \tag{3.22}$$

In other words, we can apply $\hat{H}$ to a wavefunction which is a function of both, k and y, slow and fast variables, $\varphi(k,y) \in \mathcal{H}_{\mathrm{slow}} \otimes \mathcal{H}_{\mathrm{fast}}$ and obtain another function. With such a Hamiltonian, the Schrödinger equation is indeed a meaningful expression on the space $\mathcal{H}_{\mathrm{slow}} \otimes \mathcal{H}_{\mathrm{fast}}$, $i\frac{\mathrm{d}}{\mathrm{d}t}\varphi(k,y) = \hat{H}\,\varphi(k,y)\ \forall\varphi \in \mathcal{H}_{\mathrm{slow}} \otimes \mathcal{H}_{\mathrm{fast}}$.

At first, we note that for a rapidly decreasing function we have the trivial equation

$$H = \frac{1}{(2\pi)^d} \int_{\mathbb{R}^d} \int_{\mathbb{R}^d} \mathrm{d}\eta \, \mathrm{d}\xi \, e^{i(\eta\cdot q + \xi\cdot p)} \big(\mathcal{U}_{\mathrm{F}} H\big)(\eta,\xi)$$

The crucial step in quantization procedure is an operator ordering; here this is done *implicitly* by upgrading $e^{i(\eta\cdot q+\xi\cdot p)}$ to the operator $e^{i(\eta\cdot\hat{q}+\xi\cdot\hat{p})} \otimes \mathrm{id}_{\mathcal{H}_{\mathrm{fast}}}$. If we were using $e^{i\eta\cdot\hat{q}}e^{i\xi\cdot\hat{p}} \otimes \mathrm{id}_{\mathcal{H}_{\mathrm{fast}}}$ instead, our choice of operator ordering would be equivalent to the 'usual' canonical commutation relations. The reverse order could be chosen as well, $e^{i\xi\cdot\hat{p}}e^{i\eta\cdot\hat{q}} \otimes \mathrm{id}_{\mathcal{H}_{\mathrm{fast}}}$, which is also known as 'anti-standard' commutation relations.

The choice of operator ordering is made implicitly here, because for non-commutative operators $\hat{A}$ and $\hat{B}$, whose commutator is a multiple of the identity, we do *not* have that $e^{\hat{A}+\hat{B}} = e^{\hat{A}}e^{\hat{B}}$, but rather $e^{\hat{A}+\hat{B}} = e^{\hat{A}}e^{\hat{B}}e^{\frac{1}{2}[\hat{A},\hat{B}]}$. In this sense, Weyl quantization is exactly 'in between' standard and anti-standard operator ordering.

We can interpret $e^{i(\eta\cdot\hat{k}+\xi\cdot i\varepsilon\nabla_k)} \otimes \mathrm{id}_{\mathcal{H}_{\mathrm{fast}}}$ as an operator which does not 'touch' the fast (electronic) degrees of freedom, but only changes the slow degrees of freedom we want to quantize. Since the argument $\big(\mathcal{U}_{\mathrm{F}} H\big)(\eta,\xi)$ is still an operator valued function, it combines with the second factor to $e^{i(\eta\cdot\hat{k}+\xi\cdot i\varepsilon\nabla_k)} \otimes \big(\mathcal{U}_{\mathrm{F}} H\big)(\eta,\xi)$. The first factor however is the operator which 'reacts' to the nucleonic part of the wavefunction $\psi(k)$.

$$\big(e^{i(\eta\cdot\hat{k}+\xi\cdot i\varepsilon\nabla_k)}\psi\big)(k) = e^{-i\varepsilon/2\,\eta\cdot\xi}e^{i\eta\cdot k}\psi(k-\varepsilon\xi) \qquad \forall\psi \in \mathcal{H}_{\mathrm{slow}} \tag{3.23}$$

The first phase factor results from the specific operator ordering chosen here, the second one is a translation in real space, and the last change is a translation in momentum space. The 'amplitude' of that reaction is given by the Fourier transform of the symbol which weights the response to specific eigenvalues of momentum and position.

Also, the dimensionality of the problem 'is cut in half'; classical theories label states with momentum *and* position, quantum theories represent states either with momentum *or* position in a suitable representation.

To summarize the last couple of paragraphs: Weyl quantization indeed changes the Hamiltonian to a full-fledged operator as we know it from standard quantum mechanics, an operator which acts on the space of wavefunctions $\mathcal{H}_{\text{slow}} \otimes \mathcal{H}_{\text{fast}}$. In the language of our concrete example of the Bloch electron, the stationary Schrödinger equation (in the Zak representation) reads

$$\hat{H}_{\text{Z}}\, \psi_n(k,y) = \hat{E}_n(\hat{k},\hat{r})\, \psi_n(k,y) \qquad\qquad \psi_n \in \mathcal{H}_{\text{slow}} \otimes \mathcal{H}_{\text{fast}} \tag{3.24}$$

k is the variable for the slow degrees of freedom, y is the variable of the fast degrees of freedom. The fact that we chose a momentum-like variable k and a space-like variable y is merely related to the specific problem under consideration. They are *not* conjugate to each other. $\hat{E}_n$ is the zeroth order of the effective Hamiltonian of the nth band.

3.1.4 Weyl-Moyal Product

A choice of commutation relations tells us how we have to quantize expressions like $x \cdot p = p \cdot x$ which commute classically; Weyl quantization 'symmetrizes' this to $\frac{1}{2}(\hat{x} \cdot \hat{p} + \hat{p} \cdot \hat{x})$.

On the other hand, if we consider the operator product of two operators $\hat{A}$ and $\hat{B}$, $\hat{A}\hat{B}$ is the composition of operators. What kind of product (denoted with a $\sharp$) can we define on the space of symbols such that it 'reflects' the operator structure onto the space of symbols? In other words, does there exist a composition rule $\sharp$ for which

$$\widehat{A \sharp B} = \hat{A}\hat{B}$$

holds for suitable symbols A and B? The Weyl-Moyal product *is* the product with this desired property. Before we get into the actual definition, we outline why such a (as we shall see) non-trivial product is useful in the first place.

As it turns out, it is necessary for the application of our technique of choice, space adiabatic perturbation theory, to maintain two levels: the level of symbols and the level of operators where Weyl quantization is used to go from the level of symbols to the level of operators. However the level of symbols will be used to do to *actual calculations* and our intended result is a product of operators.[3]

$$\begin{aligned} \text{calculation: } & h := \pi \sharp u \sharp H \sharp u^* \sharp \pi \\ \text{intended result: } & \hat{h} \text{ `$=$' } \hat{\pi}\, \hat{u}\, \hat{H}\, \hat{u}^*\, \hat{\pi} \end{aligned} \tag{3.25}$$

---

[3] The quotation marks should remind the reader that the expression below should not be taken literally; mathematically this statement is correct only up to an error of order $\mathcal{O}(\varepsilon^\infty)$, we refer to [PST03b] for details.

Our initial example of $x \cdot p$ shows clearly that the usual product (of real numbers) does not reflect the operator structure.

The Weyl-Moyal product of two semiclassical symbols $A(p,q)$ and $B(p,q)$ (i. e. symbols which have an expansion in terms of ε with rapidly decreasing terms, see section 3.1.2) is defined as

$$A(p,q) \sharp B(p,q) := e^{i\varepsilon/2(\nabla_p \cdot \nabla_x - \nabla_\xi \cdot \nabla_q)} A(p,q)\, B(p,q) \Big|_{\substack{x=q \\ \xi=p}} \tag{3.26}$$

For this thesis, only zeroth and first order in the power expansion are of significance. Let $\sum_{n \in \mathbb{N}_0} \varepsilon^n\, A_n$ and $\sum_{n \in \mathbb{N}_0} \varepsilon^n\, B_n$ be the asymptotic expansions of A^ε and B^ε.

$$\left(A^\varepsilon \sharp B^\varepsilon\right)_0 = A_0\, B_0 \tag{3.27}$$

$$\left(A^\varepsilon \sharp B^\varepsilon\right)_1 = A_0\, B_1 + A_1\, B_0 - \tfrac{i}{2}\{A_0, B_0\} \tag{3.28}$$

$\{\cdot\,,\cdot\}$ denotes the Poisson brackets which are defined here

$$\{A, B\} := \frac{\partial A}{\partial p_j}\frac{\partial B}{\partial q_j} - \frac{\partial A}{\partial q_j}\frac{\partial B}{\partial p_j} \tag{3.29}$$

where we have implicitly summed over j. One word of caution here. *Operator*-valued symbols do not commute in general, so we cannot swap symbols and compensate with a minus sign, $\{A, B\} \neq -\{B, A\}$, not even $\{A, A\} \neq 0$ vanishes. This is only true if one of the symbols is diagonal or a multiple of the identity (such a symbol is also called *scalar symbol*).

Now we are able to carry over all notions from the space of operators to the space of (semiclassical) symbols which are necessary to perform the computations in the next section.

3.2 Space-adiabatic Perturbation Theory

The technique of choice in this thesis is space-adiabatic perturbation theory which was conceived in a seminal paper in 2002 [PST03b]. Due to the intricate nature of the underlying mathematical structure, we will outline this technique by a relevant example.

The fruits of our efforts will be equations of motion which contain quantum corrections. There are two basic ways to obtain semiclassical equations of motion: through special semiclassical wavepackets [HJ01] [SN98] or by obtaining an effective Hamiltonian which in turn generates the dynamics. We will use the latter approach. This chapter is based on [PST03a].

3.2.1 Results

We will reconsider the Bloch electron in a slowly varying *weak*[4] electromagnetic field (confer section 3.1.2). The Zak transformed Hamiltonian depends on the parameters k and r which will be the variables of interest.

$$H_{\mathrm{Z}}(k,r) = \tfrac{1}{2}\bigl(-i\nabla_y + k - A(r)\bigr)^2 + V_\Gamma(y) + \Phi(r)$$

Our goal will be to find equations of motion of an electron which belongs to the nth band (which we assume to be non-degenerate) for the variables k and r which include quantum corrections to first order in ε. The effective Hamiltonian h which will be obtained by space-adiabatic perturbation theory describes the evolution of that electron which belongs to (and stays in) the nth band.

$$\begin{aligned} h(k,r) &= \bigl(E_{\mathrm{b}}(\kappa) + \Phi(r)\bigr) + \varepsilon\bigl(- \bigl(-\partial_{r_j}\Phi(r) + B_{jm}(r)\,\partial_{\kappa_m}E_{\mathrm{b}}(\kappa)\bigr)\mathcal{A}_{n\,j}(\kappa) \\ &\qquad - B_{jm}\,\mathrm{Re}\,\bigl(\tfrac{i}{2}\bigl\langle \partial_{\kappa_j}\psi_n(\kappa), (H_{\mathrm{per}} - E_n)(\kappa)\,\partial_{\kappa_m}\psi_n(\kappa)\bigr\rangle\bigr)\bigr) + \mathcal{O}(\varepsilon^2) \\ &= \bigl(E_{\mathrm{b}}(\kappa) + \Phi(r)\bigr) + \varepsilon\bigl(- F_{\mathrm{Lor}\,j}\,\mathcal{A}_{n\,j}(\kappa) - B_{jm}\,\mathcal{M}_{n\,jm}\bigr) + \mathcal{O}(\varepsilon^2) \end{aligned}$$

For brevity, we define the Lorentz force

$$F_{\mathrm{Lor}\,j} := -\partial_{r_j}\Phi(r) + B_{jm}\,\partial_{k_m}E_{\mathrm{b}}$$

the kinetic momentum $\kappa \equiv \kappa(k,r) := k - A(r)$ and the magnetic field two-form $B_{jl} := \partial_{r_j}A_l - \partial_{r_l}A_j$. $\mathcal{A}_n(\kappa) := +i\,\langle\psi_n(\kappa), \nabla_\kappa\psi_n(\kappa)\rangle$ is the Berry connection of the nth band. The lengthy expression in the last term will be dubbed Rammal-Wilkinson two-form $\mathcal{M}_{n\,jl}(\kappa)$. For $d = 3$ a two-form can be canonically identified with a one-form $\mathbf{B}$ so that $B_{jm}(\kappa)\,\partial_{\kappa_l}E_n(\kappa)$ (again, we remind the reader that we imply summation over repeated indices) can be identified with $\nabla_\kappa E_{\mathrm{b}}(\kappa) \wedge \mathbf{B}$.

$$\mathcal{M}_{n\,jm} := \tfrac{i}{2}\bigl\langle \partial_{\kappa_j}\psi_n(\kappa), (H_{\mathrm{per}} - E_n)(\kappa)\,\partial_{\kappa_m}\psi_n(\kappa)\bigr\rangle\bigr)$$

The dynamics which is generated by the effective Hamiltonian symbol can be computed; however the variables have to be corrected to first order in $\mathcal{O}(\varepsilon)$. Thus the final equations of motion for a single non-degenerate band are

$$\begin{aligned} \dot r &= \nabla_\kappa\bigl(E_{\mathrm{b}}(\kappa) - \varepsilon B(r)\cdot\mathcal{M}_n(\kappa)\bigr) - \varepsilon\dot\kappa \wedge \Omega_n(\kappa) \\ \dot\kappa &= -\nabla_r\bigl(\Phi(r) - \varepsilon B(r)\cdot\mathcal{M}_n(\kappa)\bigr) + \dot r \wedge B(r) \end{aligned} \tag{3.30}$$

To zeroth order, these equations of motion agree with that of a classical particle in an electromagnetic field. All quantum corrections can be cast in the form of geometric phase effects. It is important to note that each geometric phase term by itself is gauge invariant[5]. As physical effects do not depend on the specific choice of gauge, this is a

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[4] Weak means weak compared to the atomic fields which is usually the case; mathematically this condition is a prerequisite to apply space-adiabatic perturbation theory.

[5] There are actually two separate gauges to be considered here – the gauge stemming the charge (which changes the electromagnetic potentials A and Φ) and the Bloch gauge which changes the Berry connection $\mathcal{A}_n$ and the geometric potential $\Phi_n(\kappa) := -i\,\langle\psi_n(\kappa), \partial_t\psi_n(\kappa)\rangle$.

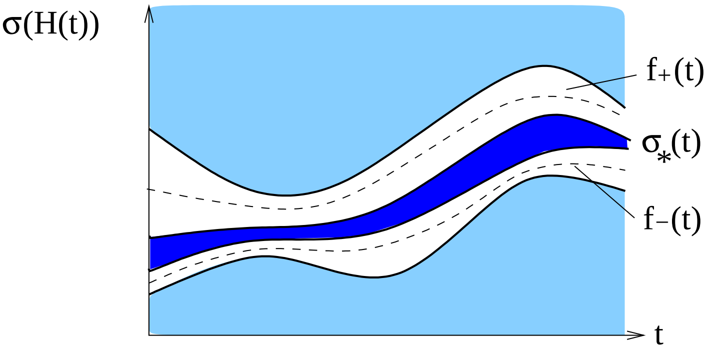

Figure 3.1: The spectral gap in the spectrum, with kind permission from the author [Teu03, p. 8].

necessary property. From the definition of $\Omega_{n\,jm} = \partial_{\kappa_j}\mathcal{A}_{n\,m} - \partial_{\kappa_m}\mathcal{A}_{n\,j}$, its gauge invariance is obvious since the pseudo-magnetic two-form $\Omega_{n\,jm}$ mimics the electromagnetic field tensor. Confirming the gauge invariance of the Rammal-Wilkinson two-form $\mathcal{M}_{n\,jm}$ is a matter of direct calculation as well.

3.2.2 General Idea

To tackle the problem we need to solve Schrödinger equation for the Hamiltonian in question; for a Bloch electron in a slowly varying field, the Hamiltonian symbol in Zak representation reads

$$\begin{aligned} H_{\mathrm{Z}}(k,r) &= \tfrac{1}{2}\big(-i\nabla_y + k - A(r)\big)^2 + V_\Gamma(y) + \Phi(r) \\ &=: H_{\mathrm{per}}(k - A(r)) + \Phi(r) \end{aligned} \tag{3.31}$$

$H_{\mathrm{per}}(k - A(r))$ is the Hamiltonian of the field-free case whose momentum was shifted by $-A(r)$, i. e. we assumed minimal coupling; analogously the band energy is split up in the same manner, $E_n(k,r) = E_{\mathrm{b}}(k - A(r)) + \Phi(r)$. E_{b} is the band energy function of the nth band of the field-free Hamiltonian H_{per}.

We assume, we have solved this Hamiltonian for all pairs of parameters (k,r). We then pick a *relevant part of the spectrum* of the zero-field Hamiltonian H_{per}, one specific energy band ('the nth band') for instance, which is separated from the remainder of the spectrum by a gap. In other words, our band does not cross other bands, it does not 'merge' into another band nor does it come 'very close' to another band. This gap inhibits transitions from the spectrum of interest to other parts which we do not include in our considerations.

Associated with this particular band there is a projector π_0 which projects onto the relevant part of the spectrum. In braket notation for a single, non-degenerate band the projector is given by $\pi_0(k, r) = |\psi_n(k, r)\rangle\, \langle\psi_n(k, r)|$ where $\psi_n(k, r)$ are the solutions of the zero-field Schrödinger equation.

$$i \frac{\mathrm{d}}{\mathrm{d}t}\, \psi_n(k - A(r)) = H_{\mathrm{per}}(k - A(r))\, \psi_n(k - A(r)) \qquad \psi_n(k - A(r)) \equiv \psi_n(k, r)$$

Then those ψ_n are also approximate solutions of the full Schrödinger equation since locally, the field $\Phi(r)$ is approximately constant and thus acts as a shift in zero energy only.

If the relevant part of the spectrum includes several bands or degenerate bands, we would have to add those to the projector as well; in case of degeneracies, a suitable orthonormal has to be chosen. In general a projector for l bands with degeneracy l_j is of the form

$$\pi_0(k, r) = \sum_{j=1}^{l} \sum_{n_j=1}^{l_j} |\psi_{n_j}(k, r)\rangle\langle\psi_{n_j}(k, r)| \tag{3.32}$$

Now we have reduced the problem to a *finite-dimensional* problem in the *fast* degrees of freedom. So we can use the representation space $\mathbb{C}^N$ where N is a suitable integer.

The dynamics within a single band with l-fold degeneracy can therefore be represented by $\mathbb{C}^l$; a unitary $u_0 \equiv u_0(k, r)$ maps functions in that band onto vectors in $\mathbb{C}^l$.

$$u_0(k, r) = \sum_{j=1}^{l} |\chi_j\rangle\, \langle\psi_j(k, r)| + u_0^{\perp}(k, r) \tag{3.33}$$

The term $u_0^{\perp}$ will not be specified and is often omitted (at least verbally, as we refer to $\sum_{j=1}^{l} |\chi_j\rangle\, \langle\psi_j(k, r)|$ as a unitarity) as we will always project onto the relevant part of the spectrum. All we need to know is that it is orthogonal to our projection, $u_0^{\perp}\, \pi_0 = 0$. We *chose* u_0 such that the vectors $\chi_j \in \mathbb{C}^l$ *do not depend on* (k, r); such a partial unitary is by no means unique.

In the remainder of this section, we will consider a single non-degenerate band only.

Our goal now is to construct an effective Hamiltonian h which describes the motion of an isolated band which is separated from the rest by a gap. A simple guess would be the direct operator product of the quantized symbols.

$$\text{guess: } \hat{h} = \hat{\pi}_0\, \hat{u}_0\, \hat{H}\, \hat{u}_0^{*}\, \hat{\pi}_0 \tag{3.34}$$

Such a choice however has several serious drawbacks, both of which lead to higher-order corrections in ε of π_0 and u_0. First and foremost $\hat{h}$ may not capture essential features of the dynamics, because the wavefunction apparently 'oscillates out' of our band of interest. To illustrate this point, we will discuss an example (Figure 3.2) which can be found in the book by Wyatt [Wya05, p. 309]. Here we see that the survival probability $|\langle\psi(k, r, t), \psi_n(k, r)\rangle|^2 = |\langle\psi(k, r, t), \pi_0\, \psi(k, r, t)\rangle|^2$ (which measures the oscillating in and out of the band) clearly oscillates quickly, but (at least on the timescale of the graph) the envelope function decays slowly.

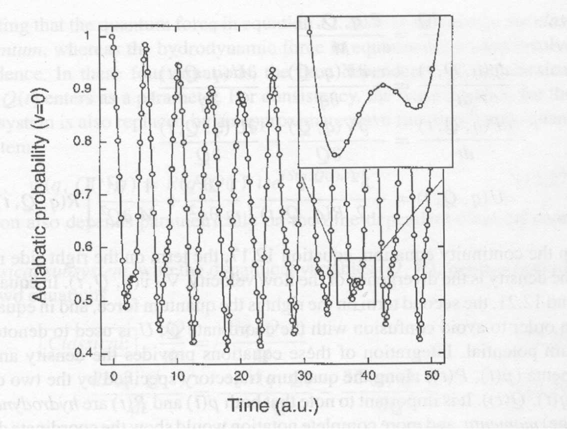

Figure 3.2: Survival probability as a function of time; the dots are obtained by a mixed quantum-classical method, the solid line is the exact quantum mechanical result.

We remedy this by 'tilting' the eigenspace a little as to accomodate for the *oscillations*. The corrected projector $\pi(k, r)$ projects onto that tilted eigenspace and the corrected unitarity $u(k, r)$ maps from the tilted space to the representation space. If $\psi(k, r, t)$ is the exact solution with $\psi(k, r, 0) = \psi_n(k, r)$, then the survival probability $|\langle\psi(k, r, t), \pi(k, r)\, \psi(k, r, t)\rangle|^2$ shows only the slow decay of the envelope function in figure 3.2.

Although we will not give the specifics of *how* we will obtain the corrected projector π and the corrected unitarity u, it is sufficient to know that there *is* a *systematic procedure* to calculate corrections to each order in ε. This procedure is mathematically exact.

The other drawback is tied to the tools we will actually use later on. If we want to give a range of validity (which is mathematically exact), we have to define a notion of closeness. General operators, i. e. those which not not necessarily admit an expansion in ε, *do not* admit such a notion. On the other hand if we consider operators which are quantizations of semiclassical symbols, i. e. symbols which admit an expansion in ε, the following definition seems 'natural': two semiclassical symbols agree up to order $\mathcal{O}(\varepsilon^{n+1})$ if

$$A^\varepsilon - B^\varepsilon = \sum_{j \in \mathbb{N}_0} \varepsilon^j \,(A_j - B_j) = \mathcal{O}(\varepsilon^{n+1}) \iff A_j - B_j = 0 \quad \forall 0 \leq j \leq n \tag{3.35}$$

and if the two symbols are close up to order $\mathcal{O}(\varepsilon^{n+1})$, so are their quantizations. However it turns out that calculations are actually easier on the level of symbols.

So the final procedure we will use has to be compatible with the product in the algebra of (semiclassical) symbols, the Moyal product, which we introduced in section

3.1.4. In this algebra π_0 is *not* a Moyal projector, i. e. $\pi_0 \sharp \pi_0 \neq \pi_0$, and similarly u_0 is not a (partial) unitary in the Moyal sense. As indicated with our terminology the principal symbols of the corrected symbols π and u will be given by π_0 and u_0, respectively. For both, π and u there are recursive formulas available which allow us to calculate corrections to any order.

Practically only first-order (and sometimes second-order) corrections are used. To put another way, we need only concern ourselves with formulas for first-order corrections here.

