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Master Thesis

Berry phase effects in the Boltzmann equation of electronic systems

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"In order to understand the world, one has to turn away from it on occasion"

Albert Camus

Abstract

The main purpose of this thesis is to study transport properties of systems involving a Berry phase using the Boltzmann equation. The Boltzmann equation is derived from the Keldysh formalism and is expressed in terms of Green's functions and self-energies. The classical Boltzmann equation can then be reobtained by performing a Wigner transformation and taking particles on-shell. This is first done for single-band systems with the added effects of a magnetic field and disorder. Afterwards, we derive the Boltzmann equation for multi-band systems, where the anomalous velocity appears due to the Berry phase. We explain that this causes the anomalous Hall effect with quantized conductivity given by Chern numbers. Then, we apply this on graphene and find that we can get a non-zero Hall conductivity for systems with broken time-reversal symmetry, as is the Haldane model. Finally, we attempt to combine the Berry phase with other effects, like disorder, a magnetic field and a spin texture, and find that it is not a trivial task, but requires further research.

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Chapter 1

Introduction

Since its introduction, the Berry phase [1] has found many applications in physics. Specifically in condensed matter physics, it has been able to describe various types of electronic transport, now collectively known as anomalous transport. The Berry phase is a geometric property, so it can describe these phenomena using concepts of topology. An important example of anomalous transport is that of the anomalous velocity, a correction to the usual group velocity of quasi-particles, that arises as a response to a weak electric field, and that is perpendicular to it. This explains the anomalous Hall effect, a Hall effect without an external magnetic field. A relatively simple model exhibiting this effect is Haldane's model for graphene [2], which breaks time-reversal symmetry. The Berry phase has also been able to explain the quantization of conductivity in the quantum Hall effect, with the use of Chern numbers [3]. Berry phase effects on transport can be studied phenomenologically using semi-classical equations of motion [4].

Alternatively, one can study Berry phase effects using the Boltzmann equation, which is the method we will use in this thesis. The Boltzmann equation describes the evolution of a system out of equilibrium, which makes it ideal for studying an electronic system under the effect of an electric field. The Boltzmann equation can be derived by Liouville's theorem in the context of statistical mechanics. However, it can also be derived form the Keldysh formalism, a formalism of quantum field theory out of equilibrium. We consider this approach more rigorous and fundamental. It results in a generalized form of the Boltzmann equation, ofter refered to as the quantum Boltzmann equation (QBE), from which the semi-classical one can be derived by performing a gradient expansion.

Within this approach, single-band systems that do not show a Berry phase can be studied. A magnetic field can be added to the system by performing minimal coupling in momentum space. A disordered system where electrons scatter with impurities can be studied by including the effect of the scattering in the collision integral of the Boltzmann equation. One of the powers of the Keldysh technique is that the collision integral is expressed with respect to self-energies, which can be known up to some order in perturbation theory. In the case of multi-band systems, effects due to the Berry phase appear in the Boltzmann equation. They are included by first applying a unitary transformation and then performing minimal coupling in real space. The final result should be in agreement with the phenomenological treatment. The Keldysh

technique allows us to also study combinations of all the aforementioned effects in a systematic way, in order to see if there is any interplay between them, as well as Berry phases in both real and momentum space. However, these phenomena are not yet well understood.

This thesis is structured as follows. In this chapter, we provide an introduction to ideas crucial to the rest of the thesis, that is the Boltzmann equation, the Wigner transformation, the Berry phase and disorder. An advanced reader can choose which parts on this chapter to read, or skip it completely. In chapter 2, we describe the basics of the Keldysh formalism for a non-equilibrium field theory with the purpose of deriving the Boltzmann equation. In chapter 3, we derive the Boltzmann equation for single-band systems, that do not exhibit any Berry phase effects, and include a magnetic field and disorder. In chapter 4, we include the Berry phase into the Boltzmann equation in the case of multi-band systems, and find that, upon applying a weak electric field, the Berry phase gives rise to the anomalous Hall effect, while in chapter 5 we do an application of this in graphene. In chapter 6, we introduce some problems that still remain open, that all attempt to combine the Berry phase with other effects. Finally, we provide our conclusions.

1.1   The Boltzmann equation in statistical physics

Studying a many-body system within the regime of classical mechanics is usually done using the tools of statistical physics. One of the fundamental notions of statistical physics is that of the *distribution function* whose time evolution is governed by the so called *Boltzmann equation*. In this section we will show a derivation of the Boltzmann equation using classical arguments before attempting a field theoretical approach in Chapter 2. Similar discussions can be found in Kittel [5] and in lectures notes by Tong [6]. Then, a simple extension of this approach can be done to include quantum effects and derive the *quantum Boltzmann equation*, a discussion of which can be found in Mahan [7].