We will not need the full machinery of space-adiabatic perturbation theory as the focus of this thesis is to *apply* it to a problem. However, we translate equation 3.34 back to the symbol level and replace u_0 and π_0 by their corrected counterparts, we obtain the effective Hamiltonian which is of the form

$$h = \pi \sharp u \sharp H \sharp u^* \sharp \pi \asymp h_0 + \varepsilon h_1 + \mathcal{O}(\varepsilon^2) \tag{3.36}$$

We can plug that into the the definition of the Moyal product and obtain principal and subprincipal symbol of the effective Hamiltonian h.

This effective Hamiltonian h (Moyal) commutes with the corrected projector π to all orders in ε,

$$[h, \pi]_\sharp := h \sharp \pi - \pi \sharp h = \mathcal{O}(\varepsilon^\infty)$$

so if we start with a wavefunction in the tilted subspace, the time-evolved wavefunction will stay in the tilted subspace up to an error of arbitrary order in ε, $\mathcal{O}(\varepsilon^\infty)$.

3.2.3 Effective Hamiltonian

Instead of trying to solve a quadruple Moyal product by brute force, we refer to 'ready-made' formulas for the zeroth and first order terms.[6] The zeroth term is the 'classical' term, the first order is a quantum mechanical correction to the classical dynamics.

To simplify the presentation, we will conveniently split up $H_Z(k, r)$ into periodic Hamiltonian H_{per} and scalar electromagnetic potential Φ.

$$\begin{aligned} H_Z(k, r) &= \tfrac{1}{2}\big(-i\nabla_y + k - A(r)\big)^2 + V_\Gamma(y) + \Phi(r) \\ &=: H_{\text{per}}(k - A(r)) + \Phi(r) \end{aligned} \tag{3.37}$$

We will consider the dynamics of a single non-degenerate band with energy $E_n(k, r)$; similarly, this band energy will be split into a band energy term of the periodic Hamiltonian E_b and a rest.

$$E_n(k, r) = E_b(k - A(r)) + \Phi(r) \tag{3.38}$$

The advantage is that H_{per} and E_b are formally the Hamiltonian and the corresponding band energy of the non-magnetic Hamiltonian which is shifted by the vector potential A.

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[6] In principle one would proceed by expanding the exponential in powers of ε and collect terms.

Furthermore we note that the expansion of H_Z in powers of ε consists only of a *principal symbol* as all ε dependence has been absorbed in r, i. e. $H_\mathrm{Z}(k,r) \equiv H_{\mathrm{Z}\,0}(k,r)$.

The general formula for the zeroth order of the effective Hamiltonian h is given by (see [PST03b, p. 20])

$$\begin{aligned} h_{0\,n}(k,r) := \langle \chi_n, h_0(k,r)\, \chi_n \rangle &= \langle \psi_n(k,r), H_{\mathrm{Z}\,0}\, \psi_n(k,r) \rangle \\ &= E_\mathrm{b}(k - A(r)) + \Phi(r) \equiv E_n(k,r) \end{aligned} \tag{3.39}$$

Here we used $\psi_n(k,r) = {u_0}^*(k,r)\, \chi_n$, χ_n being the (k,r)-independent representation of the nth band wavefunction ψ_n. Hence we obtain the energy function of the nth band.

The first-order correction h_1 consists of three terms for the singe-band case.

$$\begin{aligned} h_{1\,n}(k,r) &:= \langle \chi_n, h_1(k,r)\, \chi_n \rangle \\ &= \big\langle \chi_n, \big(u_0\, H_{\mathrm{Z}\,1}\, {u_0}^* + \big(u_0 \sharp H_{\mathrm{Z}\,0} \big)_1 {u_0}^* + \big(E_n \sharp u_0 \big)_1 {u_0}^* \big) \chi_n \big\rangle \\ &= \big\langle \chi_n, \big(0 + \big(u_0 \sharp H_\mathrm{Z} \big)_1 {u_0}^* + \big(E_n \sharp u_0 \big)_1 {u_0}^* \big) \chi_n \big\rangle \end{aligned}$$

All symbols involved consist only of a principal part so that the first order of the Moyal product can be calculated according to equation 3.28

$$\big(u_0 \sharp H_\mathrm{Z} \big)_1 = 0 + 0 - \tfrac{i}{2} \{ u_0, H_\mathrm{Z} \} \tag{3.40}$$

and similarly we obtain

$$\big(E_n \sharp u_0 \big)_1 = 0 + 0 - \tfrac{i}{2} \{ E_n, u_0 \} \tag{3.41}$$

for the second term. The Poisson bracket of a symbol and a function is defined as $\{E_n, \phi_n\} := \nabla_k E_n \cdot \nabla_r \phi_n - \nabla_r E_n \cdot \nabla_k \phi_n$. E_n is a scalar symbol (because we are dealing with a single band only) so it commutes with u_0 in the Poisson bracket and the two Moyal products can be combined. In addition to that we apply the unitaries to the vectors of the reference space χ_n.

$$\begin{aligned} h_{1\,n}(k,r) &= -\, \tfrac{i}{2} \big\langle \psi_n(k,r), \big\{ (H_\mathrm{Z} + E_n)(k,r), \psi_n(k,r) \big\} \big\rangle \\ &= -\, i \big\langle \psi_n(k,r), \big\{ (E_\mathrm{b} + \Phi(r))(k,r), \psi_n(k,r) \big\} \big\rangle \\ &\qquad - \tfrac{i}{2} \big\langle \psi_n(k,r), \big\{ (H_\mathrm{Z} - E_n)(k,r), \psi_n(k,r) \big\} \big\rangle \\ &= -\, i \big\langle \psi_n(k,r), \big\{ (E_\mathrm{b}(k - A(r)) + \Phi(r)), \psi_n(k,r) \big\} \big\rangle \\ &\qquad - \tfrac{i}{2} \big\langle \psi_n(k,r), \big\{ (H_\mathrm{per} - E_\mathrm{b})(k - A(r)), \psi_n(k,r) \big\} \big\rangle \end{aligned} \tag{3.42}$$

We have added and subtracted $i\{E_n(k,r), \psi_n(k,r)\}$ to have a suitable splitting of terms. The first term contains the (shifted) band energy of the non-magnetic Hamiltonian as well as the scalar potential Φ, the second term can also be expressed in terms of the non-magnetic case with momentum shifted by $-A(r)$. We will call $\kappa(k,r) := k - A(r)$ *kinetic momentum* and use it hereinafter.

We will solve equation 3.42 term by term. We start with the first Poisson bracket.

$$\begin{aligned}\nabla_k E_\mathrm{b} \cdot \nabla_r \psi_n =& \partial_{k_m} E_\mathrm{b}(k-A)\, \partial_{r_m} \psi_n(k-A) = \partial_{k_m} E_\mathrm{b}(k-A)\, \partial_{k_j} \psi_n(k-A)\, (-\partial_{r_m} A_j) \\ =& -\partial_{r_m} A_j\, \partial_{k_m} E_\mathrm{b}\, \partial_{k_j} \psi_n\end{aligned}$$

Similarly the converse term yields

$$\begin{aligned}\nabla_r E_\mathrm{b} \cdot \nabla_k \psi_n =& \partial_{r_j} E_\mathrm{b}(k-A)\, \partial_{k_j} \psi_n = \partial_{k_m} E_\mathrm{b}(k-A)\, (-\partial_{r_j} A_m)\, \partial_{k_j} \psi_n \\ =& -\partial_{r_j} A_m\, \partial_{k_m} E_\mathrm{b}(k-A)\, \partial_{k_j} \psi_n\end{aligned}$$

Φ depends only on r, so only one of the terms survives.

$$\nabla_r \Phi(r) \cdot \nabla_k \psi_n(k-A) = \partial_{r_j} \Phi(r)\, \partial_{k_j} \psi_n(k-A) \tag{3.43}$$

Thus the first term can be written as

$$\begin{aligned}&-i\big\langle \psi_n(k-A(r)), \big\{(E_\mathrm{b}(k-A(r)) + \Phi(r), \psi_n(k-A(r))\big\}\big\rangle \\ &\quad= -\big(\partial_{r_j} A_m - \partial_{r_m} A_j\big)\, \partial_{k_m} E_\mathrm{b}(k-A(r))\, \mathcal{A}_{n\,j}(k-A(r)) + \partial_{r_j} \Phi(r)\, \mathcal{A}_{n\,j} \\ &\quad:= \big(\partial_{r_j} \Phi(r) - B_{jm}(r)\, \partial_{k_m} E_\mathrm{b}(k-A(r))\big)\, \mathcal{A}_{n\,j}(k-A(r)) \\ &\quad:= -F_{\mathrm{Lor}\,j}\, \mathcal{A}_{n\,j}\end{aligned} \tag{3.44}$$

We introduced the magnetic field two-form $B_{jm}(r)$ and the Lorentz force F_Lor. B_{jm} is the spatial part of the (relativistic) electromagnetic field tensor F_{jm} [Jac98, p. 556]. It is important to keep in mind that we could move E_b and $\partial_{r_j} A_m(r)$ out of the scalar product, because both are *scalar symbols*.

In a completely natural way the Lorentz force F_Lor appears in our calculations. In three dimensions the definition is the force a time-indepdendent electromagnetic field exerts on a moving charge.

$$F_{\mathrm{Lor}\,j} := -\partial_{r_j} \Phi(r) + B_{jm}(r)\, \partial_{k_m} E_\mathrm{b}(k-A(r)) \overset{d=3}{\equiv} \mathbf{E} + \nabla_k \wedge \mathbf{B} \tag{3.45}$$

$H_\mathrm{per} - E_\mathrm{b}$ is *not* a scalar symbol and hence cannot be moved out of the scalar product. However we can move the gradient from one argument to the other using conservation of the norm.

$$\nabla_k \big(\langle \psi, (H_\mathrm{per} - E_\mathrm{b})\phi\rangle\big) = 0 = \langle \nabla_k \psi, (H_\mathrm{per} - E_\mathrm{b})\phi\rangle + \langle \psi, \nabla_k (H_\mathrm{per} - E_\mathrm{b})\phi\rangle \tag{3.46}$$

for all $\psi \in \ker(H_\mathrm{per} - E_\mathrm{b})$, because $H_\mathrm{per} - E_\mathrm{b}$ is symmetric. Thus, we can move one partial derivative to the first argument of the scalar product.

$$\begin{aligned}
-\tfrac{i}{2}\, &\langle \psi_n(k-A), \{H_{\mathrm{per}}(k-A) - E_{\mathrm{b}}(k-A), \psi_n(k-A)\}\rangle \\
&= -\tfrac{i}{2}\big\langle \psi_n, \nabla_k (H_{\mathrm{per}} - E_{\mathrm{b}}) \cdot \nabla_r \psi_n - \nabla_r (H_{\mathrm{per}} - E_{\mathrm{b}}) \cdot \nabla_k \psi_n \big\rangle \\
&= -\tfrac{i}{2}\big\langle \psi_n, \nabla_k (H_{\mathrm{per}} - E_{\mathrm{b}}) \cdot \nabla_r \psi_n - \nabla_r (H_{\mathrm{per}} - E_{\mathrm{b}}) \cdot \nabla_k \psi_n \big\rangle \\
&= -\tfrac{i}{2}\big\langle \psi_n, (-\partial_{r_j} A_m)\, \partial_{k_j} (H_{\mathrm{per}} - E_{\mathrm{b}})\, \partial_{k_m} \psi_n - (-\partial_{r_j} A_m)\, \partial_{k_m} (H_{\mathrm{per}} - E_{\mathrm{b}})\, \partial_{k_j} \psi_n \big\rangle \\
&= -\tfrac{i}{2}\big\langle \psi_n, (-\partial_{r_j} A_m)\, \partial_{k_j} (H_{\mathrm{per}} - E_{\mathrm{b}})\, \partial_{k_m} \psi_n - (-\partial_{r_m} A_j)\, \partial_{k_j} (H_{\mathrm{per}} - E_{\mathrm{b}})\, \partial_{k_m} \psi_n \big\rangle \\
&= \tfrac{i}{2}\big(\partial_{r_j} A_m - \partial_{r_m} A_j\big)\big\langle \psi_n, \partial_{k_j} (H_{\mathrm{per}} - E_{\mathrm{b}})\, \partial_{k_m} \psi_n \big\rangle \\
&= \tfrac{i}{2} B_{jm} \big\langle \psi_n, \partial_{k_j} (H_{\mathrm{per}} - E_{\mathrm{b}})\, \partial_{k_m} \psi_n \big\rangle = -\tfrac{i}{2} B_{jm} \big\langle \partial_{k_j} \psi_n, (H_{\mathrm{per}} - E_{\mathrm{b}})\, \partial_{k_m} \psi_n \big\rangle \\
&=: -B_{jm}\, \mathcal{M}_{n\,jm} \qquad (3.47)
\end{aligned}$$

We substituted the Rammal-Wilkinson two-form $\mathcal{M}_{n\,jm} \equiv \mathcal{M}_{n\,jm}(k - A(r,t))$ in the last step.

Altogether we obtain for $h_{1\,n}(k,r)$

$$h_{1\,n}(k,r) = -\big(-\partial_{r_j} \Phi(r) + B_{jm}(r)\, \partial_{k_m} E_{\mathrm{b}}(\kappa)\big) \mathcal{A}_{n\,j}(\kappa) - B_{jm}(r)\, \mathcal{M}_{n\,jm}(\kappa) \qquad (3.48)$$

If we assume $d = 3$ and use the canonical one-forms associated with the two-forms B_{jl} and $\mathcal{M}_{n\,jl}$, we can rewrite the equations in a more familiar way. Let $\mathbf{B}$ the magnetic field and $\mathcal{M}_n \in \mathbb{R}^3$ be the associated one-form to the Rammal-Wilkinson two-form.

$$\begin{aligned}
h_{1\,n}(k,r) &= -\big(-\nabla_k \Phi + \nabla_k E_{\mathrm{b}} \wedge \mathbf{B}\big) \cdot \mathcal{A}_n - \mathbf{B} \cdot \mathcal{M}_n \\
&= -F_{\mathrm{Lor}} \cdot \mathcal{A}_n - \mathbf{B} \cdot \mathcal{M}_n \qquad (3.49)
\end{aligned}$$

To distinguish the approximate solution including first-order correction from the full effective Hamiltonian we will define the semiclassical effective Hamiltonian $h_{\mathrm{sc}} := h_0 + \varepsilon h_1$.

$$h_{\mathrm{sc}\,n}(k,r) = \big(E_{\mathrm{b}}(\kappa) + \Phi(r)\big) + \varepsilon\big(-F_{\mathrm{Lor}\,j}\, \mathcal{A}_{n\,j}(\kappa) - B_{jm}(r)\, \mathcal{M}_{n\,jm}(\kappa)\big) \qquad (3.50)$$

This semiclassical Hamiltonian will be the starting point for the equations of motion.

3.2.4 Semiclassical Dynamics

With the semiclassical effective Hamiltonian we could proceed either fully quantum-mechanically (with the Weyl-quantized Hamiltonian $\hat{h}$) or obtain equations of motion that include quantum corrections. We will do the latter.

As a result of our efforts in the last section, we have obtained an effective Hamiltonian h_{sc} on the reference space. The first question we have to answer is whether the *truncated* effective Hamiltonian h_{sc} allows us to predict the motion of an electron *accurately*. In other words if the error is initially of order $\mathcal{O}(\varepsilon^2)$, does it stay small for macroscopic intervals of time? The answer is yes, if two flows are close up to order $\mathcal{O}(\varepsilon^2)$, they remain close and the error grows at most linearly in time [PST03a, p. 565].

Thus we can use h_{sc} to obtain the dynamics of the full effective Hamiltonian h accurately (enough). To obtain the equations of motion we could start naively and set

$$\begin{aligned} \dot{r}_l &= +\partial_{k_l} h_{\mathrm{sc}\,n}(k, r) \\ \dot{k}_l &= -\partial_{r_l} h_{\mathrm{sc}\,n}(k, r) \end{aligned} \tag{3.51}$$

and expect those to be the equations of motions. However it turns out that the variables used in the h_{sc} *are not* the physical variables, the ones that can be measured.

3.2.4.1 Heuristic Explanation For $\mathcal{O}(\varepsilon)$-correction

The representation we use for the effective Hamiltonian h differs from the representation the physical variables 'live' in. Let us compare the (quantized) operators $\hat{r}_{\mathrm{or}}$ and $\hat{k}_{\mathrm{or}}$ of the slow degrees of freedom *on the original space* with their counterparts on the *reference space*.

$$\begin{aligned} \hat{r}_{\mathrm{or}} &= i\varepsilon\nabla_k \otimes \mathrm{id}_{\mathcal{H}_{\mathrm{fast}}} & \hat{k}_{\mathrm{or}} &= \hat{k} \otimes \mathrm{id}_{\mathcal{H}_{\mathrm{fast}}} \\ \hat{r}_{\mathrm{ref}} &= i\varepsilon\nabla_k \otimes \mathrm{id}_{\mathbb{C}^l} & \hat{k}_{\mathrm{ref}} &= \hat{k} \otimes \mathrm{id}_{\mathbb{C}^l} \end{aligned}$$

If we compare $\hat{p}_{\mathrm{or}}$ and $\hat{u}^* \hat{\pi} \hat{p}_{\mathrm{ref}} \hat{\pi} \hat{u}$ with each other, which both act on the original space, we find that they agree only up to order ε.

$$\hat{p}_{\mathrm{or}} - \hat{u}^* \hat{\pi} \hat{p}_{\mathrm{ref}} \hat{\pi} \hat{u} = \mathcal{O}(\varepsilon)$$

The situation is similar to a problem in relativistic quantum mechanics, the problem of the Zitterbewegung [BD64]. A wave packet is made up of positronic and electronic contributions; the interference terms oscillate very quickly, and hence the name Zitterbewegung. If we would insist that the physical position operator is given by $\hat{q} = x$, the velocity operator would be $\hat{v} = i[\hat{H}, \hat{q}] = c\alpha$. In particular, the eigenvalues of the velocity operator are $\pm c$, which would mean that the Zitterbewegung's velocity is c, even if the particle has a mass. This implies $\hat{q}$ cannot be the 'physical' position operator.

The idea to fix the macroscopic position operator is the same, we average over the microscopic motion of the electron. This suggests we replace r with

$$r \mapsto r + \langle \psi_n(k - A(r)), \hat{r}\, \psi_n(k - A(r)) \rangle_{\mathcal{H}_{\mathrm{fast}}} = r + \varepsilon\, \mathcal{A}_n(k - A(r)) \tag{3.52}$$

The transformation for k is more intricate and can be better explained after switching to kinetic momentum.

$$k \mapsto k + \varepsilon \left(\nabla_r A_j(r) \right) \mathcal{A}_{n\,j}(k - A(r)) \tag{3.53}$$

The correction is the averaged (macroscopic) position r over one unit cell of this specific band. Although the wavefunctions have a fixed phase relation going from one unit cell to the next,

$$\psi_n(k + \gamma^*, y) = e^{-i\gamma^* \cdot y} \psi_n(k, y)$$

we expect to it change erratically on length scales of $1/\varepsilon$. Hence if we average out this 'erratic' change in phase on the microscopic level, we expect the resulting operator to have 'nicer' properties.

The kinetic momentum $\kappa(k,r) = k - A(r)$ transforms as

$$\begin{aligned}\kappa_l &\mapsto \kappa_l + \varepsilon\, B_{lj}(r)\, \mathcal{A}_{n\,j}(\kappa) \\ &\overset{d=3}{=} \kappa_l + \varepsilon\left(\mathcal{A}_n(\kappa) \wedge B(r)\right)_l\end{aligned}$$

The averaged microscopic position contributes an extra *effective angular momentum*-like term; it vanishes if the averaged microscopic position $\varepsilon\, \mathcal{A}_n$ is parallel to B.

Mathematically we can check that the transformation proposed as equations 3.53 are indeed the ones which relate the variables used in representation of the effective Hamiltonian to the physical ones [PST03a, p. 567].

3.2.4.2 Equations of Motion

The equations of motions are obtained in three steps. We first calculate the equations of motion as they are with the variables used in the representation space. We introduce new symbols of variables to clarify this distinction. Variables with a $^{-}$, e. g. $(\bar{k}, \bar{r})$, denote variables in the effective representation; variables without a bar are either physical variables or variables which agree with physical variables up to order $\mathcal{O}(\varepsilon^2)$.

$$\Phi^t_\varepsilon(\bar{k},\bar{r}) \xrightarrow{\overset{\mathcal{O}(1)}{\text{step 2}}} \Phi^t_\varepsilon(\bar{\kappa},\bar{r}) \xrightarrow{\overset{\mathcal{O}(\varepsilon)}{\text{step 3}}} \Phi^t_\varepsilon(\kappa, r) \tag{3.54}$$

Φ denotes the *geometrical* object, the Hamiltonian flow generated by h_{sc}, the effective Hamiltonian which includes first-order corrections only.

As *Step 1* we calculate the Hamiltonian equations of motion in the variables of the reference representation. In *Step 2* we change the momentum (still in the reference representation) from 'crystal momentum' to 'kinetic momentum'. The non-trivial *Step 3* corrects the variables to order $\mathcal{O}(\varepsilon)$ so they agree with the physical ones to the required degree of accuracy.

Step 1 The Hamiltonian equations of motion

$$\begin{aligned}\dot{\bar{r}}_l &= +\partial_{\bar{k}_l} h_{\mathrm{sc}}(\bar{k},\bar{r}) \\ \dot{\bar{k}}_l &= -\partial_{\bar{r}_l} h_{\mathrm{sc}}(\bar{k},\bar{r})\end{aligned}$$

are calculated in the variables of the representation space first.

$$\begin{aligned}\dot{\bar{r}}_l &= +\partial_{\bar{k}_l} h_{\mathrm{sc}}(\bar{k},\bar{r}) \\ &= \partial_{\bar{k}_l} E_{\mathrm{b}}(\bar{k}-\bar{A}) + \varepsilon\, \partial_{\bar{k}_l}\left(-F_{\mathrm{Lor}\,j}(\bar{r}, \nabla_{\bar{k}} \bar{E}_{\mathrm{b}})\, \mathcal{A}_{n\,j}(\bar{k}-\bar{A}) - B_{jm}(\bar{r})\, \mathcal{M}_{n\,jm}(\bar{k}-\bar{A})\right)\end{aligned} \tag{3.55}$$

$\bar{A}$ is a short-hand notation for $A(\bar{r}) =: \bar{A}$ and similarly for other functions of variables. Whenever we leave out the argument and add a bar, we imply that it is a function of variables in the effective representation. Furthermore $-\partial_t \bar{A}_j$ vanishes identically as $\bar{A}$ does not depend on time and hence the term will be omitted in this section.