Let us assume a system of many particles labeled by an index $i = 1, 2, \ldots, N$. The distribution function $f(t, \mathbf{r}_i, \mathbf{p}_i)$, where $\mathbf{r}_i$ and $\mathbf{p}_i$ are the position and momentum of each particle respectively, is defined on the $6N$-dimensional phase space and can be interpreted as the probability that the system can be found around the point $(\mathbf{r}_i, \mathbf{p}_i)$ of the phase space at time t. It is normalized in the phase space so that

$$\int \prod_{i=1}^{N} \mathrm{d}\mathbf{r}_i \mathrm{d}\mathbf{p}_i \, f(t, \mathbf{r}_i, \mathbf{p}_i) = 1. \tag{1.1}$$

Since probability should be conserved, the distribution function should obey a continuity equation over phase space

$$\frac{\partial f}{\partial t} + \sum_{i=1}^{N} \left(\dot{\mathbf{r}}_i \frac{\partial f}{\partial \mathbf{r}_i} + \dot{\mathbf{p}}_i \frac{\partial f}{\partial \mathbf{p}_i} \right) = 0. \tag{1.2}$$

Using Hamilton's equations

$$\dot{\mathbf{r}} = \frac{\partial H}{\partial \mathbf{p}} \qquad \dot{\mathbf{p}} = -\frac{\partial H}{\partial \mathbf{r}}, \tag{1.3}$$

where H is the total Hamiltonian of the system, the continuity equation can be rewritten as

$$\frac{\partial f}{\partial t} + \sum_{i=1}^{N} \left(\frac{\partial H}{\partial \mathbf{p}_i} \frac{\partial f}{\partial \mathbf{r}_i} - \frac{\partial H}{\partial \mathbf{r}_i} \frac{\partial f}{\partial \mathbf{p}_i} \right) = 0, \tag{1.4}$$

or more compactly as

$$\frac{\partial H}{\partial t} = \{H, f\}, \tag{1.5}$$

where $\{,\}$ denotes the Poisson bracket. This is the *Liouville equation*. It is a manifestation of the *Liouville theorem* stating that the distribution function remains constant along trajectories in phase space, or in other words behaves as an incompressible fluid.

We have derived an equation that describes the evolution of the distribution function. However, we need to know the position and momentum of N particles. To avoid that, we can integrate out most coordinates and define the *single-particle distribution function*

$$f_1(t, \mathbf{r}, \mathbf{p}) = N \int \prod_{i=2}^{N} \mathrm{d}\mathbf{r}_i \mathrm{d}\mathbf{p}_i \, f(t, \mathbf{r}, \mathbf{r}_2, \ldots, \mathbf{r}_N, \mathbf{p}, \mathbf{p}_2, \ldots, \mathbf{p}_N). \tag{1.6}$$

This is normalized to the number of particles

$$\int \mathrm{d}\mathbf{r}\mathrm{d}\mathbf{p} \, f_1(t, \mathbf{r}, \mathbf{p}) = N. \tag{1.7}$$

In general, a Hamiltonian of a system of N particles can be written as

$$H = \sum_{i=1}^{N} H_i^0 + \sum_{i \neq j} U(\mathbf{r}_i, \mathbf{r}_j) \tag{1.8}$$

where H_i^0 is the single-particle Hamiltonian, i.e. the non-interacting Hamiltonian of the i-th particle and $U(\mathbf{r}_i, \mathbf{r}_j)$ describes collisions between particles i and j. Then we can rewrite eq.(1.4) in terms of the single-particle distribution function and the single-particle Hamiltonian, where we drop all indices

$$\frac{\partial f}{\partial t} + \frac{\partial H}{\partial \mathbf{p}} \frac{\partial f}{\partial \mathbf{r}} - \frac{\partial H}{\partial \mathbf{r}} \frac{\partial f}{\partial \mathbf{p}} = \left(\frac{\partial f}{\partial t} \right)_{coll}. \tag{1.9}$$

This is the *Boltzmann equation* or *Boltzmann transport equation*. Obviously, the single-particle Hamiltonian does not include collisions between particles and, as a result, collisions have to be included as an extra term. It usually appears in the right hand side of the Boltzmann equation and it is known as the *collision integral*, often denoted as I_{coll}, while the left hand side is often referred to as the *kinetic term* of the Boltzmann equation. The first way to calculate the collision integral is the so called BBGKY hierarchy which iteratively uses the distribution function containing one more particle. Then, Boltzmann made a big simplification on this assuming that the collision term is dominated by two-particle collision whose momenta are uncorrelated before the

collision. This assumption is known as molecular chaos. Using Hamilton's equations (1.3) again, we get a more insightful from of the Boltzmann equation

$$\frac{\partial f}{\partial t} + \mathbf{v} \cdot \nabla_{\mathbf{r}} f + \mathbf{F} \cdot \nabla_{\mathbf{p}} f = \left(\frac{\partial f}{\partial t} \right)_{coll}, \tag{1.10}$$

where $\mathbf{v}$ is the velocity and $\mathbf{F}$ is an external force applied to the system.