Similarly, we obtain the equation for $\dot{\bar{k}}_l$.

$$\begin{aligned}
\dot{\bar{k}}_l &= -\,\partial_{\bar{r}_l} h_{\mathrm{sc}}(\bar{k},\bar{r}) \\
&= -\,(-\partial_{\bar{r}_l}\bar{A}_j)\,\partial_{\bar{k}_j} E_{\mathrm{b}}(\bar{k}-\bar{A}) - \partial_{\bar{r}_l}\bar{\Phi} + \varepsilon\,\partial_{\bar{k}_m}\big(\bar{F}_{\mathrm{Lor}\,j}\,\bar{\mathcal{A}}_{n\,j} + \bar{B}_{jc}\,\bar{\mathcal{M}}_{n\,jc}\big)(-\partial_{\bar{r}_l}\bar{A}_m) \\
&\quad + \varepsilon\,\partial_{\bar{r}_l}\bar{F}_{\mathrm{Lor}\,j}\,\bar{\mathcal{A}}_{n\,j} + \varepsilon\partial_{\bar{r}_l}\bar{B}_{jm}\,\bar{\mathcal{M}}_{n\,jm} \\
&= -\,\partial_{\bar{r}_l}\bar{\Phi} + \partial_{\bar{r}_l}\bar{A}_j\,\dot{\bar{r}}_j + \varepsilon\,\partial_{\bar{r}_l}\bar{F}_{\mathrm{Lor}\,j}\,\bar{\mathcal{A}}_{n\,j} + \varepsilon\,\partial_{\bar{r}_l}\bar{B}_{jm}\,\bar{\mathcal{M}}_{n\,jm}
\end{aligned} \tag{3.56}$$

Step 2 Now we will transform the momentum variable from ‘crystal momentum’ to ‘kinetic momentum’ (the quotation marks should indicate that the result will *not* be the physical kinetic momentum, but the kinetic momentum in the effective representation), $\bar{k}_l \mapsto \bar{\kappa}(\bar{k},\bar{r}) := \bar{k}_l - \bar{A}_l$.

$$\begin{aligned}
\dot{\bar{\kappa}}_l &= \dot{\bar{k}}_l - \partial_{\bar{r}_j}\bar{A}_l\,\dot{\bar{r}}_j \\
&= -\,\partial_{\bar{r}_l}\bar{\Phi} + \big(\partial_{\bar{r}_l}\bar{A}_j - \partial_{\bar{r}_j}\bar{A}_l\big)\,\dot{\bar{r}}_j + \varepsilon\,\partial_{\bar{r}_l}\bar{F}_{\mathrm{Lor}\,j}\,\bar{\mathcal{A}}_{n\,j} + \varepsilon\,\partial_{\bar{r}_l}\bar{B}_{jm}\,\bar{\mathcal{M}}_{n\,jm} \\
&= -\,\partial_{\bar{r}_l}\bar{\Phi} + \bar{B}_{lj}\,\dot{\bar{r}}_j + \varepsilon\,\partial_{\bar{r}_l}\bar{F}_{\mathrm{Lor}\,j}\,\bar{\mathcal{A}}_{n\,j} + \varepsilon\,\partial_{\bar{r}_l}\bar{B}_{jm}\,\bar{\mathcal{M}}_{n\,jm}
\end{aligned} \tag{3.57}$$

The other coordinate, $\bar{r}$, will not be changed.

$$\dot{\bar{r}}_l = \partial_{\bar{\kappa}_l} E_{\mathrm{b}}(\bar{\kappa}) + \varepsilon\,\partial_{\bar{\kappa}_l}\big(-F_{\mathrm{Lor}\,j}(\bar{r},\nabla_{\bar{\kappa}}\bar{E}_{\mathrm{b}})\,\mathcal{A}_{n\,j}(\bar{\kappa}) - B_{jm}(\bar{r})\,\mathcal{M}_{n\,jm}(\bar{\kappa})\big) \tag{3.58}$$

Step 3 As motivated in the introduction, we will now transform our variables by ‘averaging’ on the microscopic scale. Both are exact up to order $\mathcal{O}(\varepsilon^2)$.

$$\begin{aligned}
\bar{r}_l &\mapsto r_l(\bar{\kappa},\bar{r}) := \bar{r}_l + \varepsilon\,\mathcal{A}_{n\,l}(\bar{\kappa}) \\
\bar{\kappa}_l &\mapsto \kappa_l(\bar{\kappa},\bar{r}) := \bar{\kappa}_l + \varepsilon\,B_{lj}(\bar{r})\,\mathcal{A}_{n\,j}(\bar{\kappa})
\end{aligned} \tag{3.59}$$

The inverse transformations are

$$\begin{aligned}
\bar{r}_l &= r_l - \varepsilon\,\mathcal{A}_{n\,l}(\kappa) \\
\bar{\kappa}_l &= \kappa_l - \varepsilon\,B_{lj}(r)\,\mathcal{A}_{n\,j}(\kappa)
\end{aligned} \tag{3.60}$$

Since the variables’ corrections are of order $\mathcal{O}(\varepsilon)$, we can replace all barred variables in $\mathcal{O}(\varepsilon)$-terms by their non-barred counterparts (in the original representation space).

We start with $\dot{r}_l$.

$$\begin{aligned}
\dot{r}_l &= \dot{\bar{r}}_l + \varepsilon\,\partial_{\bar{\kappa}_j}\mathcal{A}_{n\,l}(\bar{\kappa})\,\dot{\bar{\kappa}}_j = \dot{\bar{r}}_l + \varepsilon\,\partial_{\kappa_j}\mathcal{A}_{n\,l}\,\dot{\kappa}_j + \mathcal{O}(\varepsilon^2) \\
&= \partial_{\bar{\kappa}_l}\big(E_{\mathrm{b}} - \varepsilon\,B_{jm}\,\partial_{\kappa_j}E_{\mathrm{b}}\,\mathcal{A}_{n\,m}\big) + \varepsilon\,\partial_{\bar{\kappa}_l}\big(-\bar{F}_{\mathrm{Lor}\,j}\,\bar{\mathcal{A}}_{n\,j} - \bar{B}_{jm}\,\bar{\mathcal{M}}_{n\,jm}\big) + \varepsilon\,\partial_{\kappa_j}\mathcal{A}_{n\,l}\,\dot{\kappa}_j + \mathcal{O}(\varepsilon^2) \\
&= \partial_{\kappa_j}E_{\mathrm{b}}\,\partial_{\bar{\kappa}_l}\kappa_j + \varepsilon\,\partial_{\kappa_l}\big(-B_{jm}\,\partial_{\kappa_j}E_{\mathrm{b}}\,\mathcal{A}_{n\,m} - F_{\mathrm{Lor}\,j}\,\mathcal{A}_{n\,j} - B_{jm}\,\mathcal{M}_{n\,jm}\big) + \varepsilon\,\partial_{\kappa_j}\mathcal{A}_{n\,l}\,\dot{\kappa}_j + \mathcal{O}(\varepsilon^2) \\
&= \partial_{\kappa_j}E_{\mathrm{b}}\,\partial_{\bar{\kappa}_l}\kappa_j + \varepsilon\,\partial_{\kappa_l}\big(+B_{jm}\,\partial_{\kappa_m}E_{\mathrm{b}}\,\mathcal{A}_{n\,j} - F_{\mathrm{Lor}\,j}\,\mathcal{A}_{n\,j} - B_{jm}\,\mathcal{M}_{n\,jm}\big) + \varepsilon\,\partial_{\kappa_j}\mathcal{A}_{n\,l}\,\dot{\kappa}_j + \mathcal{O}(\varepsilon^2)
\end{aligned}$$

In the last line we have used the antisymmetry of the magnetic two-form B_{lj}. Now we expand $\partial_{\bar{\kappa}_l}\kappa_j$ and combine terms suitably.

$$\begin{aligned}
\dot{r}_l =&\partial_{\kappa_j} E_{\mathrm{b}} \left(\delta_{jl} + \varepsilon\, B_{jm}\, \partial_{\kappa_l} \mathcal{A}_{n\,m}\right) + \varepsilon\, \partial_{\kappa_l} \big(\partial_{r_j} \Phi\, \mathcal{A}_{n\,j} - B_{jm}\, \mathcal{M}_{n\,jm}\big) + \varepsilon\, \partial_{\kappa_j} \mathcal{A}_{n\,l}\, \dot{\kappa}_j + \mathcal{O}(\varepsilon^2) \\
=&\partial_{\kappa_l} E_{\mathrm{b}} + \varepsilon\big(-B_{jm}\, \partial_{\kappa_l} \mathcal{M}_{n\,jm} + \partial_{r_j} \Phi\, \partial_{\kappa_l} \mathcal{A}_{n\,j} + B_{jm}\, \partial_{\kappa_j} E_{\mathrm{b}}\, \partial_{\kappa_l} \mathcal{A}_{n\,m} + \partial_{\kappa_j} \mathcal{A}_{n\,l}\, \dot{\kappa}_j\big) + \mathcal{O}(\varepsilon^2) \\
=&\partial_{\kappa_l} E_{\mathrm{b}} + \varepsilon\big(-B_{jm}\, \partial_{\kappa_l} \mathcal{M}_{n\,jm} + \partial_{r_j} \Phi\, \partial_{\kappa_l} \mathcal{A}_{n\,j} - B_{jm}\, \partial_{\kappa_m} E_{\mathrm{b}}\, \partial_{\kappa_l} \mathcal{A}_{n\,j} + \partial_{\kappa_j} \mathcal{A}_{n\,l}\, \dot{\kappa}_j\big) + \mathcal{O}(\varepsilon^2) \\
=&\partial_{\kappa_l} E_{\mathrm{b}} + \varepsilon\big(-B_{jm}\, \partial_{\kappa_l} \mathcal{M}_{n\,jm} - F_{\mathrm{Lor}\,j}\, \partial_{\kappa_l} \mathcal{A}_{n\,j} + \partial_{\kappa_j} \mathcal{A}_{n\,l}\, \dot{\kappa}_j\big) + \mathcal{O}(\varepsilon^2) \\
=&\partial_{\kappa_l} E_{\mathrm{b}} + \varepsilon\big(-B_{jm}\, \partial_{\kappa_l} \mathcal{M}_{n\,jm} - \dot{\kappa}_j\, \partial_{\kappa_l} \mathcal{A}_{n\,j} + \partial_{\kappa_j} \mathcal{A}_{n\,l}\, \dot{\kappa}_j\big) + \mathcal{O}(\varepsilon^2) \\
=&\partial_{\kappa_l} E_{\mathrm{b}} + \varepsilon\big(-B_{jm}\, \partial_{\kappa_l} \mathcal{M}_{n\,jm} - \Omega_{n\,lj} \dot{\kappa}_j\big) + \mathcal{O}(\varepsilon^2)
\end{aligned} \tag{3.61}$$

Up to an error of first order in ε, we have $F_{\mathrm{Lor}\,j} = -\partial_{r_j} \Phi(r) + B_{jm}(r)\, \dot{r}_m + \mathcal{O}(\varepsilon) \equiv \dot{\kappa}_j$, so we can replace $F_{\mathrm{Lor}\,j}$ by $\dot{\kappa}_j$ in $\mathcal{O}(\varepsilon)$ terms. $\Omega_{n\,jl}$ is the gauge-invariant Berry curvature two-form which was introduced earlier. For $d = 3$, it can be canonically identified with the one-form $\nabla_\kappa \wedge \mathcal{A}_n$.

The second equation of motion is calculated in a similar fashion.

$$\begin{aligned}
\dot{\kappa}_l =&\dot{\bar{\kappa}}_l + \varepsilon \tfrac{\mathrm{d}}{\mathrm{d}t} \big(\bar{B}_{lj} \bar{\mathcal{A}}_{n\,j}\big) + \mathcal{O}(\varepsilon^2) = \dot{\bar{\kappa}}_l + \varepsilon \tfrac{\mathrm{d}}{\mathrm{d}t} \big(B_{lj} \mathcal{A}_{n\,j}\big) + \mathcal{O}(\varepsilon^2) \\
=& - \partial_{\bar{r}_l} \bar{\Phi} + \bar{B}_{lj} \dot{\bar{r}}_j + \varepsilon\big(\partial_{\bar{r}_l} \bar{F}_{\mathrm{Lor}\,j}\, \bar{\mathcal{A}}_{n\,j} + \partial_{\bar{r}_l} \bar{B}_{jm}\, \bar{\mathcal{M}}_{n\,jm} + \partial_{r_m} B_{lj}\, \mathcal{A}_{n\,j} \dot{r}_m + B_{lj}\, \partial_{\kappa_m} \mathcal{A}_{n\,j} \dot{\kappa}_m\big) + \mathcal{O}(\varepsilon^2) \\
=& - \partial_{\bar{r}_l} \big(\Phi - \varepsilon\, \partial_{r_j} \Phi\, \mathcal{A}_{n\,j}\big) + \big(B_{lj} - \varepsilon\, \partial_{r_m} B_{lj}\, \mathcal{A}_{n\,m}\big) \big(\dot{r}_j - \varepsilon\, \partial_{\kappa_m} \mathcal{A}_{n\,j}\, \dot{\kappa}_m\big) \\
&+ \varepsilon\big(\partial_{r_l} F_{\mathrm{Lor}\,j}\, \mathcal{A}_{n\,j} + \partial_{r_l} B_{jm}\, \mathcal{M}_{n\,jm} + \partial_{r_m} B_{lj}\, \mathcal{A}_{n\,j} \dot{r}_m + B_{lj}\, \partial_{\kappa_m} \mathcal{A}_{n\,j} \dot{\kappa}_m\big) + \mathcal{O}(\varepsilon^2) \\
=& - \partial_{\bar{r}_l} \Phi + B_{lj}\, \dot{r}_j + \varepsilon\big(-\partial_{r_m} B_{lj}\, \mathcal{A}_{n\,m}\, \dot{r}_j + \partial_{r_l} \partial_{r_j} \Phi\, \mathcal{A}_{n\,j} + \partial_{r_j} \Phi\, \partial_{\kappa_m} \mathcal{A}_{n\,j} (-\partial_{r_l} A_m) + \\
&+ \partial_{r_l} F_{\mathrm{Lor}\,j}\, \mathcal{A}_{n\,j} + \partial_{r_m} B_{lj}\, \mathcal{A}_{n\,j} \dot{r}_m + \partial_{r_l} B_{jm}\, \mathcal{M}_{n\,jm}\big) + \mathcal{O}(\varepsilon^2) \\
=& - \partial_{r_j} \Phi\, \partial_{\bar{r}_l} r_j + B_{lj}\, \dot{r}_j + \varepsilon\, \partial_{r_l} B_{jm}\, \mathcal{M}_{n\,jm} + \varepsilon\, \partial_{r_j} \Phi\, \partial_{\kappa_m} \mathcal{A}_{n\,j} (-\partial_{r_l} A_m) + \\
&+ \varepsilon\big(-\partial_{r_j} B_{lm}\, \mathcal{A}_{n\,j}\, \dot{r}_m + \partial_{r_l} B_{jm}\, \dot{r}_m\, \mathcal{A}_{n\,j} + \partial_{r_m} B_{lj}\, \mathcal{A}_{n\,j} \dot{r}_m + \big) + \mathcal{O}(\varepsilon^2) \\
=& - \partial_{r_j} \Phi\, \big(\delta_{lj} + \partial_{r_j} \Phi\, \partial_{\kappa_m} \mathcal{A}_{n\,j} (-\partial_{r_l} A_m)\big) + \partial_{r_j} \Phi\, \partial_{\kappa_m} \mathcal{A}_{n\,j} (-\partial_{r_l} A_m) + B_{lj}\, \dot{r}_j + \\
&+ \varepsilon\, \partial_{r_l} B_{jm}\, \mathcal{M}_{n\,jm} + \varepsilon\big(\partial_{r_j} B_{ml} + \partial_{r_l} B_{jm} + \partial_{r_m} B_{lj}\big)\, \dot{r}_m\, \mathcal{A}_{n\,j} + \mathcal{O}(\varepsilon^2) \\
=& - \partial_{r_l} \Phi + B_{lj}\, \dot{r}_j + \varepsilon\, \partial_{r_l} B_{jm}\, \mathcal{M}_{n\,jm} + \mathcal{O}(\varepsilon^2)
\end{aligned} \tag{3.62}$$

In the last step, we used that the sum of all cyclic permutations of the indices j, m and l vanishes identically as can be seen by direct computation and plugging in $B_{lj} = \partial_{r_l} A_j - \partial_{r_j} A_l$.

$$\partial_{r_j} B_{ml} + \partial_{r_l} B_{jm} + \partial_{r_m} B_{lj} = 0$$

3.2.5 Interpretation

We have started from a fairly general scenario and derived equations of motion for a single electron in a periodic potential which is subjected to a slowly varying electromagnetic potential. This superimposed electromagnetic field will induce a ‘drift current’, caused by a small shift in phase at the border of neighboring cells. The slight mismatch in boundary conditions means that a Bloch wave is slightly out of phase; this phase difference in turn induces a current density.

The equations of motion

$$\dot{r}_l = + \partial_{\kappa_l} E_{\mathrm{b}}(\kappa) - \varepsilon \, \Omega_{n\,lj}(\kappa) \, \dot{\kappa}_j - \varepsilon \, B_{jm}(r) \, \partial_{\kappa_l} \mathcal{M}_{n\,jm}(\kappa) \tag{3.63}$$

$$\dot{\kappa}_l = - \partial_{\bar{r}_l} \Phi(r) + B_{lj}(r) \, \dot{r}_j + \varepsilon \, \partial_{r_l} B_{jm}(r) \, \mathcal{M}_{n\,jm}(\kappa) \tag{3.64}$$

are intrinsically gauge invariant (with respect to gauge transformations of the Berry connection $\mathcal{A}_n$ as well as electromagnetic gauge transformations).

To zeroth order in ε, the equations of motion are identical to the classical result. Also if the electromagnetic field is trivial, i. e. gauge invariant to $A = 0$ and $\Phi = 0$, the first order corrections vanish and we are left with

$$\dot{r}_l = \partial_{\kappa_l} E_{\mathrm{b}}(\kappa)$$
$$\dot{\kappa}_l = 0$$

as expected.

Thus, in the simplest limiting cases, vanishing field and $\varepsilon \longrightarrow 0$, we recover the classical results. To see the 'symmetry' of the corrections, we will rewrite the equations of motion for $d = 3$ first; we have identified the two-forms $\Omega_{n\,lj}$ and B_{lj} canonically with the corresponding one-forms Ω_n and B.

$$\dot{r}_l = + \big(\partial_{\kappa_l} E_{\mathrm{b}}(\kappa) - \varepsilon \, (\dot{\kappa} \wedge \Omega_n(\kappa))_l - \varepsilon \, \partial_{\kappa_l} (B(r) \cdot \mathcal{M}_n(\kappa)) \big) \tag{3.65}$$

$$\dot{\kappa}_l = - \big(\partial_{r_l} \Phi(r) - (\dot{r} \wedge B(r))_l - \varepsilon \, \partial_{r_l} (B(r) \cdot \mathcal{M}_n(\kappa)) \big) \tag{3.66}$$

As we can see, the form and direction of the Berry curvature term $-\varepsilon \, \dot{\kappa} \wedge \Omega_n$ is identical to the deflection of a charged particle in a magnetic field, $-\dot{r} \wedge B$. This once more suggests the name 'pseudo-magnetic field' for Ω. The sign of the two terms is the same, so we even have a Lentz' Rule for the pseudomagnetic field Ω_n.

In addition to the circular motion of the electron, there is a wobbling motion along the orbit which is due to the small corrections (proportional to ε) of $\dot{r}$.

The last term is more difficult to interpret. The form suggests $\mathcal{M}_n$ to be a band-dependent magnetic dipole moment which tries to 'align' the magnetic dipole and the magnetic field. The equation for r and κ measure the deviation of the dipole from the direction given by the magnetic field.

The quantum corrections become significant for transport phenomena, in particular for transport phenomena of semiconductors and insulators. Assume a filled band, then we know from classical arguments that it does not contribute to direct conduction [AM01]; mathematically, we know that the energy function E_{b} is periodic in k and the integral over the gradient of a periodic function vanishes. If we integrate $\dot{r}_l$ over the first Brillouin zone M^* to get the total contribution to the current density, we get for the physically interesting case $d = 3$

$$j_{n\,l} = \int_{M^*} \mathrm{d}k \, \dot{r}_l = -\varepsilon \int_{M^*} \mathrm{d}k \, \big(\dot{\kappa} \wedge \Omega_n \big)_l \tag{3.67}$$

$\nabla_\kappa \mathcal{M}_n(\kappa)$ is a periodic function in κ, it does not contribute for the same reason that the $-\nabla_\kappa E_\mathrm{b}$ term does not: if we integrate an odd function (with respect to inversions in κ space) over the torus, the integral vanishes identically.

Transport phenomena of filled bands cannot be understood classically, they are intrinsically quantum effects. If a uniform strong magnetic field is added, equation 3.67 can also be used to understand the quantum Hall effect, using geometric arguments [SW89].

3.3 Time-adiabatic Theory Revisited

Time-adiabatic theory is an established tool of quantum mechanics and as such is covered by standard textbooks in quantum mechanics [Sak94, p. 464 ff.] and with mathematical rigor [Kat95] [FMV92]. We can rephrase time-adiabatic perturbation theory so we can treat it within the framework of space-adiabatic perturbation theory.

While this may seem cumbersome and unnecessary at first, an extension of space-adiabatic perturbation theory is straight-forward and allows to solve new problems are not accessible to time-adiabatic perturbation theory.

3.3.1 Extension Of The Concepts

If classical theories are to be extended to time-dependent problems, phase space is extended to include time and energy as (conjugate) variables [KS04, p. 114 ff.].

$$\mathsf{q} := (t, q) \qquad\qquad \mathsf{p} := (E, p)$$

The canonical symplectic one-form is extended in the same fashion, $\Theta = p_j \, \mathrm{d}q_j - H \, \mathrm{d}t$, as are the Poisson brackets and the Hamiltonian vector field $X = X_H + \partial_t$ for instance.

This is also the right approach for a generalization in quantum theory. In particular we are interested in problems which vary slowly in time only, so we will replace $i\partial_t$ with $i\varepsilon\partial_t$ in the Schrödinger equation where ε controls the separation of timescales.

$$i\varepsilon \frac{\mathrm{d}}{\mathrm{d}t} \Psi = H(t) \, \Psi$$

First of all, we have to introduce a 'new' Hamiltonian on extended phase space; if $H(t)$ is the time-dependent Hamiltonian we are interested in, the symbol

$$K(\eta, t) := \eta + H(t) \tag{3.68}$$

depends on the energy-like variable η and time in a very simple fashion. η will later be quantized to $-i\varepsilon\partial_t$ so that $\hat{K} \, \Psi = 0$ is nothing but the usual Schrödinger equation.

The framework of symbols is also quickly adapted to extended phase space. The generalized Poisson brackets of two symbols A and B (which we will denote by $\{ \cdot \, , \, \cdot \}_{\eta,t}$

to differentiate between the Poisson brackets in regular and extended phase space) are given by

$$\begin{aligned}\{A,B\}_{\eta,t} &= \frac{\mathrm{d}A}{\mathrm{d}\mathsf{p}_j}\frac{\mathrm{d}B}{\mathrm{d}\mathsf{q}_j} - \frac{\mathrm{d}A}{\mathrm{d}\mathsf{q}_j}\frac{\mathrm{d}B}{\mathrm{d}\mathsf{p}_j} \\ &= \{A,B\} + \frac{\mathrm{d}A}{\mathrm{d}\eta}\frac{\mathrm{d}B}{\mathrm{d}t} - \frac{\mathrm{d}A}{\mathrm{d}t}\frac{\mathrm{d}B}{\mathrm{d}\eta} \end{aligned} \tag{3.69}$$

The symbols may of course depend on all variables (p,q), including time and energy.

The Moyal product on extended phase space $\sharp_{\eta,t}$ of two semiclassical symbols is given by

$$\begin{aligned}\big(A\sharp_{\eta,t}B\big)_0 &= A_0\,B_0 \\ \big(A\sharp_{\eta,t}B\big)_1 &= A_1\,B_0 + A_0\,B_1 - \tfrac{i}{2}\{A_0,B_0\}_{\eta,t} = \big(A\sharp B\big)_1 + \tfrac{i}{2}\big(\tfrac{\mathrm{d}A_0}{\mathrm{d}\eta}\tfrac{\mathrm{d}B_0}{\mathrm{d}t} - \tfrac{\mathrm{d}A_0}{\mathrm{d}t}\tfrac{\mathrm{d}B_0}{\mathrm{d}\eta}\big)\end{aligned}$$

to zeroth and first order in ε. We will see how the extra term for the subprincipal symbol yields a very simple correction term.

To see that we will introduce the effective Hamiltonian k which is defined completely analogous to equation 3.36

$$k = u\sharp_{\eta,t}K\sharp_{\eta,t}u^* \asymp k_0 + \varepsilon\,k_1 + \mathcal{O}(\varepsilon^2) \tag{3.70}$$

Instead of going through the whole calculation once more, we will motivate each term. The zeroth order term k_0 is trivial.

$$k_0 = u_0\,K\,{u_0}^* = \eta + u_0\,H\,{u_0}^* = \eta + h_0(t) \tag{3.71}$$

The first non-trivial order can be expressed in terms of the known first order correction from space-adiabatic theory $h_1^{\mathrm{space}}(t)$ and an additional correction $h_1^{\mathrm{time}}(t)$.

$$\begin{aligned}k_1 &= u_0\,K_1\,{u_0}^* + u_1\,K_0\,{u_0}^* + k_0\,u_0\,{u_1}^* + \big(u_0\sharp_{\eta,t}K_0\big)_1\,{u_0}^* - \big(k_0\sharp_{\eta,t}u_0\big)_1\,{u_0}^* \\ &= u_0\,H_1\,{u_0}^* + u_1\,K_0\,{u_0}^* + k_0\,u_0\,{u_1}^* + \big(u_0\sharp_{\eta,t}K_0\big)_1\,{u_0}^* - \big(k_0\sharp_{\eta,t}u_0\big)_1\,{u_0}^* \\ &= h_1^{\mathrm{space}}(t) + u_1\,\eta\,{u_0}^* + \eta\,u_0\,{u_1}^* - \tfrac{i}{2}\big(\tfrac{\partial u_0}{\partial\eta}\tfrac{\partial K_0}{\partial t} - \tfrac{\partial u_0}{\partial t}\tfrac{\partial K_0}{\partial\eta}\big)\,{u_0}^* + \tfrac{i}{2}\big(\tfrac{\partial k_0}{\partial\eta}\tfrac{\partial u_0}{\partial t} - \tfrac{\partial k_0}{\partial t}\tfrac{\partial u_0}{\partial\eta}\big)\,{u_0}^*\end{aligned}$$

If we consider only a single band, analysis shows we can neglect the terms containing the first correction to the unitarity u_1. Also, we can explicitly calculate the first two terms as $k_0 = \eta + h(t)$ and $K_0 = \eta + H_0(t)$; the only thing we need to know is that the (effective) Hamiltonians and the unitarity u_0 do not depend on η. Hence we get $\partial_\eta k_0 = \mathrm{id}$, $\partial_\eta K_0 = \mathrm{id}$ and $\partial_\eta u_0 = 0$ which simplifies the first-order correction for a single band to

$$\begin{aligned}\pi_{\mathrm{r}}\,k_1\,\pi_{\mathrm{r}} &= h_1^{\mathrm{space}}(t) - \tfrac{i}{2}\big(0 - \tfrac{\mathrm{d}u_0}{\mathrm{d}t}\mathrm{id}\big)\,{u_0}^* + \tfrac{i}{2}\big(\mathrm{id}\tfrac{\mathrm{d}u_0}{\mathrm{d}t} - 0\big)\{k_0,u_0\}\,{u_0}^* \\ &= h_1^{\mathrm{space}}(t) + \tfrac{i}{2}\big(\dot{u}_0 \;- u_0\,\dot{u}_0^*\,u_0\big){u_0}^* \\ &= h_1^{\mathrm{space}}(t) + \tfrac{i}{2}\big(\dot{u}_0\,{u_0}^* \;- u_0\,\dot{u}_0^*\big) && (3.72) \\ &=: h_1^{\mathrm{space}}(t) + h_1^{\mathrm{time}}(t) && (3.73)\end{aligned}$$

One important property of h_1^{time} is that it is *independent of the symbol under consideration* as the only quantity which enters is the unitarity chosen in the beginning.

For later use we will evaluate the symbol $h_{1\,n}^{\mathrm{time}}$ with respect to a specific band.

Representation Of h_1^{time} For the calculation of the time contribution, we will switch to the braket notation as one should use the most efficient tool for the job. It acts as a schein force contribution, i. e. forces which are due to the moving coordinate system. The first order *does not depend on the symbol under consideration*.

Furthermore, it is sufficient to calculate one of the two terms of the time contribution, because they are the adjoint of one another. Hence, the term will be the imaginary part of the first operator, up to a sign.

$$h_{1\,n}^{\text{time}} = \tfrac{i}{2}\,\langle \chi_n, (u_0\,\dot{u}_0^* - \dot{u}_0\,u_0^*)\chi_n\rangle \tag{3.74}$$

Our unitaries in braket notation are given by

$$u_0 = |\chi_n\rangle\,\langle\psi_n(k - A(r,t))| \tag{3.75}$$
$$u_0^* = |\psi_n(k - A(r,t))\rangle\,\langle\chi_n| \tag{3.76}$$
$$\dot{u}_0 = |\chi_n\rangle\langle\dot{\psi}_n(k - A(r,t))| \tag{3.77}$$

Now we calculate the first term by using $\dot{u}_0^* = -u_0\,\dot{u}_0\,u_0$. (As we are *not* dealing with symmetric operators, it is inappropriate to use $\langle\psi|u_0|\varphi\rangle$ here.)

$$\begin{aligned}\langle\chi_n|u_0\,\dot{u}_0^*\,\chi_n\rangle &= -\,\langle\chi_n|u_0\,u_0^*\,\dot{u}_0\,u_0^*\,\chi_n\rangle = -\,\langle\psi_n|u_0^*\,\dot{u}_0\,\psi_n\rangle \\ &= -\,\langle\psi_n|\;|\psi_n(k-A(r,t))\rangle\,\langle\chi_n|\;|\chi_n\rangle\langle\dot{\psi}_n(k-A(r,t))|\,|\psi_n\rangle \qquad (3.78)\\ &= -\,\underbrace{\langle\psi_n|\psi_n(k-A(r,t))\rangle}_{=\text{id}}\,\underbrace{\langle\chi_n|\chi_n\rangle}_{=\text{id}}\langle\dot{\psi}_n(k-A(r,t))|\psi_n\rangle \\ &= -\,\langle\dot{\psi}_n|\psi_n\rangle = +\langle\psi_n|\dot{\psi}_n\rangle \qquad (3.79)\end{aligned}$$

In the last step, we used norm conservation, $\partial_t\,\langle\psi_n|\psi_n\rangle = 0$; we also conclude that the last term is purely imaginary and hence we can omit Im as well as shuffle the time derivative to the other argument of the scalar product.

$$\begin{aligned}h_{1\,n}^{\text{time}} &= \ldots = \tfrac{i}{2}\,2\mathrm{Im}\,\langle\psi_n|\dot{\psi}_n\rangle = +i\,\langle\psi_n|\dot{\psi}_n\rangle \\ &=: -\Phi_n(k - A(r,t)) \qquad (3.80)\end{aligned}$$

Here we have defined the geometric scalar potential $\Phi_n := -i\,\langle\psi_n, \partial_t\psi_n\rangle$ which has a similar meaning than the scalar potential in electromagnetism (confer section 2.3).

3.3.2 Time-adiabatic Problems In A Space-adiabatic Framework

If the Hamiltonian symbol depends on time only, i. e. $H \equiv H(t)$, the first-order correction reduces to $u_0\,H_1\,u_0{}^* + h_1^{\text{space}}$ as the Hamiltonian does not depend on p and q. Thus all Poisson brackets $\{\cdot,\cdot\}$ (in regular phase space) vanish and we are left with

$$h_1(t) = u_0\,H_1\,u_0 + h_1^{\text{time}}(t) = u_0\,H_1\,u_0 - \Phi_n \tag{3.81}$$

The semiclassical dynamics is governed by the effective Hamiltonian

$$h_{\text{sc}\,n}(t) = h_{0\,n}(t) - \varepsilon\,\Phi_n = h + \mathcal{O}(\varepsilon^2) \tag{3.82}$$

The advantage of using space-adiabatic perturbation theory as technique of choice is that we can treat far more general problems.

3.3.3 New Types Of Problems

Space-adiabatic perturbation theory *does not single out* time as a special type of variable. So if we assume a system of variables εx which is conjugate to $\hat{k}$ that scale the same way as time and energy, $\hat{E} = -i\varepsilon\partial_t$, we can treat both simultaneously, although they are physically very different.

Assume a system similar to the one discussed before, a system in a slowly varying field whose potential depends slowly on time, i. e. $t = \varepsilon t_\mu$ where t_μ denotes the microscopic time. The specific time-dependence is not important here, only that the potential's change in time is controlled by the same ε which separates the microscopic and macroscopic scale in real space. This may seem artificial at first, but as we will see, we can recast the problem we are interested in in this thesis – direct piezoelectricty – in exactly this form.

$$H(\varepsilon x, \varepsilon t_\mu) = \tfrac{1}{2}\big(\hat{p} - A(\varepsilon x, \varepsilon t_\mu)\big)^2 + V(y, \varepsilon t_\mu) + \Phi(\varepsilon x, \varepsilon t_\mu)$$

Then we can treat the variable $\mathsf{r} := (\varepsilon t_\mu, \varepsilon x)$, which is conjugate to $\mathsf{k} := (-i\partial_t, -i\nabla_x)$, with the formulas we have outlined above.

Direct piezoelectricity can be understood in terms of a potential which changes slowly in time *only*, although we expect that this holds only if the deformations of the crystal are not too large [PST].

If we allow for deformations of the periodicity lattice, (standard) time-adiabatic theory cannot be used to tackle this question.

3.4 Time-dependent Dilations

Time-independent dilations are fairly standard in quantum mechanics; nevertheless, we want to state some general facts. For a more thorough take on the subject, see [insert references here].

We begin by defining a suitably generalized time-dependent dilation operator.

Definition 3.4.1 *Let $D(t) \in \mathrm{Gl}(d, \mathbb{R})$ for all t such that $D(0) = \mathrm{id}_{\mathbb{R}^d}$ and each of its components is a smooth bounded function in t. Then we define the time-dependent dilation to given by*

$$\big(\mathcal{D}_t \Psi\big)(x) := \left|\det D(t)\right|^{1/2} \, \Psi(D(t)x) \tag{3.83}$$

It defines a mapping from $L^2(\mathbb{R}^d)$ to $L^2(\mathbb{R}^d)$.

This generalization is straight-forward; however, since D did not appear explicitly in the generator of the time-*in*dependent dilation $\mathcal{D}$, we expect an additional term which can be attributed to the time-dependence of $D(t)$. The condition $D(0) = \mathrm{id}$ is merely for coherence with our treatment of polarization later on (at $t = 0$, the system is assumed to be unperturbed).

Theorem 3.4.2 *$\mathcal{D}_t$ defines a unitary operator for all t and its generator is given by*

$$\begin{aligned} \mathsf{d}_t &= \tfrac{1}{2}\big(\dot{D}(t)x \cdot iD^{-1}(t)\nabla_x + iD^{-1}(t)\nabla_x \cdot \dot{D}(t)x\big) \\ &= \dot{D}(t)x \cdot iD^{-1}(t)\nabla_x + \tfrac{i}{2}\mathrm{tr}\left({D^{-1}}^{\mathrm{T}}(t)\dot{D}(t)\right) \end{aligned} \tag{3.84}$$

Proof First, we show that $\big[Mx, -iN\nabla_x\big] = i\ \mathrm{tr}\left(N^{\mathrm{T}}M\right) = i\ \mathrm{tr}\left(N\,M^{\mathrm{T}}\right)$ where M and N are two arbitrary d-dimensional matrices.

By direct computation, we obtain

$$\begin{aligned} \big[Mx, -iN\nabla_x\big] &= -\, Mx \cdot iN\nabla_x + iN\nabla_x \cdot Mx \\ &= -\, Mx \cdot iN\nabla_x + i\sum_b\Big(\sum_c N_{bc}\partial_{x_c}\Big)\,\Big(\sum_d M_{bd}x_d\Big) \\ &= -\, Mx \cdot iN\nabla_x + i\sum_{b\,c\,d} \underbrace{N_{bc}}_{{N_{cb}}^{\mathrm{T}}}\, M_{bd} \quad \underbrace{\partial_{x_c}x_d}_{=\delta_{cd}+x_d\partial_{x_c}} \\ &= i\sum_{b\,c} {N_{cb}}^{\mathrm{T}}M_{bc} = i\,\mathrm{tr}\left(N^{\mathrm{T}}\,M\right) \\ &= i\sum_{b\,c} N_{bc}M^{\mathrm{T}}_{cb} = i\,\mathrm{tr}\left(N\,M^{\mathrm{T}}\right) \end{aligned} \tag{3.85}$$

It is trivial to check that $-i\nabla|_{x=D(t)x} = -iD^{-1}\nabla_x|_{x=x} \equiv -iD^{-1}\nabla_x$. (Thus, the momentum scales as expected; scale everything by $\lambda\mathrm{id}$, then the momentum scales as $1/\lambda$).

Let Ψ be such that $i\partial_t\Psi = 0$ for simplicity; deriving $D_t\Psi$ with respect to t, we get

$$\begin{aligned} i\frac{\mathrm{d}}{\mathrm{d}t}\big(\mathcal{D}_t\Psi\big)(x) &= i\frac{\mathrm{d}}{\mathrm{d}t}\big(\left|\det D(t)\right|^{1/2}\Psi(D(t)x)\big) \\ &= i\big(\partial_t\left|\det D(t)\right|^{1/2}\big)\Psi(D(t)x) + \left|\det D\right|^{1/2}\dot{D}x \cdot i\nabla_x\Psi|_{x=Dx} \\ &= \frac{i}{2}\frac{\partial_t\left|\det D(t)\right|}{\left|\det D(t)\right|}\left|\det D(t)\right|^{1/2}\Psi(D(t)x) + \left|\det D\right|^{1/2}\dot{D}x \cdot iD^{-1}\nabla_x\Psi|_{x=x} \\ &= \underbrace{\Big(\tfrac{i}{2}\ \mathrm{tr}\left({D^{-1}}^{\mathrm{T}}\dot{D}\right) + \dot{D}x \cdot iD^{-1}\nabla_x)\Big)}_{=:\mathsf{d}_t}\big(\mathcal{D}_t\Psi\big) \end{aligned} \tag{3.86}$$

where we have used a same trick to derive $\partial_t \det D(t)$; we rewrite $\det D(t)$ and then use $\partial_t \ln D(t) = D^{-1}_{jl}\,\dot{D}_{jl} = \mathrm{tr}\,{D^{-1}}^{\mathrm{T}}\,\dot{D}$.

$$\begin{aligned} i\frac{\mathrm{d}}{\mathrm{d}t}\big(\det D\big) &= i\frac{\mathrm{d}}{\mathrm{d}t}\big(\exp(\mathrm{tr}\ \ln D)\big) = i\exp(\mathrm{tr}\ \ln D)\cdot\mathrm{tr}\,({D^{-1}}^{\mathrm{T}}\,\dot{D}) \\ &= i\det D\cdot\mathrm{tr}\,({D^{-1}}^{\mathrm{T}}\,\dot{D}) \end{aligned}$$

The absolute value sign does not give any (Dirac delta) contributions, because $\det$ is a continuous function on $\mathrm{Gl}(d,\mathbb{R})$; we have assumed that D is invertible for all t and hence it cannot cross from one part of $\mathrm{Gl}(d,\mathbb{R})$ to the other (there is no path joining the two patches, because the image of $\det$ is $\mathrm{ran}(\det) = \mathbb{R}\backslash\{0\}$).

Next, we use the commutation relation derived above with $M = \dot{D}$ and $N = D^{-1}$ to 'symmetrize' the generator.

$$\begin{aligned}\mathsf{d}_t =& \tfrac{i}{2}\,\mathrm{tr}\left({D^{-1}}^{\mathrm{T}}\dot{D}\right) + \dot{D}x \cdot iD^{-1}\nabla_x \\ =& \tfrac{1}{2}\left(-\dot{D}x \cdot iD^{-1}\nabla_x + iD^{-1}\nabla_x \cdot \dot{D}x\right) + \dot{D}x \cdot iD^{-1}\nabla_x \\ =& \tfrac{1}{2}\left(\dot{D}x \cdot iD^{-1}\nabla_x + iD^{-1}\nabla_x \cdot \dot{D}x\right) \end{aligned} \tag{3.87}$$

For $\mathcal{D}_t$ to be unitary, we have to show that $\mathsf{d}_t^* = \mathsf{d}_t$, but this is obvious if d_t is cast in its symmetric form.

It is straight-forward to show that $\mathcal{D}_t$ is really a unitarity pointwise in t, mapping from $L^2(\mathbb{R}^d)$ to $L^2(\mathbb{R}^d)$. □

Remark 3.4.3 It is important to note that d_t does not commute at different times; the calculation of the commutator is lengthy and the details of the calculation will be omitted.

$$\begin{aligned}[\mathsf{d}_t, \mathsf{d}_{t'}] = & \, i\,\mathrm{tr}\left({D^{-1}}^{\mathrm{T}}(t)\,\dot{D}(t')\right)\dot{D}(t)x \cdot iD^{-1}(t')\nabla_x \\ & - i\,\mathrm{tr}\left({D^{-1}}^{\mathrm{T}}(t')\,\dot{D}(t)\right)\dot{D}(t')x \cdot iD^{-1}(t)\nabla_x \end{aligned} \tag{3.88}$$

Formally $\mathcal{D}_t$ is given by the Dyson series, although we caution to take this formula at face value. To prove its existence and equality to $\mathcal{D}_t$ is mathematically a formidable task.

$$\mathcal{D}_t = \mathrm{id} + \sum_{n=1}^{\infty} \int_0^t \mathrm{d}t_1 \int_0^{t_1} \mathrm{d}t_2 \cdots \int_0^{t_{n-1}} \mathrm{d}t_n \, \mathsf{d}_{t_1} \cdots \mathsf{d}_{t_n} \tag{3.89}$$

We will derive the behavior of our fundamental operators under this transformation, namely q and p. As usual, q is the multiplication operator by x and $p = -i\nabla_x \equiv -i\nabla_x|_{x=x}$ (we will suppress $\Box|_{x=x}$ if it is unambiguous from the context).

$$\mathcal{D}_t\, q\, \mathcal{D}_t^{-1} = D(t)\, q \tag{3.90}$$

$$\mathcal{D}_t\, p\, \mathcal{D}_t^{-1} = D^{-1}(t)\, p \tag{3.91}$$

4 Slowly Deformed Lattice

In this section we will deduce the change of polarization per unit cell from a given deformation of the crystal. In other words we focus on the *direct piezoelectric effect* and treat it with the machinery of space-adiabatic perturbation theory for periodic potentials.

Our goal is to *reduce the problem to one we are already familiar with*. Hence we start by defining our objects and the corresponding Hilbert spaces. Then we rescale the Hamiltonian, using the theory developed in section 3.4. The rescaled problem is then accessible to the standard tools from space-adiabatic perturbation theory (see [PST03a], section 3.2), i. e. we compute the effective Hamiltonian of the Zak transformed rescaled Hamiltonian and Weyl-quantize the result. Finally, we will discuss the semiclassics of the problem and calculate the piezocurrent induced by the deformation of the crystal.

4.1 Fundamental Definitions

Consider a solid whose d-dimensional periodicity lattice is initially given by Γ_0 (the 'undeformed' lattice); over time, the periodicity lattice is deformed, the primitive lattice vectors are 'bent', where the transformation law on the microscopic timescale (microscopic times are denoted with t_μ to avoid confusion) is given by a d-dimensional matrix $D(\varepsilon t_\mu)$.

$$\Gamma(\varepsilon t_\mu) := \Gamma(\varepsilon t_\mu) := \left\{ \gamma(\varepsilon t_\mu) \in \mathbb{R}^d \mid \gamma(\varepsilon t_\mu) = \textstyle\sum_{j=1}^{d} n_j \, a_j(\varepsilon t_\mu), \, n_j \in \mathbb{N}_0 \right\} \tag{4.1}$$

The dilation matrix D maps primitive lattice vectors at time $t_\mu = 0$ to primitive lattice vectors at εt_μ.

$$D(\varepsilon t_\mu) \, a_j(0) = a_j(\varepsilon t_\mu)$$

More succinctly we could reformulate this relationship between primitive lattice vectors at different times as $\Gamma(\varepsilon t_\mu) = D(\varepsilon t_\mu) \, \Gamma_0$.

ε controls the speed of the deformation compared to the microscopic timescale. The timescales are related by $t = \varepsilon t_\mu$, t_μ and t being the microscopic and macroscopic time, respectively. Physically we usually have $d \leq 3$. We assume the potential is given by the sum over the atomic potentials $V_{a,s}$ where s denotes the different atoms in a unit cell.

$$V_{\Gamma(\varepsilon t_\mu)}(x, \varepsilon t_\mu) := \sum_{\gamma(\varepsilon t_\mu) \in \Gamma(\varepsilon t_\mu), \, s} V_{a,s}(x + \gamma(\varepsilon t_\mu), \varepsilon t_\mu) = \sum_{\gamma \in \Gamma_0, \, s} V_{a,s}(x + D(\varepsilon t_\mu)\gamma, \varepsilon t_\mu) \tag{4.2}$$

The index $\Gamma(\varepsilon t_\mu)$ of the total potential $V_{\Gamma(\varepsilon t_\mu)}$ denotes its periodicity,

$$V_{\Gamma(\varepsilon t_\mu)}(x + \gamma(\varepsilon t_\mu), \varepsilon t_\mu) = V_{\Gamma(\varepsilon t_\mu)}(x, \varepsilon t_\mu) \qquad \gamma(\varepsilon t_\mu) \in \Gamma(\varepsilon t_\mu)$$

There are two contributions to the time-dependence of the potential: the first part can be solely attributed to the change in shape of the (translational) unit cell. The second contribution is the back reaction of the system to the change in shape, i. e. reconstruction of the potential *within* a unit cell.

Thus the Hamiltonian of our system is defined by

$$\hat{H} \equiv \hat{H}(\varepsilon t_\mu) := -\tfrac{1}{2}\Delta_x + V_{\Gamma(\varepsilon t_\mu)}(x, \varepsilon t_\mu) \tag{4.3}$$

The hat on top of the Hamiltonian indicates that it is an operator and *not* an operator-valued symbol. Those two notions need to be carefully distinguished. However unlike in section 3, we will *omit the hats* $\hat{}$ *on top of multiplication operators* such as k and r (instead of $\hat{k}$ and $\hat{r}$) to simplify the presentation. It should be clear from the context whether we deal with an operator-valued symbol, which acts on the Hilbert space of the fast degrees of freedom $\mathcal{H}_{\mathrm{fast}}$, or an operator on the full Hilbert space $\mathcal{H}_{\mathrm{slow}} \otimes \mathcal{H}_{\mathrm{fast}}$.