If quantum effects are important, then particles behave also as waves. This means that the distribution function should have an extra dependence on the energy E, or frequency ω, and the classical momentum $\mathbf{p}$ should be replaced by the wave-vector $\mathbf{k}$, so that $f = f(t, \mathbf{r}, E, \mathbf{k})$. f is often called the *Wigner distribution function*, for reasons that will become apparent in Chapter 2. The classical distribution function can then be obtained again by integrating out the extra energy argument

$$f(t, \mathbf{r}, \mathbf{k}) = \int_{-\infty}^{+\infty} \frac{\mathrm{d}E}{2\pi} f(t, \mathbf{r}, E, \mathbf{k}). \tag{1.11}$$

Also, macroscopic observables will use the distribution function as weight in their definitions, for example the particle density

$$n(t, \mathbf{r}) = \int \frac{\mathrm{d}E}{2\pi} \int \frac{\mathrm{d}^d k}{(2\pi)^d} f(t, \mathbf{r}, E, \mathbf{k}) \tag{1.12}$$

and current density

$$\mathbf{j}(t, \mathbf{r}) = \int \frac{\mathrm{d}E}{2\pi} \int \frac{\mathrm{d}^d k}{(2\pi)^d} \mathbf{v}(\mathbf{k}) f(t, \mathbf{r}, E, \mathbf{k}), \tag{1.13}$$

where d is the dimensionality of the system.

Due to the extra coordinate, a term like $\dot{E} \partial f / \partial E$ will be generated in the Liouville equation. This leads to

$$\frac{\partial f}{\partial t} + \mathbf{v} \cdot \nabla_{\mathbf{r}} f + \mathbf{v} \cdot \mathbf{F} \frac{\partial f}{\partial E} + \mathbf{F} \cdot \nabla_{\mathbf{k}} f = \left(\frac{\partial f}{\partial t} \right)_{coll}, \tag{1.14}$$

which is known as the *quantum Boltzmann equation* and $\mathbf{v} \cdot \mathbf{F}$ is the Joule heating due to the force $\mathbf{F}$. It was introduced by Mahan and Hänsch [**?**].

In the rest of the thesis, the Boltzmann equation will be derived using non-equilibrium field theory. That way, generalized versions of the velocity ad force terms will be found for various systems. Also, the collision integral will be formulated using self-energies arising from the Dyson equation.

1.2   Wigner transformation

In this section we will introduce a tool that will prove useful throughout the thesis, the Wigner transformation. It is a transformation for two-point $A(x_1, x_2)$ where x_1 and x_2 are space-time variables $x = (t, \mathbf{r})$.

As a first step, a transformation can be made from the two coordinates x_1 and x_2 to the center of mass coordinate and the relative coordinate, namely

$$x = \frac{1}{2}(x_1 + x_2) \qquad x' = x_1 - x_2, \qquad (1.15)$$

meaning that

$$x_1 = x + \frac{x'}{2} \qquad x_2 = x - \frac{x'}{2}. \qquad (1.16)$$

Then, a Fourier transform can be performed in the relative coordinate which results in

$$A(x, p) = \int dx' \, e^{-ipx'} A\left(x + \frac{x'}{2}, x - \frac{x'}{2}\right). \qquad (1.17)$$

This is called the Wigner transformation of $A(x_1, x_2)$ and provides a representation of it with respect to the center of mass coordinate and the relative momentum $p = (E, \mathbf{k})$. The inverse transformation is given by

$$A(x_1, x_2) = \sum_p e^{ip(x_1 - x_2)} A\left(\frac{x_1 + x_2}{2}, p\right). \qquad (1.18)$$

The main advantage of the Wigner transformation is to simplify products between two-point functions that contain integration over the intermediate variable, i.e.

$$C(x_1, x_2) = \int dx_3 \, A(x_1, x_3) B(x_3, x_2). \qquad (1.19)$$

This type of product will appear in the Boltzmann equation, when derived from the Keldysh formalism. The Wigner transform of $C(x_1, x_2)$ is given by

$$C(x, p) = A(x, p) e^{\frac{i}{2}\left(\overleftarrow{\partial}_x \overrightarrow{\partial}_p - \overleftarrow{\partial}_p \overrightarrow{\partial}_x\right)} B(x, p) \qquad (1.20)$$

where $\partial_x \partial_p = -\partial_t \partial_E + \nabla_\mathbf{r} \cdot \nabla_\mathbf{k}$. This is the Moyal product, written as $C = A \star B$, and is a product of two functions in phase space. A derivation of this can be found in Appendix A.