4.2 Overview Of Calculations And Results

In a first step, we will rescale the Hamiltonian from ‘physical’ space to a space so the potential will be a Γ_0-periodic function for all times, the time-dependence which is attributed to the reshaping is shifted from the potential to the momentum. We rewrite the initial Hamiltonian in the new, rescaled coordinates.

$$\hat{H}_{\mathrm{rse}}(\varepsilon t_\mu) = -\tfrac{1}{2}\big(D(\varepsilon t_\mu)\nabla_x\big)^2 + V_{\Gamma_0}(x, \varepsilon t_\mu)$$

We then obtain the equivalent of the Schrödinger equation for a rescaled wavefunction; the Hamiltonian which governs the dynamics of rescaled wavefunctions serves as input for the machinery of space-adiabatic perturbation theory.

$$\hat{H}_{\mathrm{rs}} = \hat{H}_{\mathrm{rse}} - \tfrac{1}{2}\varepsilon\left(\dot{D}^{-1}\, x \cdot (-iD\nabla_x) + (-iD\nabla_x) \cdot \dot{D}^{-1}\, x\right)$$

The problem is now very similar to that of a Bloch electron which moves in a slowly varying electromagnetic field (see section 3.2 for details). The Zak-transformed Hamiltonian is given by

$$\begin{aligned}\hat{H}_{\mathrm{Z}} &= \tfrac{1}{2}\big(D(-i\nabla_y + k - A(i\varepsilon\nabla_k, t))\big)^2 + V_{\Gamma_0}(y,t) - \tfrac{1}{2}\big(D\,A(i\varepsilon\nabla_k, t)\big)^2 \\ &= \hat{H}_{\mathrm{per}}(k - A(i\varepsilon\nabla_k, t), t) - \tfrac{1}{2}\big(D\,A(i\varepsilon\nabla_k, t)\big)^2\end{aligned}$$

where the shaping momentum $A(i\varepsilon\nabla_k, \varepsilon t)$ is defined as

$$A(i\varepsilon\nabla_k, t) := D^{-1}(t)\dot{D}^{-1}(t)\, i\varepsilon\nabla_k$$

Applying equations 3.39 and 3.42 to the Zak-transformed Hamiltonian yields an effective Hamiltonian on a relevant part of the spectrum which is separated from the remainder by a gap to prevent the wavefunction from ‘flowing out to other bands’.

$$\begin{aligned} h_{\mathrm{sc}\,n}(k,r,t) :=& h_{0\,n}(k,r,t) + \varepsilon\, h_{1\,n}(k,r,t) \\ =& \big(E_{\mathrm{b}} - \tfrac{1}{2}\big(D\,A\big)^2\big) + \varepsilon\big(-F_{\mathrm{Lor}\,j}\,\mathcal{A}_{n\,j} - B_{jm}\,\mathcal{M}_{n\,jm} - \Phi_n\big) \end{aligned}$$

$B_{jm} := \partial_{r_j} A_m - \partial_{r_m} A_j$ is the shaping two-form and $F_{\mathrm{Lor}\,j}$ is the pseudo Lorentz force defined as in equation 4.21.

$$F_{\mathrm{Lor}\,j} = +\tfrac{1}{2}\partial_{r_j}\big(DA\big)^2 - \partial_t A_j + B_{jm}\,\partial_{k_m} E_{\mathrm{b}} \tag{4.4}$$

However we caution to *not* interpret A and B as electromagnetic quantities, the shaping momentum and two-form only formally resemble their electromagnetic counterparts.

$\mathcal{A}_n := +i\,\langle\psi_n, \nabla_\kappa \psi_n\rangle$ is the Berry connection of the nth band and $\mathcal{M}_{n\,jm}$ the jm component of the Rammal-Wilkinson two-form (equation 3.47). It can be interpreted as ‘effective angular momentum’ of a wavepacket which belongs to that band [DDSN03].

$$\mathcal{M}_{n\,jm} = \tfrac{i}{2}\big\langle\partial_{k_j}\psi_n, (H_{\mathrm{per}} - E_{\mathrm{b}})\,\partial_{k_m}\psi_n\big\rangle \tag{4.5}$$

From this effective Hamiltonian h_{sc} we will derive the semiclassical dynamics of an electron, taking into account that we have to correct the variables to first order in ε to obtain physically meaningful results. Before scaling back to physical space, the equations of motion are given by

$$\begin{aligned} \dot r_l &= \partial_{\kappa_l} E_{\mathrm{b}} - \varepsilon\big(B_{jm}\,\partial_{\kappa_l}\mathcal{M}_{n\,jm} + \Omega_{n\,lj}\,\dot\kappa_j + \Theta_{n\,l}\big) + \mathcal{O}(\varepsilon^2) \\ \dot\kappa_l &= +\tfrac{1}{2}\partial_{r_l}\big(D\,A\big)^2 - \partial_t A_l + B_{lj}\,\dot r_j + \mathcal{O}(\varepsilon^2) \end{aligned}$$

For our intents and purposes we only need to scale back the position r.

$$q_l := D_{lj}\,r_j \implies \dot q_l = \dot D_{lj}\,r_j + D_{lj}\,\dot r_j \tag{4.6}$$

To close the circle and compare our result with that of King-Smith–Vanderbilt as well as Panati et al, we will give an explicit formula for the piezocurrect, i. e. the current which is induced by the squeezing of our system.

$$j_l = \int_{M_0^*} \mathrm{d}k\,\dot q_l = -\varepsilon\int_{M_0^*}\mathrm{d}k\,D_{lj}\,\big(\Theta_{n\,j} + \Omega_{n\,jm}\,\dot\kappa_m\big) + \int_{M_0^*}\mathrm{d}k\,\dot D_{lj}\,r_j \tag{4.7}$$

In the limiting case of vanishing deformation of the unit cell, we recover the result by King-Smith–Vanderbilt.

4.3 Calculations

4.3.1 Rescaled Hamiltonian

We start by rescaling the Hamiltonian using equations 3.90 and 3.91; however, we will work in microscopic time, so we have to replace t by εt_μ so that each derivative with respect to time contributes an extra ε as a prefactor.

We stress that all time-dependent effects are contained in the rescaled Hamiltonian as the Zak transform is time-independent. Technically we could also compute $\mathcal{U}_{\mathrm{Z}} \circ \mathcal{D}_{\varepsilon t_\mu}$ directly, but doing so would obscure this distinction and make it harder to relate the result to the case of a time-dependent potential (confer section 2.3).

Since we start in the scaled space, the computation of the rescaled Hamiltonian involves $\mathcal{D}_{\varepsilon t_\mu}^{-1}$ which is given by replacing D with its inverse D^{-1} as can be seen by direct computation.

$$\begin{aligned}
\hat{H}_{\mathrm{rse}}(\varepsilon t_\mu) &:= \big(\mathcal{D}_{\varepsilon t_\mu}^{-1}\big)\, H(\varepsilon t_\mu)\, \big(\mathcal{D}_{\varepsilon t_\mu}^{-1}\big)^{-1} \\
&= \mathcal{D}_{\varepsilon t_\mu}^{-1}\, H(\varepsilon t_\mu)\, \mathcal{D}_{\varepsilon t_\mu} = \tfrac{1}{2}\big(-D(\varepsilon t_\mu)\, i\nabla_x\big)^2 + V_{\Gamma(\varepsilon t_\mu)}(D^{-1}(\varepsilon t_\mu)\, x, \varepsilon t_\mu) \\
&= -\tfrac{1}{2}\big(D(\varepsilon t_\mu)\nabla_x\big)^2 + V_{\Gamma_0}(x, \varepsilon t_\mu)
\end{aligned} \tag{4.8}$$

Now let ψ_t be a solution of the Schrödinger equation, $i\dot{\psi}_{t_\mu} = \hat{H}(\varepsilon t_\mu)\, \psi_{t_\mu}$ and let Φ be the rescaled wavefunction $\Phi := \mathcal{D}_{\varepsilon t_\mu}^{-1} \psi_{t_\mu}$. Then Φ solves the following equation.

$$\begin{aligned}
i\frac{\mathrm{d}}{\mathrm{d}t_\mu}\Phi(x) &= i\frac{\mathrm{d}}{\mathrm{d}t_\mu}\big(\mathcal{D}_{\varepsilon t_\mu}^{-1}\, \psi_{t_\mu}\big)(x) = -\dot{\mathcal{D}}_{\varepsilon t_\mu}\, \mathcal{D}_{\varepsilon t_\mu}\, \Phi(x) + \mathcal{D}_{\varepsilon t_\mu}^{-1}\, \hat{H}\, \mathcal{D}_{\varepsilon t_\mu}\, \Phi(x) \\
&= i\frac{\mathrm{d}}{\mathrm{d}t_\mu}\Big(|\det D^{-1}|^{1/2}\, \psi_{t_\mu}(D^{-1}(\varepsilon t_\mu)\, x)\Big) \\
&= \Big(i\tfrac{\partial}{\partial t_\mu}|\det D^{-1}|^{1/2}\Big)\, \psi_{t_\mu}(D^{-1}\, x) + i\,\varepsilon\, |\det D^{-1}|^{1/2} \dot{D}^{-1} x \cdot \nabla_x \psi_t(D^{-1}\, x) \\
&\quad + |\det D^{-1}|^{1/2}\, i\dot{\psi}_{t_\mu}(D^{-1} x) \\
&= i\,\varepsilon \operatorname{tr}\big(D^{\mathrm{T}}\, \dot{D}^{-1}\big)\, \Phi(x) - \varepsilon\, |\det D^{-1}|^{1/2}\, \dot{D}^{-1}\, x \cdot (-iD\, \nabla_x)\psi_{t_\mu} + \mathcal{D}_{\varepsilon t_\mu}^{-1}\, \hat{H}\, \mathcal{D}_{\varepsilon t_\mu}\, \Phi(x) \\
&= \Big(i\,\varepsilon \operatorname{tr}\big(D^{\mathrm{T}} \dot{D}^{-1}\big) - \varepsilon\, \dot{D}^{-1}\, x \cdot (-iD\, \nabla_x) + \hat{H}_{\mathrm{rse}}\Big)\, \Phi(x) \\
&=: \hat{H}_{\mathrm{rs}}\, \Phi(x)
\end{aligned} \tag{4.9}$$

For brevity, we have defined $\varepsilon\, \dot{D}^{-1}(\varepsilon t_\mu) := \partial_{t_\mu}(D^{-1}(\varepsilon t_\mu))$, the dot indicates that the *inverse* was derived with respect to time. Scaling back in space shifts the time-dependence from the potential energy to the kinetic energy. As suggested earlier, the only contribution in the potential is due to reconstruction *within* a translational unit cell.

The dilation terms – which are completely analogous to those in section 3.4 – are not self-adjoint term by term, but only as a whole. For simplicity, we will sometimes resort to the symmetrized version and sometimes to the version which includes the purely imaginary trace term, depending on the context.

$$\begin{aligned}\hat{H}_{\mathrm{rs}} &= \hat{H}_{\mathrm{rse}} - \varepsilon\, \dot{D}^{-1}\, x \cdot (-iD\nabla_x) + i\,\varepsilon\, \mathrm{tr}\,\big(D^{\mathrm{T}} \dot{D}^{-1}\big) \\ &= \hat{H}_{\mathrm{rse}} - \varepsilon\, \tfrac{1}{2}\big(\dot{D}^{-1}\, x \cdot (-iD\nabla_x) + (-iD\nabla_x) \cdot \dot{D}^{-1}\, x\big) \qquad (4.10)\end{aligned}$$

4.3.2 Zak-transformed Hamiltonian

Before we continue our considerations, we *switch to macroscopic time* t, i. e. we replace εt_μ by t. In macroscopic time, there is an additional ε in front of the time derivative of the Schrödinger equation.

$$i\varepsilon\, \frac{\mathrm{d}}{\mathrm{d}t}\Psi = \hat{H}_{\mathrm{rs}}(t)\,\Psi$$

Continuing with the standard recipe of space-adiabatic perturbation theory, we compute the Zak transform as defined in section 3.1.2.

$$\begin{aligned}\mathcal{F}\,\hat{H}_{\mathrm{rs}}\,\mathcal{F}^{-1} &= \tfrac{1}{2}\big(D(-i\nabla_y + k)\big)^2 + V_{\Gamma_0}(y) - \varepsilon\, \tfrac{1}{2}\big(\dot{D}^{-1} i\nabla_k \cdot D(-i\nabla_y + k) + D(-i\nabla_y + k) \cdot \dot{D}^{-1} i\nabla_k\big) \\ &= \tfrac{1}{2}\big(D(-i\nabla_y + k)\big)^2 + V_{\Gamma_0}(y) - \varepsilon\, \dot{D}^{-1} i\nabla_k \cdot D(-i\nabla_y + k) + i\,\varepsilon\, \mathrm{tr}\,\big(D^{\mathrm{T}}\, \dot{D}^{-1}\big) \\ &=: \hat{H}_{\mathrm{Z}} \qquad (4.11)\end{aligned}$$

Here, for all times t_μ the variables y and k take values in the undeformed Wigner-Seitz cell M_0 and the undeformed first Brillouin zone M_0^*, repsectively, $y \in M_0$ and $k \in M_0^*$.

The specific form of the first-order correctioin suggests to define the scaling momentum operator as

$$\hat{A} \equiv A(i\varepsilon\nabla_k, t) := D^{-1}\dot{D}^{-1}\, i\varepsilon\nabla_k \qquad (4.12)$$

Now we can rewrite the Hamiltonian as

$$\begin{aligned}\hat{H}_{\mathrm{Z}} &= \tfrac{1}{2}\big(D(-i\nabla_y + k)\big)^2 + V_{\Gamma_0}(y,t) - \varepsilon\, \tfrac{1}{2}\big(D\hat{A} \cdot D(-i\nabla_y + k) + D(-i\nabla_y + k) \cdot D\hat{A}\big) \\ &= \tfrac{1}{2}\big(D(-i\nabla_y + k - A(i\varepsilon\nabla_k, t))\big)^2 - \tfrac{1}{2}\big(D\,A(i\varepsilon\nabla_k, t)\big)^2 + V_{\Gamma_0}(y,t) \qquad (4.13)\end{aligned}$$

Instead of working with operators, we will go back to operator-valued symbols, i. e. we replace $i\varepsilon\nabla_k$ by r and take k to be a vector and not an operator. These two form a second set of variables with commutation relation $[k, i\varepsilon\nabla_k] = -i\,\varepsilon\,\mathrm{id}$. ε was absorbed into r as later, it will be Weyl-quantized by setting r to $r \mapsto i\varepsilon\nabla_k$ again and taking k to be its conjugate operator. In favor of an abbreviated notation, we will often suppress the arguments of various quantities, in case of the shaping momentum $A(r,t)$ we will often simply write A. Since the ε-dependence has been absorbed by A, so formally our Zak-transformed Hamiltonian consists only of a principal symbol, i. e. $H_{\mathrm{Z}\,j} \equiv 0$ $\forall j \in \mathbb{N}$.

To simplify the presentation, let H_{per} be defined as

$$H_{\mathrm{per}}(k - A(r,t), t) := \tfrac{1}{2}\big(D(-i\nabla_y + k - A)\big)^2 + V_{\Gamma_0}(y,t) \qquad (4.14)$$

Quantity	*Bloch Electron*		*Piezoelectricity*	
	Interpretation	Variables	Interpretation	Variables
H_{Z}	Zak-transformed Hamiltonian	k, r	Zak-transformed Hamiltonian	k, r, t
H_{per}	periodic Hamiltonian	$k - A$	Zak-transformed Hamiltonian	$k - A$, t
A	electromagnetic vector potential	r	shaping momentum	r, t
B	magnetic two-form	r	shaping two-form	t
Φ	electrostatic potential	r	$\Phi = -\frac{1}{2}(D\,A)^2$	r, t
$\mathcal{A}_n$	geometric vector potential	$k - A$	geometric vector potential	$k - A$, t
Φ_n	geometric scalar potential	$k - A$	geometric scalar potential	$k - A$, t

Table 4.1: The analogous quantities of the piezoelectric case compared to the case of a Bloch electron in a slowly varying electromagnetic field.

Unless explicitly stated otherwise, all band energies are the eigenvalues of H_{per}. Furthermore, the Hamiltonian in question only has a principal symbol which simplifies calculations tremendously.

$$H(k,r,t) \equiv H_0(k,r,t) = H_{\mathrm{per}}(k - A(r,t),t) - \tfrac{1}{2}\big(D(t)A(r,t)\big)^2 \tag{4.15}$$

4.3.3 Effective Hamiltonian

The effective Hamiltonian is calculated using the formulas derived in section 3.3. For any details as to how to obtain these formulas, we refer to that section or [PST03b].

$$h \asymp \sum_{n\in\mathbb{N}_0} \varepsilon^n \Big(\sum_{j+k+l=n} u_j\, H_k\, u_l^* + \tfrac{i}{2} \sum_{j+k+1=n} \big(u_j \,\big(\tfrac{\mathrm{d}}{\mathrm{d}t} u_k^*\big) - \big(\tfrac{\mathrm{d}}{\mathrm{d}t} u_j\big)\, u_k^* \big) \Big) \tag{4.16}$$

We will calculate the first and the second term separately which we will dub space contribution and time contribution. It is important to note that we are in the framework of time-adiabatic theory coming from a space-adiabatic point of view.

Instead of re-deriving everything from scratch, we will quote the appropriate formulas from sections 3.2 and 3.3 which will be adapted to the present case.

The zeroth order effective Hamiltonian for a Bloch electron in a slowly varying electromagnetic field is given by equation 3.39.

$$h_{0\,n}(k,r) = E_{\mathrm{b}}(k - A(r)) + \Phi(r) \equiv E_n(k,r) \tag{4.17}$$

To relate the two problems, we can identify the electromagnetic vector potential with the shaping momentum and the electrostatic potential $\Phi(r)$ with $-\frac{1}{2}(DA)^2$. We have juxtaposed all relevant quantities in Table 4.1 including the variables they depend on.

$$\begin{aligned} h_{0\,n}(k,r,t) &= E_{\mathrm{b}}(k - A(r,t),t) + \Phi(r,t) \equiv E_n(k,r,t) \\ &= E_{\mathrm{b}}(k - A(r,t),t) - \tfrac{1}{2}\big(D(t)\,A(r,t)\big)^2 \end{aligned} \tag{4.18}$$

The space part of the first-order correction can be obtained by equation 3.48; however, we need to modify equation 3.80 because $A \equiv A(r,t)$ *and* the projector $u_0 \equiv u_0(k - A(r,t), t)$ depend on time. In the notation of section 3.3, we get

$$\begin{aligned}
\pi_\mathrm{r}\, k_1\, \pi_\mathrm{r} &= h_1^{\mathrm{space}}(t) - \tfrac{i}{2}\big(0 - \tfrac{\mathrm{d}u_0}{\mathrm{d}t}\mathrm{id}\big)\, {u_0}^* + \tfrac{i}{2}\big(\mathrm{id}\tfrac{\mathrm{d}u_0}{\mathrm{d}t} - 0\big)\{k_0, u_0\}\, {u_0}^* \\
&= h_1^{\mathrm{space}}(t) + \tfrac{i}{2}\big(\dot{u}_0 \;- u_0\, \dot{u}_0^*\, u_0\big){u_0}^* + i\big(\partial_{k_j} u_0\, (-\partial_t A_j)\;\big){u_0}^* \\
&= h_1^{\mathrm{space}}(t) + \tfrac{i}{2}\big(\dot{u}_0\, {u_0}^* \;- u_0\, \dot{u}_0^*\big) - \partial_t A_j\, \mathcal{A}_{n\,j} \\
&= h_1^{\mathrm{space}}(t) - \Phi_n(k - A(r,t), t) - \partial_t A_j(r,t)\, \mathcal{A}_{n\,j}(k - A(r,t), t) \\
&=: h_1^{\mathrm{space}}(t) + h_1^{\mathrm{time}}(t)
\end{aligned} \tag{4.19}$$

The geometric scalar potential Φ_n is defined similarly to the Berry connection $\mathcal{A}_n$.

$$\Phi_n := -i\,\langle \psi_n, \partial_t \psi_n \rangle$$

To obtain the first-order correction, we need equations 3.48 and 4.19 and combine the two. Although the interpretation differ, formally we obtain a Lorentz force term, a Rammal-Wilkinson term $B_{jm}\, \mathcal{M}_{n\,jm}$ and a geometric scalar potential term $-\Phi_n$; those terms were derived in sections 3.2 and 3.3.

$$\begin{aligned}
h_{1\,n}(k,r,t) =& h_{1\,n}^{\mathrm{space}}(k,r,t) + h_{1\,n}^{\mathrm{time}}(k,r,t) \\
=& \big(-\partial_{r_j}\Phi - \partial_t A_j + B_{jm}\, \partial_{k_m} E_\mathrm{b}\big)\, \mathcal{A}_{n\,j} - B_{jm}\, \mathcal{M}_{n\,jm} - \Phi_n \\
=& \big(+\tfrac{1}{2}\partial_{r_l}\big(D\,A\big)^2 - \partial_t A_j + B_{jm}\, \partial_{k_m} E_\mathrm{b}\big)\, \mathcal{A}_{n\,j} - B_{jm}\, \mathcal{M}_{n\,jm} - \Phi_n \\
=& -F_{\mathrm{Lor}\,j}\, \mathcal{A}_{n\,j} - B_{jm}\, \mathcal{M}_{n\,jm} - \Phi_n
\end{aligned} \tag{4.20}$$

Despite the familiar shape of the equations, the meaning of the individual terms differ in the piezoelectric case from the electromagnetic case. There is no notion of gauge for the shaping momentum, it is physically observable. Also the shaping two-form $B_{jl} \equiv B_{jl}(t) := \partial_{r_j} A_l - \partial_{r_l} A_j$ is a function of time only as r is linear in the shaping momentum $A(r,t) = D^{-1} \dot{D}^{-1}\, r$ so that all derivatives of B with respect to anything other than time vanish.

We have introduced the *pseudo* Lorentz force F_Lor in analogy with equation 3.45 to simplify the presentation and speed up calculations.

$$F_{\mathrm{Lor}\,j} := -\partial_{r_j}\Phi - \partial_t A_j + B_{jm}\, \partial_{k_m} E_\mathrm{b} \tag{4.21}$$

In section 3.2 the Rammal-Wilkinson term was introduced (equation 3.47); it can be interpreted as an intrinsic magnetic dipole moment of the electron.

$$\mathcal{M}_{n\,jm} := \tfrac{i}{2}\big\langle \partial_{k_j}\psi_n, (H_\mathrm{per} - E_\mathrm{b})\, \partial_{k_m}\psi_n \big\rangle$$

One word of caution: we have to differentiate between the shaping potential

$$\Phi(r,t) = -\tfrac{1}{2}\big(D(t)\, A(r,t)\big)^2$$

and the scalar geometric potential

$$\Phi_n(k - A(r,t),t) = -i \left\langle \psi_n(k - A(r,t),t), \partial_t \psi_n(k - A(r,t),t) \right\rangle \tag{4.22}$$

of the nth band. $\mathcal{A}_n$ is the Berry connection of the nth band.

$$\mathcal{A}_n(k - A(r,t),t) = +i \left\langle \psi_n(k - A(r,t),t), \nabla_k \psi_n(k - A(r,t),t) \right\rangle \tag{4.23}$$

The semiclassical Hamiltonian $h_{\mathrm{sc}\,n}$ which governs the dynamics up to order $\mathcal{O}(\varepsilon^2)$ is given by

$$\begin{aligned} h_{\mathrm{sc}\,n}(k,r,t) :=& h_{0\,n}(k,r,t) + \varepsilon\, h_{1\,n}(k,r,t) \\ &= \big(E_{\mathrm{b}} - \tfrac{1}{2}\big(D\,A\big)^2\big) + \varepsilon\big(\big(+\tfrac{1}{2}\partial_{r_l}\big(D\,A\big)^2 - \partial_t A_j + B_{jm}\,\partial_{k_m} E_{\mathrm{b}}\big)\,\mathcal{A}_{n\,j} - B_{jm}\,\mathcal{M}_{n\,jm} - \Phi_n\big) \\ &= \big(E_{\mathrm{b}} - \tfrac{1}{2}\big(D\,A\big)^2\big) - \varepsilon\big(F_{\mathrm{Lor}\,j}\,\mathcal{A}_{n\,j} + B_{jm}\,\mathcal{M}_{n\,jm} + \Phi_n\big) \end{aligned} \tag{4.24}$$

We will use this effective Hamiltonian to obtain equations of motion which include quantum corrections.

4.3.4 Semiclassical Limit

Now that the semiclassical Hamiltonian symbol $h_{\mathrm{sc}\,n}$ has been obtained we have two way we can continue our analysis: in principle we can continue with a fully quantum mechanical treatment of the problem in the reference space or we can derive semiclassical equations of motion for a Bloch electron in a deformed crystal lattice. We will follow the latter approach.

We already have all the ingredients and checked the prerequisites, but we will recap the most important points once again here. We refer to section 3.2 and [Teu03] for details. First and foremost we know that the flow generated by the truncated expansion $h_{\mathrm{sc}\,n}$ compared to the flow of the full effective Hamiltonian h_n (projected onto the nth band) stays $\mathcal{O}(\varepsilon^2)$-close and the error grows at most linearly in time. To put another way, we can use $h_{\mathrm{sc}\,n}$ in our calculations instead of the full expansion and still obtain the 'same' results (up to errors of order $\mathcal{O}(\varepsilon^2\,|t - t_0|)$). This statement is mathematically exact [PST03a, p. 565].

The second ingredient is the fact that we have to correct the initial variables in the representation space, the initial variables *are not* the physical variables (i. e. those we can measure). We can show that the transformation used in [PST03a] can be used here as well, *if we choose parallel transport gauge*, i. e. a gauge in which the geometric scalar potential vanishes $\Phi_n(k - A(r,t),t) = 0$. This is always possible [PST].

We have to amend the *three step-program* of section 3.2.4 with a *fourth step*: we have to scale back to physical space. In the first step of the calculation, section 4.3.1, we have rescaled our spaces such that the translation lattice does not depend on time anymore. To get back to real space, we have to undo this scaling.

$$\Phi^t_\varepsilon(\bar{k},\bar{r}) \xrightarrow[]{\overset{\mathcal{O}(1)}{\text{step 2}}} \Phi^t_\varepsilon(\bar{\kappa},\bar{r}) \xrightarrow[]{\overset{\mathcal{O}(\varepsilon)}{\text{step 3}}} \Phi^t_\varepsilon(\kappa,r) \xrightarrow{\text{step 4}} \Phi^t_\varepsilon(p,q) \tag{4.25}$$

4.3.4.1 Step 1: Equations Of Motion In Effective Variables

First of all, we choose a gauge such that $\Phi_n \equiv 0$; this guarantees that we can formally use the same transformation proposed in [PST03a] and [PST].

We would like to remind the reader of the notation used in section 3.2.4: all bar variables are associated with variables in the effective representation.

The starting point are the usual semiclassical equations of motion.

$$\begin{aligned}\dot{\bar{r}}_l &= +\partial_{\bar{k}_l} h_{\mathrm{sc}\,n}\\ \dot{\bar{k}}_l &= -\partial_{\bar{r}_l} h_{\mathrm{sc}\,n}\end{aligned}$$

where $h_{\mathrm{sc}\,n}$ in parallel transport gauge is given by

$$\begin{aligned}h_{\mathrm{sc}\,n}(k,r,t) =& \big(E_\mathrm{b} - \tfrac{1}{2}\big(D\,A\big)^2\big) + \varepsilon\big(-F_{\mathrm{Lor}\,j}\,\mathcal{A}_{n\,j} - B_{jm}\,\mathcal{M}_{n\,jm} - \Phi_n\big)\\ \overset{\text{gauge}}{=}& \big(E_\mathrm{b} + \Phi\big) + \varepsilon\big(-F_{\mathrm{Lor}\,j}\,\mathcal{A}_{n\,j} - B_{jm}\,\mathcal{M}_{n\,jm}\big)\end{aligned}$$

The pseudo Lorentz force F_Lor is *not* the *physical* Lorentz force, because A and B_{jm} have assumed entirely different meanings. Furthermore we have defined the scalar shaping potential $\Phi := -\frac{1}{2}\big(D\,A\big)^2$.

Now we can rewrite the Hamiltonian so that it formally resembles the effective Hamiltonian of the Bloch electron in the slowly varying electromagnetic field (equation 3.50).

$$\begin{aligned}h_{\mathrm{sc}\,n} =& \big(E_\mathrm{b} + \Phi\big) + \varepsilon\big(\big(\partial_{r_j}\Phi(r) - \partial_t A_j - B_{jm}\,\partial_{k_m}E_\mathrm{b}\big)\mathcal{A}_{n\,j} - B_{jm}\,\mathcal{M}_{n\,jm}\big)\\ =& \big(E_\mathrm{b} + \Phi\big) + \varepsilon\big(F_{\mathrm{Lor}\,j}\,\mathcal{A}_{n\,j} - B_{jm}\,\mathcal{M}_{n\,jm}\big) \qquad (4.26)\end{aligned}$$

Because of the obvious similarity, we will not repeat the calculations in section 3.2.4 in full detail.

We start with the equation for $\dot{\bar{r}}_l$. A straight-forward calculation yields equation 3.55.

$$\begin{aligned}\dot{\bar{r}}_l =& \partial_{\bar{k}_l}\bar{E}_\mathrm{b} + \varepsilon\,\partial_{\bar{k}_l}\big(-F_{\mathrm{Lor}\,j}(\bar{r},\nabla_{\bar{k}}\bar{E}_\mathrm{b})\,\bar{\mathcal{A}}_{n\,j} - \bar{B}_{jm}\,\bar{\mathcal{M}}_{n\,jm}\big)\\ =& \partial_{\bar{k}_l}\bar{E}_\mathrm{b} + \varepsilon\,\partial_{\bar{k}_l}\big(-\tfrac{1}{2}\partial_{\bar{r}_j}\big(\bar{D}\,\bar{A}\big)^2\,\bar{\mathcal{A}}_{n\,j} - \bar{B}_{jm}\,\partial_{\bar{k}_m}\bar{E}_\mathrm{b}\,\bar{\mathcal{A}}_{n\,j} - \bar{B}_{jm}\,\bar{\mathcal{M}}_{n\,jm}\big) \qquad (4.27)\end{aligned}$$

Similarly, we get from equation 3.56

$$\begin{aligned}\dot{\bar{k}}_l =& -\partial_{\bar{r}_l}\bar{\Phi} + \partial_{\bar{r}_l}\bar{A}_j\,\dot{\bar{r}}_j + \varepsilon\,\partial_{\bar{r}_l}\bar{F}_{\mathrm{Lor}\,j}\,\bar{\mathcal{A}}_{n\,j} + \varepsilon\,\partial_{\bar{r}_l}\bar{B}_{jm}\,\bar{\mathcal{M}}_{n\,jm}\\ =& -\partial_{\bar{r}_l}\bar{\Phi} + \partial_{\bar{r}_l}\bar{A}_j\,\dot{\bar{r}}_j + \varepsilon\,\partial_{\bar{r}_l}\bar{F}_{\mathrm{Lor}\,j}\,\bar{\mathcal{A}}_{n\,j} \qquad (4.28)\end{aligned}$$

We have used that $\bar{B}_{jm}$ does *not* depend on r (we refer to table 4.1 for a complete list of functions and their variables).

4.3.4.2 Step 2: Change To Kinetic Momentum

We now switch from the ‘crystal momentum’ to the ‘kinetic momentum’.

$$(\bar{k},\bar{r}) \longmapsto (\bar{\kappa},\bar{r}) := (\bar{k} - \bar{A},\bar{r})$$

$\bar{A}$ does not depend on $\bar{k}$, so we can replace every $\partial_{\bar{k}_l}$ by $\partial_{\bar{\kappa}_l}$. We get two additional terms in the equation of motion. The equation for $\dot{\bar{r}}_l$ becomes

$$\dot{\bar{r}}_l = \partial_{\bar{\kappa}_l} \bar{E}_\mathrm{b} + \varepsilon\, \partial_{\bar{\kappa}_l} \big(-F_{\mathrm{Lor}\, j}\, \bar{\mathcal{A}}_{n\, j} - \bar{B}_{jm}\, \bar{\mathcal{M}}_{n\, jm} \big) \tag{4.29}$$

$\bar{E}_\mathrm{b}$ and $\bar{\mathcal{M}}_{n\, jm}$ are now functions of $\bar{\kappa} = \bar{k} - \bar{A}(\bar{r}, t)$ and (macroscopic) time t only. Because of the additional time dependence, we get an additional term compared to the corresponding Bloch electron result (equation 3.57).

$$\begin{aligned} \dot{\bar{\kappa}}_l &= \dot{\bar{k}}_l - \partial_t \bar{A}_l - \dot{\bar{r}}_m\, \partial_{\bar{r}_m} \bar{A}_l \\ &= \tfrac{1}{2} \partial_{\bar{r}_l} \big(\bar{D}\, \bar{A} \big)^2 - \partial_t \bar{A}_l + \partial_{\bar{r}_l} \bar{A}_j\, \dot{\bar{r}}_j - \dot{\bar{r}}_j\, \partial_{\bar{r}_j} \bar{A}_l + \varepsilon\, \partial_{\bar{r}_l} \bar{F}_{\mathrm{Lor}\, j}\, \bar{\mathcal{A}}_{n\, j} \\ &=: \bar{E}_{\mathrm{sh}\, l} + \bar{B}_{lj}\, \dot{\bar{r}}_j + \varepsilon\, \partial_{\bar{r}_l} \bar{F}_{\mathrm{Lor}\, j}\, \bar{\mathcal{A}}_{n\, j} \end{aligned} \tag{4.30}$$

In the last line we have defined the shaping field $\bar{E}_\mathrm{sh}$ which is defined in the same way as the electric field in electromagnetism and inserted the definition of $\bar{B}_{lj} = \partial_{\bar{r}_l} \bar{A}_j - \partial_{\bar{r}_j} \bar{A}_l$.

$$\bar{E}_{\mathrm{sh}\, l} := -\partial_{\bar{r}_l} \bar{\Phi} - \partial_t \bar{A}_l$$

In this notation the pseudo-Lorentz force reduces to

$$\bar{F}_{\mathrm{Lor}\, l} = \bar{E}_{\mathrm{sh}\, l} + \bar{B}_{lj}\, \partial_{\bar{\kappa}_j} \bar{E}_\mathrm{b} \tag{4.31}$$

4.3.4.3 Step 3: $\mathcal{O}(\varepsilon)$ Correction

We can show that the transformation used to correct the coordinates in the case of the Bloch electron in the slowly varying electromagnetic field can be applied here as well if we switch to the parallel transport gauge, $\Phi_n \equiv 0$.

$$r_l := \bar{r}_l + \varepsilon \bar{\mathcal{A}}_{n\, l} \tag{4.32}$$

$$\kappa_l := \bar{\kappa}_l + \varepsilon \bar{B}_{lj}\, \bar{\mathcal{A}}_{n\, j} + \mathcal{O}(\varepsilon^2) \tag{4.33}$$

The inverse transformations (which are needed for the Taylor expansion to convert functions of the bar variables to functions of variables without bar) are given by

$$\bar{r}_l = r_l - \varepsilon \mathcal{A}_{n\, l} + \mathcal{O}(\varepsilon^2) \tag{4.34}$$

$$\bar{\kappa}_l = \kappa_l - \varepsilon B_{lj}\, \mathcal{A}_{n\, j} + \mathcal{O}(\varepsilon^2) \tag{4.35}$$

We will break down the calculation in several parts and comment on it. The calculation is completely analogous to that in equation 3.61 with the exception of the additional $\partial_t \mathcal{A}_n$ term.

$$\begin{aligned} \dot{r}_l &= \dot{\bar{r}}_l + \varepsilon\, \frac{\mathrm{d}}{\mathrm{d}t} \bar{\mathcal{A}}_{n\, l} = \dot{\bar{r}}_l + \varepsilon\, \frac{\mathrm{d}}{\mathrm{d}t} \mathcal{A}_{n\, l} + \mathcal{O}(\varepsilon^2) \\ &= \dot{\bar{r}}_l + \varepsilon \left(\partial_{\kappa_j} \mathcal{A}_{n\, l}\, \dot{\kappa}_j + \partial_t \mathcal{A}_{n\, l} \right) + \mathcal{O}(\varepsilon^2) = \ldots = \\ &= \partial_{\kappa_l} E_\mathrm{b} + \varepsilon \big(-B_{jm}\, \partial_{\kappa_l} \mathcal{M}_{n\, jm} - \Omega_{n\, lj}\, \dot{\kappa}_j + \partial_t \mathcal{A}_{n\, l} \big) + \mathcal{O}(\varepsilon^2) \end{aligned} \tag{4.36}$$

A simple calculation shows that $\partial_t \mathcal{A}_{n\,l} = 2\mathrm{Im}\,\langle \partial_t \psi_n, \partial_{\kappa_l} \psi_n \rangle$ can be identified with the pseudo-electric field Θ_n in our gauge of choice, $\Phi_n \equiv 0$.

$$\begin{aligned}
\partial_t \mathcal{A}_{n\,l} &= \partial_t\big(i\,\langle \psi_n, \partial_{\kappa_l}\psi_n\rangle\big) = i\,\langle \partial_t\psi_n, \partial_{\kappa_l}\psi_n\rangle + i\,\langle \psi_n, \partial_t\partial_{\kappa_l}\psi_n\rangle \\
&= i\,\langle \partial_t\psi_n, \partial_{\kappa_l}\psi_n\rangle + i\,\langle \psi_n, \partial_{\kappa_l}\partial_t\psi_n\rangle = i\,\langle \partial_t\psi_n, \partial_{\kappa_l}\psi_n\rangle - i\,\langle \partial_{\kappa_l}\psi_n, \partial_t\psi_n\rangle \\
&= 2\mathrm{Im}\,\langle \partial_t\psi_n, \partial_{\kappa_l}\psi_n\rangle \equiv -\Theta_{n\,l}
\end{aligned} \tag{4.37}$$

If we combine the last two equations, we get

$$\dot{r}_l = \partial_{\kappa_l} E_\mathrm{b} - \varepsilon\big(\Theta_{n\,l} + \Omega_{n\,lj}\,\dot{\kappa}_j + B_{jm}\,\partial_{\kappa_l}\mathcal{M}_{n\,jm}\big) + \mathcal{O}(\varepsilon^2) \tag{4.38}$$

Θ_n is a gauge-invariant quantity as can be seen from an equivalent definition

$$\Theta_n := -\partial_t \mathcal{A}_n - \nabla_\kappa \Phi_n \tag{4.39}$$

which is formally the same equation as the dynamical equation for the electric field. This is not coincidental, the symmetry groups of both are $U(1)$.

The calculation of $\dot{\kappa}_l$ requires a little more effort. Again, we can replace all quantities in the effective representation (with bar) with quantities in the physical representation (without bar).

$$\begin{aligned}
\dot{\kappa}_l =& \dot{\bar{\kappa}}_l + \varepsilon\,\frac{\mathrm{d}}{\mathrm{d}t}\big(\bar{B}_{lj}\,\bar{\mathcal{A}}_{n\,j}\big) + \mathcal{O}(\varepsilon^2) = \dot{\bar{\kappa}}_l + \varepsilon\,\frac{\mathrm{d}}{\mathrm{d}t}\big(B_{lj}\,\mathcal{A}_{n\,j}\big) + \mathcal{O}(\varepsilon^2) \\
=& \dot{\bar{\kappa}}_l + \varepsilon\,\big(\partial_t B_{lj}\,\mathcal{A}_{n\,j} + B_{lj}\,\tfrac{\mathrm{d}}{\mathrm{d}t}\mathcal{A}_{n\,j}\big) + \mathcal{O}(\varepsilon^2) \\
=& \bar{E}_{\mathrm{sh}\,l} + \bar{B}_{lj}\,\dot{\bar{r}}_j + \varepsilon\,\big(B_{lj}\,\tfrac{\mathrm{d}}{\mathrm{d}t}\mathcal{A}_{n\,j} + \partial_{\bar{r}_l}\bar{F}_{\mathrm{Lor}\,j}\,\bar{\mathcal{A}}_{n\,j} + \partial_t B_{lj}\,\mathcal{A}_{n\,j}\big) + \mathcal{O}(\varepsilon^2)
\end{aligned}$$

We Taylor-expand the remaining bar terms to first order and simplify the remaining terms. $\bar{B}_{lj}$ does not need to be expanded as it does not depend on $\bar{r}$.

$$\begin{aligned}
\dot{\kappa}_l =& \big(E_{\mathrm{sh}\,l} - \varepsilon\partial_{r_j}E_{\mathrm{sh}\,l}\,\mathcal{A}_{n\,j}\big) + B_{lj}\,\big(\dot{r}_j - \varepsilon\,\tfrac{\mathrm{d}}{\mathrm{d}t}\mathcal{A}_{n\,j}\big) + \\
& + \varepsilon\,\big(B_{lj}\,\tfrac{\mathrm{d}}{\mathrm{d}t}\mathcal{A}_{n\,j} + \partial_{r_l}F_{\mathrm{Lor}\,j}\,\mathcal{A}_{n\,j} + \partial_t B_{lj}\,\mathcal{A}_{n\,j}\big) + \mathcal{O}(\varepsilon^2) \\
=& E_{\mathrm{sh}\,l} + B_{lj}\,\dot{r}_j + \varepsilon\big(-B_{lj}\,\tfrac{\mathrm{d}}{\mathrm{d}t}\mathcal{A}_{n\,j} + B_{lj}\,\tfrac{\mathrm{d}}{\mathrm{d}t}\mathcal{A}_{n\,j}\big) + \\
& + \varepsilon\,\big(-\partial_{r_j}E_{\mathrm{sh}\,l}\,\mathcal{A}_{n\,j} + \partial_{r_l}F_{\mathrm{Lor}\,j}\,\mathcal{A}_{n\,j} + \partial_t B_{lj}\,\mathcal{A}_{n\,j}\big) + \mathcal{O}(\varepsilon^2) \\
=& E_{\mathrm{sh}\,l} + B_{lj}\,\dot{r}_j + \varepsilon\,\big(-\partial_{r_j}E_{\mathrm{sh}\,l} + \partial_{r_l}E_{\mathrm{sh}\,j} + \mathcal{O}(\varepsilon) + \partial_t B_{lj}\big)\mathcal{A}_{n\,j} + \mathcal{O}(\varepsilon^2) \\
=& E_{\mathrm{sh}\,l} + B_{lj}\,\dot{r}_j + \mathcal{O}(\varepsilon^2) = -\partial_{r_l}\Phi - \partial_t A_l + B_{lj}\,\dot{r}_j + \mathcal{O}(\varepsilon^2) \\
=& \tfrac{1}{2}\partial_{r_l}\big(D\,A\big)^2 - \partial_t A_l + B_{lj}\,\dot{r}_j + \mathcal{O}(\varepsilon^2)
\end{aligned} \tag{4.40}$$

Since $F_{\mathrm{Lor}\,j} = E_{\mathrm{sh}\,j} + B_{jm}\,\dot{r}_m + \mathcal{O}(\varepsilon)$ and the shaping two-form B_{jm} does not depend on r, we have that

$$\partial_{r_l}F_{\mathrm{Lor}\,j} = \partial_{r_l}E_{\mathrm{sh}\,j}$$

It is easy to verify by direct calculation that the last term indeed vanishes identically,

$$-\partial_{r_j}E_{\mathrm{sh}\,l} + \partial_{r_l}E_{\mathrm{sh}\,j}\ + \partial_t B_{lj} \equiv 0$$

4.3.4.4 Step 4

We will only scale back the position as the calculations are easier with the momentum k which is an element of the undeformed first Brillouin zone. However since the integral of a periodic function does not change when the function is shifted by a fixed amount, we can continue to use κ.

We set $q := D(t)\,r$; q is the position in physical space. Deriving q_l with respect to time yields

$$\begin{aligned}\dot{q}_l =& D_{lj}\,\dot{r}_j + \dot{D}_{lj}\,r_j \\ =& D_{lj}\left(\partial_{\kappa_j}E_{\mathrm{b}} - \varepsilon\big(\Theta_{n\,j} + \Omega_{n\,jm}\,\dot{\kappa}_m + B_{mc}\,\partial_{\kappa_j}\mathcal{M}_{n\,mc}\big)\right) + \dot{D}_{lj}\,r_j \end{aligned} \tag{4.41}$$

Thus we get an additional term, $\dot{D}_{lj}\,r_j$, which describes the motion of the electrons which adiabatically follow the crystal lattice which is deformed in time.

4.3.5 Piezocurrent

In order to obtain the contribution of the nth band to the piezocurrent density, we integrate $\dot{q}$ over the *undeformed* first Brillouin zone M_0^*.

$$j_l = \int_{M_0^*} \mathrm{d}k\,\dot{q}_l = \int_{M_0^*} \mathrm{d}\kappa\,\dot{q}_l \tag{4.42}$$

We will now assume that our band of interest, the nth band, is filled, i. e. $\hat{\psi}_n(k) = 1$. This is physically plausible since we have assumed to deal with an insulator which means that all bands below the Fermi level are completely filled.

Since E_{b} and $B_{jm}\,\mathcal{M}_{n\,jm}$ are periodic functions in κ (with respect to the reciprocal undeformed lattice Γ_0^*), the integral of their derivatives with respect to κ, ∂_{κ_l}, vanishes. This means we have three contributing terms.

$$j_l = -\varepsilon \int_{M_0^*} \mathrm{d}\kappa\,D_{lj}\big(\Theta_{n\,j} + \Omega_{n\,jm}\,\dot{\kappa}_m\big) + \int_{M_0^*} \mathrm{d}\kappa\,\dot{D}_{lj}\,r_j \tag{4.43}$$

$\dot{\kappa}_m$ is given by equation 4.40 where we replace r by $D^{-1}q$ and all derivatives in r, ∇_r by $D\,\nabla_q$.

$$\dot{\kappa}_l = +\tfrac{1}{2}D_{lj}\partial_{q_j}\big(D\,A(D^{-1}q)\big)^2 + B_{lj}\,D^{-1}_{jc}\big(\dot{q}_c - \dot{D}_{lm}D^{-1}_{mc}\,q_c\big) - \partial_t A_l(D^{-1}q) \tag{4.44}$$

We will interpret this result in the Conclusion of our calculations.

4.4 Comments On The Quantum Corrections

It is interesting to comment on the quantum corrections as to ascribe a meaning to them and anticipate the effect they will have on the motion of the electron. The analogy to an electron moving in a slowly varying electromagnetic potential will help us gain insight.