The exponential can be expanded, which to first order leads to the following identities

$$A \star B \approx AB + \frac{i}{2}\left(\partial_x A \, \partial_p B - \partial_p A \, \partial_x B\right) \qquad (1.21)$$

$$[A, B]^\star \approx [A, B] + \frac{i}{2}\{\partial_x A, \partial_p B\} - \frac{i}{2}\{\partial_p A, \partial_x B\} \qquad (1.22)$$

$$\{A, B\}^\star \approx \{A, B\} + \frac{i}{2}[\partial_x A, \partial_p B] - \frac{i}{2}[\partial_p A, \partial_x B] \qquad (1.23)$$

where $[\,,\,]$ denotes the commutator and $\{\,,\,\}$ the anti-commutator. These identities are known as the gradient expansion. The gradient expansion is accurate for functions that change slowly in the central coordinate x, and fast in the relative coordinate x'. In the context of Boltzmann equation, one of the functions will be a Green's function, and the gradient expansion becomes an expansion over $\hbar$. Then it is equivalent to a

semi-classical approximation. In the special case that the functions A and B (anti-)commute eq. (1.22) reduces to

$$[A, B]^\star \approx i(\partial_x A \, \partial_p B - \partial_p A \, \partial_x B), \tag{1.24}$$

or, in other words, the commutator reduces to a Poisson bracket. This is evidence that the gradient expansion is in fact a semi-classical expansion.

1.3 Berry phase

A concept that is of of primary interest in this thesis is that of the Berry phase, that was introduced by Michael Berry [1]. It is a phase picked up by a wave function after cyclic adiabatic evolution of its parameters. Its importance lies on the fact that it is a geometric object, which makes it suitable for topological descriptions of various phenomena. Also, it exhibits many similarities to a $U(1)$ gauge field theory, which allows for use of the known formulation of quantum electrodynamics. In this section we will provide an basic introduction to the Berry phase and quantities related to it. Other discussions can be found in the lecture notes by Tong [8], in books by Wen [9] and Bernevig and Hughes [10], and in the review by Xiao, Chang and Niu [4].

1.3.1 The Berry phase and adiabatic evolution

Let us look at a Hamiltonian that depends on a set of parameters $\mathbf{R} = (R_1, R_2, \dots)$ that evolve in time, namely

$$H = H(\mathbf{R}), \qquad \mathbf{R} = \mathbf{R}(t). \tag{1.25}$$

A quantum state can always be expressed as a superposition of instantaneous eigenstates

$$|\psi(\mathbf{R}(t))\rangle = \sum_n a_n(t)|n(\mathbf{R}(t))\rangle \tag{1.26}$$

where

$$H(\mathbf{R})|n(\mathbf{R})\rangle = E_n(\mathbf{R})|n(\mathbf{R})\rangle. \tag{1.27}$$

$|\psi(t)\rangle$ obeys the time-dependent Schrödinger equation, i.e.

$$i\hbar \frac{\partial}{\partial t}|\psi(t)\rangle = H(\mathbf{R}(t))|\psi(t)\rangle, \tag{1.28}$$

$$i\hbar \sum_n \left(\dot{a}_n |n(\mathbf{R}(t))\rangle + a_n \frac{\partial}{\partial t}|n(\mathbf{R}(t))\rangle \right) = \sum_n a_n E_n(t)|n(\mathbf{R}(t))\rangle. \tag{1.29}$$

Taking the overlap with another eigenstate

$$\langle m(\mathbf{R}(t))| \sum_n \left(i\hbar \dot{a}_n |n(\mathbf{R}(t))\rangle + i\hbar a_n \frac{\partial}{\partial t}|n(\mathbf{R}(t))\rangle - a_n E_n(t)|n(\mathbf{R}(t))\rangle \right) = 0. \tag{1.30}$$

According to the adiabatic theorem of quantum mechanics, for a Hamiltonian with a gapped spectrum, the system remains in its instantaneous eigenstate under a slow enough evolution of its parameters. This implies that

$$\langle m(\mathbf{R}(t))|\frac{\partial}{\partial t}|n(\mathbf{R}(t))\rangle = \langle m(\mathbf{R}(t))|\frac{\partial}{\partial t}|n(\mathbf{R}(t))\rangle \delta_{nm} \tag{1.31}$$

which leads to

$$\sum_n \left(i\hbar \dot{a}_n \delta_{nm} + i\hbar a_n \langle m(\mathbf{R}(t))|\frac{\partial}{\partial t}|n(\mathbf{R}(t))\rangle \delta_{nm} - a_n E_n(t)\delta_{nm} \right) = 0, \tag{1.32}$$

$$\dot{a}_n + a_n \langle n(\mathbf{R}(t))|\frac{\partial}{\partial t}|n(\mathbf{R}(t))\rangle + \frac{i}{\hbar} E_n(t) = 0. \tag{1.33}$$

This differential equation is solved by

$$a_n(t) = a_n(0) e^{-\frac{i}{\hbar}\int_0^t dt' E_n(t')} e^{-\int_0^t dt' \langle n(\mathbf{R}(t))|\frac{\partial}{\partial t'}|n(\mathbf{R}(t))\rangle}. \tag{1.34}$$

Then it follows that after some time T, the quantum state obtains two types of phases

$$|\psi(T)\rangle = e^{-\frac{i}{\hbar}\int_0^T dt E_n(t)} e^{i\gamma_n} |\psi(0)\rangle. \tag{1.35}$$

The first one is known as the dynamical phase that is present in every time evolution, even if the parameters don't change and then it simply reduces to $e^{-iE_nT/\hbar}$. The second one is a new type of phase, that exists only when the parameters are time-dependent and is given by

$$\gamma_n(T) = i\int_0^T dt \, \langle n(\mathbf{R}(t))|\partial_t|n(\mathbf{R}(t))\rangle. \tag{1.36}$$

In general, the wave function is determined up to an arbitrary phase that we can change at will. However, if we evolve the parameters in a way that they return to their initial values, i.e. $\mathbf{R}(T) = \mathbf{R}(0)$, the phase $e^{i\gamma}$ remains unaffected by this change. The reasons for that will become apparent in the next section. The first to notice that was Michael Berry [1] and that's why under cyclic evolution the phase $e^{i\gamma}$ is called the *Berry phase*. Another interesting property is that it does not depend on the rate at which the parameters change, provided that it is slow enough that the adiabatic theorem holds, but only on the path followed. For this reason, it is also called the *geometric phase* and can be rewritten ignoring the time arguments

$$\gamma_n = i\oint d\mathbf{R}\langle n(\mathbf{R})|\nabla_\mathbf{R}|n(\mathbf{R})\rangle. \tag{1.37}$$

1.3.2 The Berry connection and the Berry curvature

It is useful to define the object

$$A_\mathbf{R} = i\langle n(\mathbf{R})|\nabla_\mathbf{R}|n(\mathbf{R})\rangle \tag{1.38}$$

and express the Berry phase as

$$\gamma_n = \oint d\mathbf{R} \cdot A_\mathbf{R}. \tag{1.39}$$

$A_{\mathbf{R}}$ is called the *Berry connection*. It describes the adiabatic evolution that we described in the previous section, in the same way that a connection describes parallel transport on a manifold. For this reason, it is defined on each energy level.

The Berry connection can also be defined via a unitary matrix, which will prove useful in chapter 4. We can define a matrix that contains the eigenstates as columns

$$U(\mathbf{R}) = \begin{pmatrix} |n_1(\mathbf{R})\rangle & |n_2(\mathbf{R})\rangle & \dots & |n_k(\mathbf{R})\rangle \end{pmatrix} \tag{1.40}$$

and its Hermitian conjugate

$$U^{\dagger}(\mathbf{R}) = \begin{pmatrix} \langle n_1(\mathbf{R})| \\ \langle n_2(\mathbf{R})| \\ \vdots \\ \langle n_k(\mathbf{R})| \end{pmatrix}. \tag{1.41}$$

Since the eigenstates are normalized, $U(\mathbf{R})$ is unitary, i.e. $U^{\dagger}(\mathbf{R})U(\mathbf{R}) = 1$. Then, from linear algebra we know that $U(\mathbf{R})$ is the matrix that diagonalizes the Hamiltonian as

$$U^{\dagger}(\mathbf{R})H(\mathbf{R})U(\mathbf{R}) = \begin{pmatrix} E_{n_1} & & & \\ & E_{n_2} & & \\ & & \ddots & \\ & & & E_{n_k} \end{pmatrix}. \tag{1.42}$$

Then, the Berry connection can be defined as

$$A_{\mathbf{R}} = iU^{\dagger}(\mathbf{R})\nabla_{\mathbf{R}}U(\mathbf{R}). \tag{1.43}$$

Let us now look at some properties of the Berry connection. First of all it is Hermitian. This comes from the fact that the eigenstates are normalized

$$\langle n(\mathbf{R})|n(\mathbf{R})\rangle = 1. \tag{1.44}$$

Taking the derivative, we get the following relation

$$\begin{aligned} \nabla_{\mathbf{R}}\langle n(\mathbf{R})|n(\mathbf{R})\rangle &= 0 \\ \langle \nabla_{\mathbf{R}}n(\mathbf{R})|n(\mathbf{R})\rangle + \langle n(\mathbf{R})|\nabla_{\mathbf{R}}|n(\mathbf{R})\rangle &= 0 \\ \langle n(\mathbf{R})|\nabla_{\mathbf{R}}|n(\mathbf{R})\rangle^{\dagger} + \langle n(\mathbf{R})|\nabla_{\mathbf{R}}|n(\mathbf{R})\rangle &= 0. \end{aligned} \tag{1.45}$$

Then we can use this to show that

$$A_{\mathbf{R}}^{\dagger} = -i\langle n(\mathbf{R})|\nabla_{\mathbf{R}}|n(\mathbf{R})\rangle^{\dagger} = i\langle n(\mathbf{R})|\nabla_{\mathbf{R}}|n(\mathbf{R})\rangle = A_{\mathbf{R}}. \tag{1.46}$$

The Berry connection is also gauge dependent. To make obvious we can apply a gauge transformation to the eigenstates, meaning multiply with a phase that depends on the parameters $\mathbf{R}$

$$|n(\mathbf{R})\rangle \to e^{i\phi(\mathbf{R})}|n(\mathbf{R})\rangle. \tag{1.47}$$