The semiclassical effective Hamiltonian is composed of five terms: the $\mathcal{O}(1)$ terms are clear, they give the 'trivial' motion of the electron along the energy surface. Hence, to zeroth order, the effective Hamiltonian coincides with what is usually found in solid state physics textbooks [AM01].

$$h_{\mathrm{sc}\,n}(k,r,t) = \big(E_{\mathrm{b}} - \tfrac{1}{2}(D\,A)^2\big) + \varepsilon\big(-F_{\mathrm{Lor}\,j}\,\mathcal{A}_{n\,j} - B_{jm}\,\mathcal{M}_{n\,jm} - \Phi_n\big)$$

The second term $-\frac{1}{2}(DA)^2$ is quadratic in r and one could think that this harmonic repulser causes mayhem, but this is not the case. Although this term keeps on increasing the momentum of the electron, the electron will still turn at the border of the first Brillouin zone and oscillate back. In other words, all the harmonic repulser does is induce Bloch oscillations. We will expand this argument when we discuss the equations of motion.

The first $\mathcal{O}(\varepsilon)$ correction, $-F_{\mathrm{Lor}\,j}\,\mathcal{A}_{n\,j}$, is not easy to interpret as it clearly depends on the gauge.

As pointed out by Niu [DDSN03], the Rammal-Wilkinson two-form $\mathcal{M}_{n\,jm}$ can be interpreted as the internal angular momentum of a wavefunction belonging to the nth band. Thus $B_{jm}\,\mathcal{M}_{n\,jm}$ can be interpreted as the *orbital pseudo-magnetization energy*.

The last term $-\Phi_n$ is just a shift in reference point of the energy and thus does not contribute to the dynamics of the system.

To simplify the presentation, we will interpret the scaled equations of motion, equations 4.38 and 4.40, first, and then discuss the implications of scaling back to physical space. Up to order $\mathcal{O}(\varepsilon^2)$ the equation for the velocity $\dot{r}_l$ of an electron in the nth band is given by

$$\dot{r}_l = \partial_{\kappa_l} E_{\mathrm{b}} - \varepsilon\big(\Theta_{n\,l} + \Omega_{n\,lj}\,\dot{\kappa}_j + B_{jm}\,\partial_{\kappa_l}\mathcal{M}_{n\,jm}\big)$$

The gradient of the electron's band energy function in equation 4.38 dominates the motion of the electron, the electron is guided along the energy surface of the nth band. Since we have assumed the system to be in a band insulating state, this term does not contribute to the conductivity. All other terms are higher-order corrections of order $\mathcal{O}(\varepsilon)$ which may lead to a conductance even if the electrons of the crystal are in an insulating state.

The term which was discovered by King-Smith and Vanderbilt, $-\varepsilon\Theta_{n\,l}$, does give the well-known contribution to the piezocurrent. Θ_n can be dubbed pseudo-electric field as it formally satisfies the kinematic Maxwell equation for the electric field.

$-\varepsilon\Omega_{lj}\,\dot{\kappa}_j$ is new in the context of piezoelectricity. In the theory of the quantum Hall effect[1], it is this term which explains the quantization of the Hall current in terms of geometric invariants (equation (14) in [BvS94] or [TKNdN82]). The quantum Hall effect is essentially concerned with the conductivity perpendicular to both, the applied

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[1] A strong magnetic field is applied perpendicular to a current in a conductor. Then a current perpendicular to both, the magnetic and the electric field, can be measured. At low temperatures the Hall current is quantized [TKNdN82].

electric and magnetic field, so we expect a similar behavior here: this term should contribute mainly to the conductance which is perpendicular to the shaping two-forms B_{jm} and E_{sh}.

The term containing the Rammal-Wilkinson two-form, $-\varepsilon B_{jm}\,\partial_{\kappa_l}\mathcal{M}_{n\,jm}$, describes the dynamics of the total internal angular momentum of a wavefunction which belongs to the nth band. However this term will not contribute to the piezocurrent as the shaping two-form B_{jm} depends only on time and the Rammal-Wilkinson $\mathcal{M}_{n\,jm}$ is periodic in κ. The gradient of a periodic function is odd with respect to inversion and the integral of an odd function over the first Brillouin zone vanishes.

Now we turn to the equation for $\dot{\kappa}_l$, equqtion 4.40. Again, the analogy to electromagnetism will help us understand the dynamics of the system. *Formally* equation 4.40 is identical to that of a particle in an electromagnetic potential.

$$\dot{\kappa}_l = E_{\mathrm{sh}\,l} + B_{lj}\,\dot{r}_j = \tfrac{1}{2}\partial_{r_l}\big(D\,A\big)^2 - \partial_t A_l + B_{lj}\,\dot{r}_j$$

The shaping field E_{sh} will accelerate the particle; classically this would have very unphysical implications as the potential here is a harmonic repulser and a classical particle would be accelerated without bound. However E_{sh} will only induce Bloch oscillations: when the electron reaches the border of a Brillouin zone, it will be, due to the periodicity in reciprocal space, start at the opposite end of the Brillouin zone. More mathematically, the crystal momentum is defined only up to a reciprocal lattice vector $\gamma^* \in \Gamma_0^*$, and hence the momentum $\kappa = k - A(r,t)$ will always remain bounded.

The shaping two-form B_{jm} on the other hand will induce a motion perpendicular to it as a constant magnetic field forces a charge onto cyclotron orbits.

If we scale back r to real space, we get one extra term in the equation for $\dot{q}$, $q := D(t)\,r$.

$$\dot{q}_l = D_{lj}(t)\,\dot{r}_j + \dot{D}_{lj}(t)\,r_j$$

When we scale back, the ‘scaled-back’ velocity $D_{lj}\,\dot{r}_j$ contains the non-trivial dynamics. $\dot{D}_{lj} r_j$ is a schein force term that is due to the moving coordinate system. Physically it describes the tendency of the electron to adiabatically follow the nuclei.

If we integrate $\dot{q}_l$ over the first Brillouin zone, we obtain the piezocurrent in that direction. Only three terms contribute. To lowest order, the piezocurrent is just the motion of the electron which adiabatically follows the motion of the nuclei.

$$j_l = \int_{M_0^*} \mathrm{d}\kappa\,\dot{D}_{lj}\,r_j - \varepsilon \int_{M_0^*} \mathrm{d}\kappa\,D_{lj}\big(\Theta_{n\,j} + \Omega_{n\,jm}\,\dot{\kappa}_m\big) \tag{4.45}$$

The two order $\mathcal{O}(\varepsilon)$ corrections are the (rescaled) King-Smith–Vanderbilt term $-\varepsilon\Theta_{n\,j}$ and a term which is formally identical to the Kubo formula [TKNdN82], $-\varepsilon\Omega_{n\,jm}\,\dot{\kappa}_m$.

However since we can assume the changes in shape to be small, we can infer that the changes of volume are small and the shaping matrix D must be close to the identity. In a suitable matrix norm (the supremum norm for instance) we have

$$\|D(t) - \mathrm{id}_{\mathbb{R}^d}\| < \delta$$

with $\delta \ll 1$. This implies we can neglect the deformation in the order $\mathcal{O}(\varepsilon)$ terms and yield

$$j_l \simeq \int_{M_0^*} \mathrm{d}\kappa\, \dot{D}_{lj}\, r_j - \varepsilon \int_{M_0^*} \mathrm{d}\kappa \left(\Theta_{n\,l} + \Omega_{n\,lj}\, \dot{\kappa}_j\right) \tag{4.46}$$

This reduces the effect of the deformation to the inclusion of two extra terms in the integral over the first Brillouin zone M_0^*, $-\varepsilon\Omega_{n\,lj}\, \dot{\kappa}_j$ and $\dot{D}_{lj}\, r_j$.

We would like to stress that there is no notion of gauge invariance in this case. The shaping momentum A is physically observable as the shaping matrix $D(t)$ is.

$$A(r,t) = D^{-1}\dot{D}^{-1}\, r$$

Even if there is a 'gauge function χ' such that $A = \nabla_r \chi$ holds, i. e. if A is equivalent with $A = 0$, this would imply also the shaping potential

$$\Phi(r,t) = -\tfrac{1}{2}\big(DA\big)^2 \overset{\text{gauge}}{\equiv} 0 \tag{4.47}$$

vanishes identically and thus all effects due to the reshaping were not observable.

However similarly to electromagnetism, we can split A into a curl-free (A_{grad}) and a divergence-free part (A_{curl}), $A \equiv A_{\text{grad}} + A_{\text{curl}}$. We define the matrix Q to be the matrix

$$A(r,t) = D^{-1}\dot{D}^{-1}\, r =: Q\, r$$

We can split every matrix into a symmetric and an antisymmetric part, Q_{sym} and Q_{asym} with $Q = Q_{\text{sym}} + Q_{\text{asym}}$.

$$\begin{aligned} Q_{\text{sym}} &:= \tfrac{1}{2}\big(Q + Q^{\mathrm{T}}\big) \\ Q_{\text{asym}} &:= \tfrac{1}{2}\big(Q - Q^{\mathrm{T}}\big) \end{aligned}$$

A_{grad} and A_{curl} are now defined as

$$\begin{aligned} A_{\text{grad}}(r,t) &:= Q_{\text{sym}}\, r \\ A_{\text{curl}}(r,t) &:= Q_{\text{asym}}\, r \\ A(r,t) &= Q_{\text{sym}}\, r + Q_{\text{asym}}\, r \equiv Q\, r \end{aligned}$$

We can show explicitly that A_{grad} does not contribute to the shaping two-form B_{jm} and that $B_{lj} = 2Q_{\text{asym}\,lj}$.

$$\begin{aligned} B_{lj} &= \partial_{r_l} A_j - \partial_{r_l} A_j = Q_{lj} - Q_{jl} = \big(Q_{\text{sym}\,lj} - Q_{\text{asym}\,lj}\big) - \big(Q_{\text{sym}\,jl} - Q_{\text{asym}\,jl}\big) \\ &= \big(Q_{\text{sym}\,lj} - Q_{\text{sym}\,lj}\big) + \big(Q_{\text{asym}\,lj} + Q_{\text{asym}\,lj}\big) = 2Q_{\text{asym}\,lj} \end{aligned} \tag{4.48}$$

On the other hand the gradient of the potential

$$\varphi(r,t) = \tfrac{1}{2} r \cdot Q_{\text{sym}} r$$

generates A_{grad},

$$\nabla_r \varphi(r,t) = Q_{\mathrm{sym}} r \equiv A_{\mathrm{grad}}$$

Thus each shaping potential induced by a deformation D can be uniquely decomposed into two parts, a curl-free and a divergence-free part. Each of the two corresponds to a specific class of deformation and it might be useful to investigate what class of shaping matrices D lead to a purely symmetric or asymmetric matrix Q.

5 Examples

We will proceed with two simple examples: a dilation parallel to a primitive lattice vector with initial and final position as well as an oscillatory dilation along one crystal axis.

5.1 Dilation Along One Primitive Lattice Vector

We assume a cubic crystal that is dilated along one of the crystal axes. Thus the dilation matrix D is given by

$$D(t) = \begin{pmatrix} 1+\lambda t & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

λ is a small parameter, $|\lambda| \ll 1$. If T is the final time, the total (relative) displacement $|\lambda|\, T$ is also assumed to be small $|\lambda|\, T \ll 1$. Physically the total deformation is typically of the order of 10^{-3} or smaller. To yield a dimensionless number, λ has the unit of $1\ {}^{1}\!/\!\mathrm{s}$. If $\lambda < 0$, the crystal is compressed, and conversely the crystal is elongated if $\lambda > 0$

We will now calculate all quantities which are needed and then give the effective Hamiltonian. The inverse of the dilation and its time-derivative are

$$D^{-1}(t) = \begin{pmatrix} (1+\lambda t)^{-1} & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

$$\partial_t D^{-1}(t) = \dot{D}^{-1}(t) = -\frac{\lambda}{(1+\lambda t)^2} \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$$

The shaping momentum's only non-zero component is along the direction of the deformation.

$$A(r,t) := D^{-1}\, \dot{D}^{-1}\, r = -\frac{\lambda}{(1+\lambda t)^3} \begin{pmatrix} r_1 \\ 0 \\ 0 \end{pmatrix}$$

The time-derivative of the shaping momentum as well as the 'potential' generated by the deformation are calculated in a straight-forward manner.

$$\begin{aligned}\partial_t A_1(r,t) &= \frac{3\lambda^2}{(1+\lambda t)^4} r_1 - \frac{\lambda}{(1+\lambda t)^3}\dot{r}_1 \simeq 3\lambda^2(1-4\lambda t)\, r_1 - \lambda(1-3\lambda t)\,\dot{r}_1 \\ \Phi(r,t) &:= -\tfrac{1}{2}\big(D(t)\,A(r,t)\big)^2 = -\frac{1}{2}\frac{\lambda^2}{(1+\lambda t)^4}{r_1}^2 \simeq -\tfrac{1}{2}\lambda^2(1-4\lambda t)\,{r_1}^2\end{aligned}$$

This implies the shaping two-form $B_{jm}(t) = \partial_{r_j} A_m - \partial_{r_m} A_j \equiv 0$ vanishes identically. (The shaping two-form is a measure of the 'twisting' and shear due to the deformation.)

This simplifies the effective Hamiltonian and the equations of motion considerably. We plug everything into equation 4.24 and obtain

$$\begin{aligned}h_{\mathrm{sc}\,n} &= \Big(E_{\mathrm{b}} - \tfrac{1}{2}\tfrac{\lambda}{(1+\lambda t)^4}{r_1}^2\Big) + \varepsilon\Big(\tfrac{\lambda^2}{(1+\lambda t)^4} r_1\,\mathcal{A}_{n\,1} - \Phi_n\Big) \\ &\simeq \big(E_{\mathrm{b}} - \tfrac{1}{2}\lambda^2(1-4\lambda t)\,{r_1}^2\big) + \varepsilon\big(\lambda^2(1-4\lambda t)\,r_1\,\mathcal{A}_{n\,1} - \Phi_n\big)\end{aligned}$$

The equations of motion in the unscaled variables simplify in the 1-direction as $\Omega_{n\,11} \equiv 0$ due to antisymmetry of the pseudomagnetic two-form. We will use the appropriate expansions of $(1+\lambda t)^{-n}$ to simplify the results. Since $\lambda t \ll 1$, we expect these results to be reasonably accurate.

$$\begin{aligned}\dot{\kappa}_1 &= E_{\mathrm{sh}\,1} + B_{1j}\,\dot{r}_j = -\partial_{r_1}\Phi(r,t) - \partial_t A_1 \\ &= -\frac{2\lambda^2}{(1+\lambda t)^4}\,r_1 + \frac{\lambda}{(1+\lambda t)^3}\,\dot{r}_1 \simeq -2\lambda^2(1-4\lambda t)\,r_1 + \lambda(1-3\lambda t)\,\dot{r}_1 \\ \dot{\kappa}_l &= 0 && l \neq 1 \\ \dot{r}_1 &= \partial_{\kappa_1} E_{\mathrm{b}} - \varepsilon\,\Theta_{n\,1} \\ \dot{r}_l &= \partial_{\kappa_l} E_{\mathrm{b}} - \varepsilon\,\big(\Theta_{n\,l} + \Omega_{n\,l1}\big(2\lambda^2(1-4\lambda t)\,r_1 - \lambda(1-3\lambda t)\,\partial_{\kappa_1}E_{\mathrm{b}}\big)\big) && l \neq 1\end{aligned}$$

We scale back to the 'physical' coordinates $q_l := D_{lj} r_j$. Clearly since D only acts non-trivially on the first coordinate, we have $q_l = r_l$ for $l \neq 1$.

$$\begin{aligned}\dot{q}_1 &= D_{1j}\,\dot{r}_j + \dot{D}_{1j}\,r_j \\ &= (1+\lambda t)\,\partial_{\kappa_1}E_{\mathrm{b}} - \varepsilon\,(1+\lambda t)\,\Theta_{n\,1} + \lambda\,r_1\end{aligned}$$

The piezocurrent density is obtained by integrating over the first Brillouin zone of the lattice at $t = 0$ (as we did not scale back the momentum).

$$\begin{aligned}j_1 &= \int_{M_0^*} \mathrm{d}\kappa\,\dot{q}_1 = (1+\lambda t)\int_{M_0^*}\mathrm{d}\kappa\,\partial_{\kappa_1}E_{\mathrm{b}} + \int_{M_0^*}\mathrm{d}\kappa\,\lambda r_1 - \varepsilon\int_{M_0^*}\mathrm{d}\kappa\,(1+\lambda t)\,\Theta_{n\,1} \\ &\approx |M_0^*|\;\lambda r_1 - \varepsilon\int_{M_0^*}\mathrm{d}\kappa\,\Theta_{n\,1}\end{aligned}$$

For $l \neq 1$ we get up to first order in λ an additional correction which is proportional to $\dot{r} \wedge \Omega_n$. However $\lambda \ll 1$, so $\varepsilon\lambda$ is even smaller, $\varepsilon\lambda \ll 1$, and we can neglect terms of order $\mathcal{O}(\lambda\varepsilon)$

$$\begin{aligned}
j_l &= \int_{M_0^*} \mathrm{d}\kappa \, \dot{q}_l \\
&= \int_{M_0^*} \mathrm{d}\kappa \, \partial_{\kappa_l} E_\mathrm{b} - \varepsilon \int_{M_0^*} \mathrm{d}\kappa \, \big(\Theta_{n\,l} + \Omega_{n\,l1}\big(2\lambda^2(1-4\lambda t)r_1 - \lambda(1-3\lambda t)\partial_{\kappa_1} E_\mathrm{b}\big)\big) \\
&\approx -\varepsilon \int_{M_0^*} \mathrm{d}\kappa \, \big(\Theta_{n\,l} - \lambda\,\Omega_{n\,l1}\,\partial_{\kappa_1} E_\mathrm{b}\big) \approx -\varepsilon \int_{M_0^*} \mathrm{d}\kappa \, \Theta_{n\,l}
\end{aligned}$$

Thus the non-trivial contribution to the piezocurrent is due to the King-Smith–Vanderbilt term, $-\varepsilon\,\Theta_{n\,l}$, only in the 1-direction we get one extra term due to rescaling, $|M_0^*|\;\lambda r_1$.

5.2 Oscillatory Deformation

Instead of a deformation linear in time t, we assume the crystal is deformed periodically with frequency ω. Thus the dilation matrix D is given by

$$D(t) = \begin{pmatrix} 1+\lambda\sin\omega t & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

Again λ is a small parameter, $\lambda \ll 1$. Unlike in the previous case, λ is a dimensionless number from the start which quantifies the maximal relative change in length along the 1-direction. Physically we expect it to be of the order $\lambda \sim 10^{-8} - 10^{-4}$. However the frequency ω may be large, $\omega \sim 10^3 - 10^8\,{}^1\!/\mathrm{s}$, so that both combined $\lambda\omega$ cannot be neglected.

We will now calculate all quantities which are needed and then give the effective Hamiltonian. The inverse of the dilation and its time-derivative are

$$D^{-1}(t) = \begin{pmatrix} (1+\lambda\sin\omega t)^{-1} & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

$$\partial_t D^{-1}(t) = \dot{D}^{-1}(t) = -\frac{\lambda\omega\cos\omega t}{(1+\lambda\sin\omega t)^2} \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$$

The shaping momentum vanishes in the 2- and 3-direction.

$$A(r,t) := D^{-1}\,\dot{D}^{-1}\,r = -\frac{\lambda\omega\cos\omega t}{(1+\lambda\sin\omega t)^3} \begin{pmatrix} r_1 \\ 0 \\ 0 \end{pmatrix}$$

The time-derivative of the shaping momentum as well as the ‘potential’ generated by the deformation are given by

$$
\begin{aligned}
\partial_t A_1(r,t) &= \frac{3\lambda^2\omega^2\cos^2\omega t}{(1+\lambda\sin\omega t)^4} r_1 + \frac{\lambda\omega^2\sin\omega t}{(1+\lambda\sin\omega t)^3} r_1 - \frac{\lambda\omega\cos\omega t}{(1+\lambda\sin\omega t)^3}\dot{r}_1 \\
&\simeq \lambda\omega(1-3\lambda\sin\omega t)\big(\omega\sin\omega t\, r_1 - \cos\omega t\, \dot{r}_1\big) \\
\Phi(r,t) &:= -\tfrac{1}{2}\big(D(t)\,A(r,t)\big)^2 = -\frac{1}{2}\frac{\lambda^2\omega^2\cos^2\omega t}{(1+\lambda\sin\omega t)^4}{r_1}^2 \\
&\simeq -\tfrac{1}{2}\lambda^2\omega^2\cos^2\omega t\,(1-4\lambda\sin\omega t)\,{r_1}^2
\end{aligned}
$$

The shaping two-form $B_{jm}(t) = \partial_{r_j}A_m - \partial_{r_m}A_j \equiv 0$ vanishes identically. We plug everything into equation 4.24 and obtain

$$
\begin{aligned}
h_{\mathrm{sc}\,n} &= \Big(E_\mathrm{b} - \tfrac{1}{2}\tfrac{\lambda^2\omega^2\cos^2\omega t}{(1+\lambda\sin\omega t)^4}{r_1}^2\Big) + \varepsilon\Big(\tfrac{\lambda^2\omega^2\cos^2\omega t}{(1+\lambda\sin\omega t)^4} r_1\,\mathcal{A}_{n\,1} - \Phi_n\Big) \\
&\simeq \big(E_\mathrm{b} - \tfrac{1}{2}\lambda^2\omega^2\cos^2\omega t\,(1-4\lambda\sin\omega t)\,{r_1}^2\big) + \varepsilon\big(\lambda^2\omega^2\cos^2\omega t\,(1-4\lambda\sin\omega t)\,r_1\,\mathcal{A}_{n\,1} - \Phi_n\big)
\end{aligned}
$$

The equations of motion in the unscaled variables simplify in the 1-direction as $\Omega_{n\,11} \equiv 0$ due to antisymmetry of the pseudomagnetic two-form. We expand $(1+\lambda t)^{-n}$ to first order in λ to simplify the results. Since $\lambda \ll 1$, we expect these results to be reasonably accurate.

$$
\begin{aligned}
\dot{\kappa}_1 &= E_{\mathrm{sh}\,1} + B_{1j}\,\dot{r}_j = -\partial_{r_1}\Phi - \partial_t A_1 \\
&= \lambda\,\frac{\lambda\omega^2\cos^2\omega t}{(1+\lambda\sin\omega t)^4} r_1 - \lambda\,\frac{3\lambda\omega^2\cos^2\omega t}{(1+\lambda\sin\omega t)^4} r_1 + \frac{\lambda\omega^2\sin\omega t}{(1+\lambda\sin\omega t)^3} r_1 + \frac{\lambda\omega\cos\omega t}{(1+\lambda\sin\omega t)^3}\dot{r}_1 \\
&\simeq \lambda\omega(1-3\lambda\sin\omega t)\big(\omega\sin\omega t\, r_1 - \cos\omega t\,\dot{r}_1\big) \\
\dot{\kappa}_l &= 0 && l \neq 1 \\
\dot{r}_1 &= \partial_{\kappa_1}E_\mathrm{b} - \varepsilon\,\Theta_{n\,1} \\
\dot{r}_l &= \partial_{\kappa_l}E_\mathrm{b} - \varepsilon\left(\Theta_{n\,l} + \lambda\omega(1-3\lambda\sin\omega t)\,\Omega_{n\,l1}\left(\omega\sin\omega t\, r_1 - \cos\omega t\,\partial_{\kappa_1}E_\mathrm{b}\right)\right) && l \neq 1
\end{aligned}
$$

We scale back to physical space, $q_l := D_{lj}r_j$. Again, D only acts non-trivially on the first coordinate, we have $q_l = r_l$ for $l \neq 1$.

$$
\begin{aligned}
\dot{q}_1 &= D_{1j}\,\dot{r}_j + \dot{D}_{1j}\,r_j \\
&= (1+\lambda\sin\omega t)\,\partial_{\kappa_1}E_\mathrm{b} + \varepsilon\,(1+\lambda\sin\omega t)\,\Theta_{n\,1} + \lambda\omega\cos\omega t\, r_1
\end{aligned}
$$

The piezocurrent density is obtained by integrating over the first Brillouin zone of the undeformed lattice (as we did not scale back the momentum).

$$
\begin{aligned}
j_1 &= \int_{M_0^*}\mathrm{d}\kappa\,\dot{q}_1 \\
&= (1+\lambda\sin\omega t)\int_{M_0^*}\mathrm{d}\kappa\,\partial_{\kappa_1}E_\mathrm{b} + \int_{M_0^*}\mathrm{d}\kappa\,\lambda\omega\cos\omega t\, r_1 - \varepsilon\int_{M_0^*}\mathrm{d}\kappa\,(1+\lambda\sin\omega t)\,\Theta_{n\,1} \\
&= |M_0^*|\;\lambda\omega\cos\omega t\, r_1 - \varepsilon\,(1+\lambda\sin\omega t)\int_{M_0^*}\mathrm{d}\kappa\,\Theta_{n\,1} \\
&\approx |M_0^*|\;\lambda\omega\cos\omega t\, r_1 - \varepsilon\int_{M_0^*}\mathrm{d}\kappa\,\Theta_{n\,1}
\end{aligned}
$$

For $l \neq 1$ we obtain

$$\begin{aligned} j_l &= \int_{M_0^*} \mathrm{d}\kappa\, \dot{q}_l = \int_{M_0^*} \mathrm{d}\kappa\, \partial_{\kappa_l} E_\mathrm{b} - \varepsilon \int_{M_0^*} \mathrm{d}\kappa\, \big(\Theta_{n\,l} + \\ &\quad + \lambda\omega(1 - 3\lambda \sin\omega t)\, \Omega_{n\,l1}\, (\omega \sin\omega t\, r_1 - \cos\omega t\, \partial_{\kappa_1} E_\mathrm{b})\big) \\ &\approx -\varepsilon \int_{M_0^*} \mathrm{d}\kappa\, \big(\Theta_{n\,l} + \lambda\omega\, \Omega_{n\,l1}\, (\omega \sin\omega t\, r_1 - \cos\omega t\, \partial_{\kappa_1} E_\mathrm{b})\big) \end{aligned}$$

Compared to the linear case, the situation is qualitatively different. The King-Smith–Vanderbilt formula alone will not be able to describe the dynamics accurately in directions perpendicular to the deformation. Here we get a Kubo-like term $-\varepsilon\, \Omega_{n\,lj}\, \dot{\kappa}_j$ in addition to the King-Smith–Vanderbilt term which will contribute to the total polarization current (unless $\Omega_{n\,lj}$ vanishes of course) [TKNdN82].