Then it follows from its definition that the Berry connection transforms as

$$A_{\mathbf{R}} \to A_{\mathbf{R}} - \nabla_{\mathbf{R}}\phi. \tag{1.48}$$

This implies that the Berry connection can be defined only up to the gradient of a scalar quantity. This property is reminiscent of the vector potential of electrodynamics or the the gauge field of QED. This encourages as to treat the Berry connection as a gauge field and define an object similar the electromagnetic field strength tensor, the *Berry curvature*

$$\Omega_{\mu\nu} = \frac{\partial A_\nu(\mathbf{R})}{\partial R^\mu} - \frac{\partial A_\mu(\mathbf{R})}{\partial R^\nu}. \tag{1.49}$$

It is straightforward to see that the Berry curvature remains invariant under the gauge transformation (1.47). Thus, it contains information about observables, while that Berry connection does not.

For one energy level labeled by the index n, the Berry curvature can be rewritten as follows

$$\Omega_{\mu\nu}^n = i \left\langle \frac{\partial n(\mathbf{R})}{\partial R^\mu} \middle| \frac{\partial n(\mathbf{R})}{\partial R^\nu} \right\rangle - i \left\langle \frac{\partial n(\mathbf{R})}{\partial R^\nu} \middle| \frac{\partial n(\mathbf{R})}{\partial R^\mu} \right\rangle, \tag{1.50}$$

or after inserting identities

$$\Omega_{\mu\nu}^n = i \sum_m \left(\left\langle \frac{\partial n(\mathbf{R})}{\partial R^\mu} \middle| m(\mathbf{R}) \right\rangle \left\langle m(\mathbf{R}) \middle| \frac{\partial n(\mathbf{R})}{\partial R^\nu} \right\rangle \right.$$
$$\left. - \left\langle \frac{\partial n(\mathbf{R})}{\partial R^\nu} \middle| m(\mathbf{R}) \right\rangle \left\langle m(\mathbf{R}) \middle| \frac{\partial n(\mathbf{R})}{\partial R^\mu} \right\rangle \right). \tag{1.51}$$

It can be shown that

$$\langle m(\mathbf{R})| \frac{\partial}{\partial R^\mu} |n(\mathbf{R})\rangle = \frac{\left\langle m(\mathbf{R}) \middle| \frac{\partial H}{\partial R^\mu} \middle| n(\mathbf{R}) \right\rangle}{E_n - E_m}, \quad \text{for } m \neq n. \tag{1.52}$$

Then the Berry connection is expressed as

$$\Omega_{\mu\nu}^n = i \sum_{m \neq n} \frac{\langle n | \frac{\partial H}{\partial R^\mu} | m \rangle \langle m | \frac{\partial H}{\partial R^\nu} | n \rangle - \langle n | \frac{\partial H}{\partial R^\nu} | m \rangle \langle m | \frac{\partial H}{\partial R^\mu} | n \rangle}{(E_n - E_m)^2}. \tag{1.53}$$

One can notice that, under this formulation, that the Berry curvature contains a singularity when $E_n = E_m$ which can occur for some value of the parameters $\mathbf{R}$. This singularity corresponds to a monopole existing in the parameter space, that acts as a source or sink of Berry curvature flux. An example will be demonstrated in the next subsection. Additionally, from eq. (1.53) it follows that the sum of Berry curvatures over all energy levels, i.e.

$$\sum_n \Omega_{\mu\nu}^n = 0. \tag{1.54}$$

In other words, the Berry curvature is always zero in systems with one single energy level.

If the parameter space is three-dimensional, a vectorial type of Berry curvature can be defined via

$$\Omega_{\mu\nu}^n = \epsilon_{\mu\nu\rho} \, \mathbf{\Omega}_\rho^n, \tag{1.55}$$

which is, as a result, given by the curl of the Berry connection

$$\mathbf{\Omega}_n(\mathbf{R}) = \nabla_{\mathbf{R}} \times \mathbf{A}_n(\mathbf{R}). \tag{1.56}$$

This is a manifestation that $\mathbf{\Omega}_n$ behaves equivalently to the magnetic field, while $\mathbf{A}_n$ corresponds to the vector potential. Then using Stoke's theorem in eq. (1.39), we can express the Berry phase as a surface integral

$$\gamma_n = \int_{\mathcal{S}} \mathrm{d}\mathbf{S} \cdot \mathbf{\Omega}_n, \tag{1.57}$$

where $\mathcal{S}$ is a surface that has the closed contour $\mathcal{C}$ as a boundary. Under this formulation, the Berry phase represents the flux of Berry curvature that penetrates through the surface $\mathcal{S}$.

However, to use Stoke's theorem we could have chosen any surface with $\mathcal{C}$ as a boundary. If we choose a surface with opposite orientation, we get a Berry phase

$$\gamma_n' = - \int_{\mathcal{S}'} \mathrm{d}\mathbf{S}' \cdot \mathbf{\Omega}_n, \tag{1.58}$$

where the minus sign appears because of the opposite orientation of the surface $\mathcal{S}'$. Then we can subtract eqs. (1.57) and (1.58). The surfaces $\mathcal{S}$ and $\mathcal{S}'$ glued together give a closed surface $\mathcal{S}^2$, so we end up with

$$\gamma_n - \gamma_n' = \int_{\mathcal{S}^2} \mathrm{d}\mathbf{S} \cdot \mathbf{\Omega}_n. \tag{1.59}$$

The Berry phase must be uniquely defined, i.e.

$$e^{i\gamma} = e^{i\gamma'}. \tag{1.60}$$

This means that γ and γ' can only differ by an integer multiple of 2π. This integer is called the *Chern number* and is given by

$$C_n = \frac{1}{2\pi} \int_{\mathcal{S}^2} \mathrm{d}\mathbf{S} \cdot \mathbf{\Omega}_n, \quad \in \mathbb{Z}. \tag{1.61}$$

It measures the flux of Berry curvature that goes out through the closed surface.

1.3.3   Example: Spin in a magnetic field

The simplest example that manifests Berry phase and curvature is that of a single spin $1/2$ in a magnetic field that is allowed to rotate on a sphere. The Hamiltonian describing this system is

$$H = -\mathbf{B} \cdot \boldsymbol{\sigma} \tag{1.62}$$

where the magnetic field is parametrized in spherical coordinates

$$\mathbf{B} = B \begin{pmatrix} \sin\theta\cos\phi \\ \sin\theta\sin\phi \\ \cos\theta \end{pmatrix} \tag{1.63}$$

and $\boldsymbol{\sigma}$ is the vector of Pauli matrices. This system has two energy levels $E_- = -B$ and $E_+ = B$, with their corresponding eigenstates

$$|\chi_-\rangle = \begin{pmatrix} \cos\frac{\theta}{2} \\ e^{i\phi}\sin\frac{\theta}{2} \end{pmatrix} \qquad |\chi_+\rangle = \begin{pmatrix} \sin\frac{\theta}{2} \\ -e^{i\phi}\cos\frac{\theta}{2} \end{pmatrix} \tag{1.64}$$

that are well defined only up to phase.

We can now calculate the Berry connections for the two levels using $\mathbf{R} = (\theta, \phi)$ as parameter space

$$\mathbf{A}_- = i \langle \chi_- | \nabla_{\mathbf{R}} | \chi_- \rangle = -\frac{1}{B} \frac{\sin^2 \theta/2}{\sin \theta} \, \hat{\phi} \tag{1.65}$$

$$\mathbf{A}_+ = i \langle \chi_+ | \nabla_{\mathbf{R}} | \chi_+ \rangle = -\frac{1}{B} \frac{\cos^2 \theta/2}{\sin \theta} \, \hat{\phi}, \tag{1.66}$$

as well as the corresponding Berry curvatures

$$\mathbf{\Omega}_- = \nabla \times \mathbf{A}_- = -\frac{1}{2B^2} \, \hat{B} \tag{1.67}$$

and

$$\mathbf{\Omega}_+ = \nabla \times \mathbf{A}_+ = +\frac{1}{2B^2} \, \hat{B}. \tag{1.68}$$

They have the same form as magnetic monopoles existing, however, in parameter space. Indeed these monopoles are located at the singular point $\mathbf{B} = 0$, where the two energy levels coincide. The two monopoles have opposite 'charge' of $-1/2$ and $+1/2$, acting as sources and sinks of Berry curvature and satisfying eq. (1.54). The Chern number in this case will count how many monopoles exists in each energy level, resulting in $C_- = -1$ and $C_+ = +1$.

1.3.4   Non-abelian Berry connection

The Hamiltonians we have looked at so far, contain no degeneracies. It was shown by Wilczek and Zee [11] that, if the system's energy levels are degenerate, then the Berry connection and curvature become non-abelian.

Lets us assume a ground state that is N-fold degenerate. Then, the corresponding eigenstates are

$$|n_a(\mathbf{R})\rangle, \qquad a = 1, \dots, N. \tag{1.69}$$

Starting from the ground state, the adiabatic theorem states that the system should remain in the ground state for slow evolution of the parameters, but does not restrict it to remain in the same eigenstate. Instead, it can be in any of the degenerate eigenstates (1.69). This means, that under time evolution, the wave function, instead of a phase, will acquire a unitary matrix

$$|\psi_a(t)\rangle = U_{ab}(t)|n_b(t)\rangle \tag{1.70}$$

The Berry connection then becomes an $N \times N$ matrix

$$A_\mu^{ab} = i \langle n^b(\mathbf{R}) | \frac{\partial}{\partial R^\mu} | n^a(\mathbf{R}) \rangle \tag{1.71}$$

A_μ has the same structure as the gauge field of an $SU(N)$ theory. It follows that the Berry curvature should also have the same structure as that of an $SU(N)$ theory, namely

$$\Omega_{\mu\nu} = \frac{\partial A_\nu}{\partial R^\mu} - \frac{\partial A_\mu}{\partial R^\nu} - i \left[A_\mu, A_\nu \right]. \tag{1.72}$$

Comparing with the non-degenerate case, the Berry curvature now contains an extra commutator, accounting for the matrix nature of the Berry connection.