5.3 Comment On Further Toy Models

We have given two simple toy models in which the shaping two-form B_{jm} vanishes identically. These two models correspond to two common applications of piezoelectric materials: the linear deformation corresponds to a pressure-sensitive sensor for instance, when a sample's pressure is measured. In this case, we found that we expect King-Smith and Vanderbilt's formula to hold.

The periodic deformation could model a microphone made of a piezoelectric material or a piezotransducer which transforms voltages. In this case our corrections are essential to predict the piezocurrent accurately. Furthermore we expect the piezocurrent in all directions to be quantized, although the explanation is beyond the scope of this thesis[1] [PST] [TKNdN82]. This might be essential for the detection of our corrections, because our correction, the Kubo term, cannot be small as it is quantized. In other words,

$$-\varepsilon \int_{M_0^*} \mathrm{d}\kappa\, \Omega_{n\,lj}\, \dot{\kappa}_j = c\, z \qquad\qquad c \in \mathbb{R},\ z \in \mathbb{Z} \tag{5.1}$$

where c is a constant independent of the integer z. $c\,z$ cannot decrease smoothly from a non-zero value to zero, but only in increments of z. If the constant $\lambda\omega$ is adjusted correctly, one should be able to see that the current changes in discrete values only.

---

[1] This has geometric reasons and can be readily understood in the language of fiber bundles, see [SW89] for details.

6 Research Directions And Further Perspectives

We would like to close this paper by giving a brief outlook as to what questions might be asked next. We will start with some theoretical questions and then propose an experimental test of our equations and the new corrections on fermionic ultra-cold gases.

6.1 Further Theoretical Research

Although it is *conceptually* fairly easy to model the direct piezoelectric effect using the squeezing matrices $D(t)$, which transform the initial periodicity lattice Γ_0 to the lattice at time t, $\Gamma(t)$, one cannot *a priori* anticipate the reaction of a crystal when it is subjected to a certain potential difference. In this sense, direct piezoelectricity is easier to understand as the shape of the unit cell is 'prescribed' in the model of chapter 4. The problem of determining the equilibrium structure of a solid which is subjected to an electric (or electromagnetic) field is beyond the scope of the technique presented here and presents a formidable challenge to theoretical solid-state physicists [MO97].

A second interesting application is to use piezoelectricity as a model to introduce noise into the framework of space-adiabatic perturbation theory. By noise we think of either impurities and defects of the lattice structure or the small oscillatory motion of the nuclei at a finite temperature. Since we are dealing with an essentially time-adiabatic problem, we expect this to be easier than a space-adiabatic problem in full generality. In a first step our results on direct piezoelectricity may be expanded to quasi-periodic potentials.

6.2 Ultra-cold Gases As Models For A Crystalline Solid

In an attempt to test the formulas developed in chapter 4, we would like to propose the following experiment on ultra-cold gases in periodic potentials. Before we detail the experimental setup, we will give a brief overview of the relevant scientific progress in the field of ultra-cold gases.

If a gas consisting of a certain isotope is cooled down to very low temperatures in the $1\,\mathrm{mK}$ range or lower, quantum effects will dominate the physical properties. In particular the behavior will be very different depending on whether the isotopes are fermions or bosons; at sufficiently low temperatures a bosonic gas may form a Bose-Einstein condensate. These gases are confined by a magneto-optical trap which acts as a container. Recently ultra-cold quantum gases have become an important tool to deepen the understanding of fundamental physical effects, such as quantum statics, as well as opening up entirely new possibilities in quantum information processing. The experimentator has unprecedented freedom to manipulate parameters such as particle density, and geometry and strength of the potential.

In order to subject the ultra-cold gas to a periodic potential, optical lattices are created by counter-propagating laser beams. Depending on the relative polarization, the frequency of the photons and the angles of the beams relative to each other, the gas can either be cooled, the so-called *molasses configuration*, or the gas can be trapped in a periodic potential without cooling it down any further [GR01]. For a lattice in d dimensions, at least $d + 1$ lasers are necessary, e. g. a 2d lattice requires at least 3 lasers.

The range of possible configurations includes standard cubic lattices, hexagonal lattices [DDL03] and kagomé lattices [SBC^{+}04a]. In particular ultra-cold gases can be subjected to a periodic potential whose unit cell lacks a center of inversion (see figure 6.1). The parameters, which determine the geometry of the lattice, can be *adjusted in real-time during the experiment*, allowing for changes in lattice geometry during the experiment [DFE^{+}05].

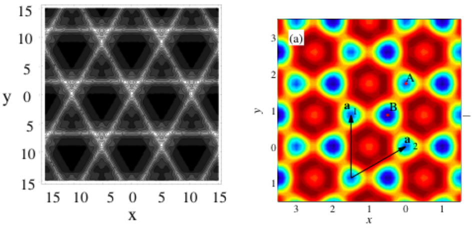

Figure 6.1: A kagomé lattice [SBC^{+}04a] and a hexagonal lattice [DDSN03] (the opposing sites are inequivalent) without center of inversion.

Experiments with fermionic and bosonic gases in optical lattices have been performed. If the applied electromagnetic field (and thus the depth of the potential well) reaches a critical value, a gas composed of bosons undergoes a phase transition from a superfluid phase to a *Mott insulator*, i. e. an insulator whose 'charge' carriers (the atoms) are localized at a specific lattice site [GME^{+}02]. In the *superfluid phase*, the condensate is described by a single collective wave function, the 'charge' carriers are delocalized, whereas in the Mott insulator phase the atoms are distributed evenly among the different lattice sites with no phase coherence between atoms located at different lattice sites.

Band insulators[1] cannot be formed with bosonic atoms as the weak transverse confinement (of the trap) inhibits the creation of a large band gap. However in recent

---

[1] A band insulator has no direct conductance, because all energy bands below the Fermi energy are filled and the charge carriers oscillate back and forth if an electric field is applied (Bloch oscillations). Bloch oscillating charge carriers have no net movement and so they do not contribute to macroscopic conductance. Mott insulators on the other hand show no conductance, as their charge carriers are localized so strongly within a unit cell that transitions to neighboring unit cells are suppressed [AM01].

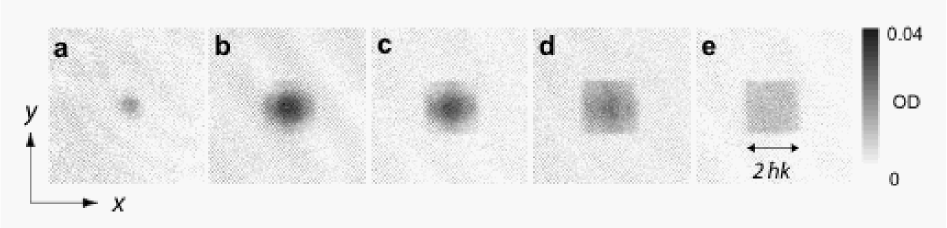

Figure 6.2: A Mott insulator (images a and b) will still have spherical distribution of momentum whereas in a band insulator (d and e) all momenta are populated equally [SBC+04b].

experiments with fermionic potassium isotopes the system undergoes a phase transition to a band insulator if the confinement energy reaches a critical value [SBC+04b]; alternatively fermionic gases may form a Mott insulator as well [PPS+04].

As the amount of ultra-cold gas used in experiments is usually small to be detected directly, one standard method to observe effects is *ballistic expansion*. The confining potential and the optical lattice are switched off and the gas is allowed to expand for a few milliseconds (see figure 6.3). In a way, the 'crystal momentum is mapped onto the momentum in real space', so the crystal momentum can actually be measured directly. After expansion, the optical absorption is measured, which, in turn, can be related to the particle density of the gas [GME+02] [SBC+04b]. If a discrete interference pattern is visible after the expansion, only a few discrete values of momenta are populated. The particles who populated a certain state then expand at that fixed momentum; particles with higher momenta will expand more rapidly and hence each maximum of the particle density in the interference pattern corresponds to a specific momentum.

Now we are in a position to propose an experiment to simulate the analog of piezoelectric effect in ultra-cold fermionic gases. In principle all the necessary tools are available. A fermionic[2] gas is cooled down to ultra-low temperatures and subjected to a periodic lattice without center of inversion. The strength of the potential is adjusted such that the gas is in a band insulator state. Slow adjustments in the relative phases and the wavelengths of the lasers then change the geometry of the lattice adiabatically.[3] The separation of timescales can thus be controlled by increasing or decreasing the rate of change of the parameters which determine the lattice geometry. In this way the range of validity of the adiabatic approximation may be tested. Finally, the piezocurrent may be observed by free expansion of the gas after the confining field of the trap as well as the optical lattice have been shut off. If there is a current that is induced by the deformation, it should be visible by comparing the momentum distribution to the 'square-shaped' momentum distribution (see figure 6.3) of a band insulator.

---

[2] Bosonic ultra-cold gases cannot form a band insulator.

[3] The typical time-scales for other significant processes such as rephasing and electron tunneling are well-known [GME+02] [SBC+04b].

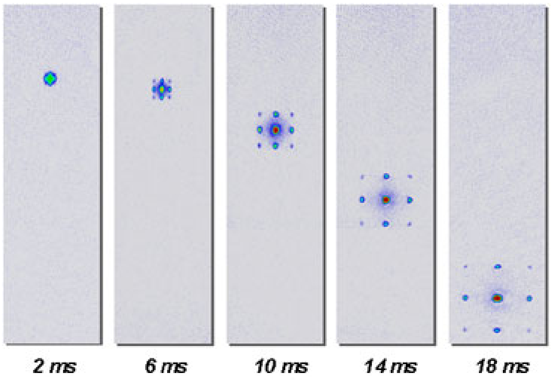

Figure 6.3: Ballistic expansion of a Bose-Einstein condensate previously subjected to a three-dimensional optical lattice; the interference pattern is a direct consequence of the quanization of the momentum distribution [uni05].

Any currents should be visible as changes in particle density of a given crystal momentum k.

If the lattice is periodically deformed, we would also expect to see corrections beyond the King-Smith–Vanderbilt formula as well as quantization of the current.

A Brief Introduction To Geometric Phases

As geometric phases are at the heart of first (and higher-order) corrections to the effective Hamiltonians derived in sections 3.2 and 4.3.3, we will give a brief digression on the significance of geometric phases in quantum systems. It is based on a recent book by Bohm et al. which is dedicated to that subject [BMK$^+$03]. We will not go into full detail here; in particular we omit a few, but important subjects such as topological phases and the geometric interpretation of geometric phases.

One of the most famous manifestations of geometric phases is the Aharonov-Bohm effect [AB59] which was predicted as early as 1959. But it was only in 1983 and 1984 when Berry [Ber84] and Simon [Sim83] rediscovered the topic and gave a coherent explanation for seemingly disparate effects in different fields such as optics and molecular dynamics.

Assume a particle in a strong magnetic field which we slowly rotate. Then we have a Hamiltonian which depends on three parameters (one for each spatial direction) and is given by

$$H(\mathbf{B}) = H_0 + c\mathbf{B} \cdot \mathbf{J} =: H_0 + h(\mathbf{B}) \tag{A.1}$$

where c is a constant and $\mathbf{J}$ the angular momentum operator; H_0 gives the 'trivial' dynamics which does not depend on $\mathbf{B}$. If we keep the strength of the magnetic field constant and just consider changes in direction, the parameter space is given by the unit sphere in three dimensions (as only the direction of the magnetic field matters).

If we neglect the dynamics generated by H_0 for the moment, we can obtain a set of eigenfunctions of the Schrödinger equation depending on the parameter $\mathbf{B}$.

$$i\frac{\mathrm{d}}{\mathrm{d}t}\psi_{\mathbf{B}}(t) = h(\mathbf{B})\,\psi_{\mathbf{B}}(t) \tag{A.2}$$

In braket notation we obtain a complete set of solutions for each parameter $\mathbf{B}$ separately.

$$h(\mathbf{B})\,|n,\mathbf{B}\rangle = E_n(\mathbf{B})\,|n,\mathbf{B}\rangle \qquad\qquad \langle n,\mathbf{B}|m,\mathbf{B}\rangle = \delta_{nm} \tag{A.3}$$

Now lets assume we slowly rotate $\mathbf{B}$ along a closed circular path – slow enough so that the system remains in an eigenstate at all times, i. e. we assume an adiabatic change of $\mathbf{B}$. In other words, after one period T we have $\mathbf{B}(0) = \mathbf{B}(T)$. Berry's insight was that although the system is in an eigenstate of $h(T) \equiv h(0)$ again, we *cannot* conclude $|n,\mathbf{B}(T)\rangle = |n,\mathbf{B}(0)\rangle$, but that they equal only up to a phase.

$$|n,\mathbf{B}(T)\rangle = e^{i\varphi(\mathbf{B})}\,|n,\mathbf{B}(0)\rangle \tag{A.4}$$

Physically speaking, we cannot measure phases, only *differences in phases*, and $|n,\mathbf{B}\rangle$ and $c\,|n,\mathbf{B}\rangle$, $c\in\mathbb{C}$, $|c|=1$, are actually one and the same physical state. It is important to note that $\varphi(\mathbf{B})$ depends on the *path in parameter space*, so we cannot expect it to depend only on initial and final datum. This is the very reason for the occurrence of nontrivial geometric phases.

Assume the system is initially in the state $|n,\mathbf{B}(0)\rangle$, then by adiabaticity assumption, the system is in the state $c(t)\,|n,\mathbf{B}(t)\rangle$ at time t, $c(0)=1$. Thus $c(t)\,|n,\mathbf{B}(t)\rangle$ satisfies the following Schrödinger equation

$$\begin{aligned} i\frac{\mathrm{d}}{\mathrm{d}t}\big(c(t)\,|n,\mathbf{B}(t)\rangle\big) &= i\partial_t c(t)\;|n,\mathbf{B}(t)\rangle + c(t)\,i\partial_t\,|n,\mathbf{B}(t)\rangle \\ &= i\partial_t c(t)\;|n,\mathbf{B}(t)\rangle + c(t)\,h(\mathbf{B}(t))\,|n,\mathbf{B}(t)\rangle \end{aligned} \tag{A.5}$$

Sandwiching both sides with $\langle n,\mathbf{B}(t)|$ and regrouping the terms, we get a differential equation for $c(t)$.

$$i\frac{\mathrm{d}}{\mathrm{d}t}c(t) = c(t)\big(E_n(\mathbf{B}(t)) + i\,\big\langle n,\mathbf{B}(t)\big|\tfrac{\mathrm{d}}{\mathrm{d}t}\big|n,\mathbf{B}(t)\big\rangle\big) \tag{A.6}$$

The first phase factor is called *dynamical phase factor*, the second one is the *geometric phase*. The solution of this equation is given by

$$c(t) = e^{-i\int_0^t \mathrm{d}\tau E(\mathbf{B}(\tau))}\,e^{i\gamma_n(t)} \tag{A.7}$$

with

$$\begin{aligned} \gamma_n(t) &= \int_0^t \mathrm{d}\tau\;\big\langle n,\mathbf{B}(\tau)\big|\tfrac{\mathrm{d}}{\mathrm{d}\tau}\big|n,\mathbf{B}(\tau)\big\rangle = \int_{\mathbf{B}(0)}^{\mathbf{B}(t)} \mathrm{d}\mathbf{B}\;\langle n,\mathbf{B}|i\nabla|n,\mathbf{B}\rangle \\ &=: \int_{\mathbf{B}(0)}^{\mathbf{B}(t)} \mathrm{d}\mathbf{B}\,\mathcal{A}_n(\mathbf{B}) \end{aligned} \tag{A.8}$$

$\mathcal{A}_n$ is the Berry connection of the nth band. All the integrals above are *path integrals*.

If $\mathcal{A}_n$ *were* integrable, then the integral would only depend on initial and final point in phase space. So if we consider a closed path, the geometric phase would vanish. However, in general $\mathcal{A}_n$ is *not integrable*, so the Berry phase can assume 'any' value.

To illustrate this point more explicitly, let us change the gauge to $|n,\mathbf{B}(t)\rangle' := e^{i\varphi_n(\mathbf{B}(t))}\,|n,\mathbf{B}(t)\rangle$ where $\varphi_n(\mathbf{B}(t))$ is an arbitrary function which is periodic in t (modulo 2π), in other words, $\varphi_n(\mathbf{B}(T)) = \varphi_n(\mathbf{B}(0)) + n\,2\pi$, $n\ \in\mathbb{N}_0$. Now we calculate $\gamma_n'(t)$ and find

$$\gamma_n'(t) = \int_{\mathbf{B}(0)}^{\mathbf{B}(t)} \mathrm{d}\mathbf{B}\,\mathcal{A}_n'(\mathbf{B}) = \gamma_n(t) - \big(\varphi_n(\mathbf{B}(t)) - \varphi_n(\mathbf{B}(0))\big) \tag{A.9}$$

since $\mathcal{A}_n' = \mathcal{A}_n - \nabla\varphi_n$. Thus for $t=T$, we get $\gamma_n'(T) = \gamma_n(t) - n\,2\pi$, $n\in\mathbb{N}_0$. This implies that the value of the geometric phase *essentially* does not change even if we choose another gauge. It also means if the Berry connection is exact, e. g. $\nabla\wedge A = 0$

in three dimensions, there are no geometric phase effects; we then call $\mathcal{A}_n$ trivial. On the other hand, we cannot *a priori* assume the triviality of $\mathcal{A}_n$.

The similarity to electromagnetism is no coincidence as both theories have the same symmetry group, $U(1)$, and thus have to abide by the same laws. The gauge transformations are the same, too. This motivates the introduction of a field tensor

$$\Omega_{n\,jl} := \partial_{k_j}\mathcal{A}_k - \partial_{k_l}\mathcal{A}_j \tag{A.10}$$

which is a *gauge invariant* quantity as can be shown by direct computation (and using that partial derivatives commute).

Assume we want to integrate the Berry connection $\mathcal{A}_n$ over a closed curve C; then we can use Stoke's theorem to convert it to an integral over any surfaces enclosed by the path.

$$\gamma_n(C) = \oint_C \mathcal{A}_n(\mathbf{B}) = \int_S \Omega(\mathbf{B}) \tag{A.11}$$

In general, i. e. when Stoke's theorem cannot be directly applied, the statement is still true, but only modulo 2π. Since the right-hand side is essentially gauge-invariant, the phase has to be gauge-invariant as well.

Until now physicists might have the impression that geometric phases do not have consequences for the zeroth-order dynamics, but this is not the case. Assume a neutral molecule in the Born-Oppenheimer approximation [Teu03, p. 61 f.]. If we apply a strong constant magnetic field, we would expect no separation of charge.

$$H_{\mathrm{BO}}(P,Q) = \sum_{n=1}^{N} \frac{1}{2m_{\mathrm{nuc}}} P^2 + H_{\mathrm{e}}(Q) \tag{A.12}$$

After all, the whole molecule is neutral, so the quantity which gives the 'reaction' to the magnetic field is the magnetic (dipole) moment of the molecule.

However if we neglect geometric phase effects in the semiclassical equations of motion and naively introduce the magnetic field through minimal substitution, electrons and nuclei *seem* to move on circular orbits (in opposite directions) and the charges would separate. This unphysical prediction is remedied when we correctly include geometric phase effects which *exactly cancel* the magnetic vector potential, $\mathcal{A}_n = A$. To put another way, the Berry connection describes the screening of the bare charges by the electrons.

There are two origins of the geometric phases: conditions we impose on a system (as discussed before) and – as in the Born-Oppenheimer case – the mere 'separation' of degrees of freedom. Often such a separation is intuitively and physically very clear: for a Born-Oppenheimer-type problem a distinction between electrons and ionic cores is the physically reasonable choice. However it is an inseparable system, we cannot treat ionic cores and electrons separately, and then superpose the results, but we have to include geometric phases to relate the two systems properly.

To make the connection to the present case of operator-valued symbols, consider the Bloch electron in the slowly varying electromagnetic field (see section 3.2 for details).

The Hamiltonian symbol H depended on two variables k and r. If we consider (k, r) as parameters and assume we have solved the (semi)classical equations of motion for k and r, we get functions $k(t)$ and $r(t)$ in phase space of the slow variables.

When we plug in these solutions into the Hamiltonian, we get a *time*-dependent Hamiltonian.

$$H(t) := H(k(t), r(t))$$

From this point of view, it is clear why we come to expect geometric phase effects: symbols can be considered as parameter-depenent Hamiltonians on the fast degrees of freedom and geometric phases are a consequence of 'imposing' certain conditions on the system.

These examples should serve as a reminder that geometric phase effects may be the key to understanding even simple physical effects.

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