As in the abelian case, we can apply a gauge transformation since the eigenstates are not uniquely defined. The difference is that now the transformation is a unitary matrix

$$|n_a(\mathbf{R})\rangle \to \Phi_{ab}(\mathbf{R})|n_b(\mathbf{R})\rangle. \tag{1.73}$$

As expected, the Berry connection transforms under the gauge transformation, but in a slightly more complicated way

$$A_\mu \to \Phi^\dagger A_\mu \Phi + i\Phi^\dagger \frac{\partial \Phi}{\partial R^\mu}. \tag{1.74}$$

As for the Berry curvature, it transforms as

$$\Omega_{\mu\nu} \to \Phi^\dagger \Omega_{\mu\nu} \Phi. \tag{1.75}$$

Contrary to the abelian case, the Berry curvature is not gauge invariant so it cannot correspond to an observable quantity. Gauge invariant objects can be created by tracing over the matrix indices, for example $\text{Tr}\,\Omega_{\mu\nu}$.

1.4   Disorder

Every solid in real life is far from ideal and contains impurities and other defects. We then say that such a solid is disordered. Applying an electric field will try to drive the system out of equilibrium and create a current. In this process, however, electrons will get scattered by impurities. Because of this, disorder tends to relax the system and bring it back to its equilibrium state.

In order to study the problem of disorder we have to make a few assumptions. First of all, we assume that impurities have no internal degree of freedom, meaning that they remain unaffected from scattering with the electrons and from external fields. We also assume that they are are static, i.e. time-independent, so each impurity creates a potential $v(\mathbf{r} - \mathbf{r}_j)$, where $\mathbf{r}_j$ is its position, resulting in a total potential $v(\mathbf{r}) = \sum_j v(\mathbf{r} - \mathbf{r}_j)$. Scattering of electrons with static impurities is elastic, meaning that they exchange momentum but not energy. One last assumption is that impurities are dilute and randomly distributed inside the system. Therefore, it is impossible to know the location of all individual impurities to calculate the full disorder potential. However, if we are interested in macroscopic properties of the system, it is more than enough to calculate average values with respect to the disorder configuration. This procedure is called disorder average and was first done by Kohn and Luttinger [12].

Impurity scattering will enter the Boltzmann equation in the collision integral. As we will see in chapter 2, expressed in Keldysh formalism, the collision integral involves self-energies, so this is what we will try to calculate. Surprisingly, this can be done with a lot of different methods that are described in Mahan [7], Bruus and Flensberg [13], Altland [14] and Kamenev [15]. In this discussion, we will first calculate the self-energy using perturbation theory up to second order in the disorder potential and the perform disorder average.

1.4.1 Perturbation theory over the disorder potential

Let us assume a potential $v(\mathbf{r})$ that describes the total disorder configuration. For a more compact notation, from now on we will write $v(x)$, where $x = (t, \mathbf{r})$ but remember that the disorder potential is time-independent. This adds a quadratic term in the action

$$S_{dis} = -\int dx \, v(x) \bar{\psi}(x) \psi(x). \tag{1.76}$$

Then, the Green's function is no longer the bare one, but it is dressed with a self-energy originating from the disorder action. In general it is

$$G(x, x') = -i\langle \psi(x) \bar{\psi}(x') \rangle, \tag{1.77}$$

where $\langle \dots \rangle$ is the so-called thermal average, or average with respect to the partition function $\mathcal{Z}$. It can be calculated within perturbation theory, which gives as a result Dyson's equation

$$G(x, x') = G_0(x, x') + \int dx_1 \, G_0(x, x_1) v(x_1) G(x_1, x'). \tag{1.78}$$

Expanding Dyson's equation up to second order we get

$$\begin{aligned}
G(x, x') = G_0(x, x') &+ \int dx_1 \, G_0(x, x_1) v(x_1) G_0(x_1, x') \\
&+ \int dx_1 dx_2 \, G_0(x, x_1) v(x_1) G_0(x_1, x_2) v(x_2) G_0(x_2, x')
\end{aligned} \tag{1.79}$$

that can also be expressed in diagrammatic language in figure 1.1.

For the first order contribution the self-energy is

$$\Sigma(x_1, x_2) = v(x_1) \, \delta(x_1 - x_2) \tag{1.80}$$

or in Fourier space

$$\Sigma(p) = v_0 \tag{1.81}$$

where v_0 is the strength of the disorder potential. The self-energy is first order is therefore just a constant that only provides a shift in the energy of the Green's function.

For this reason, we will focus on the second order contribution. The self-energy is then

$$\Sigma(x_1, x_2) = v(x_1) G_0(x_1, x_2) v(x_2) \tag{1.82}$$

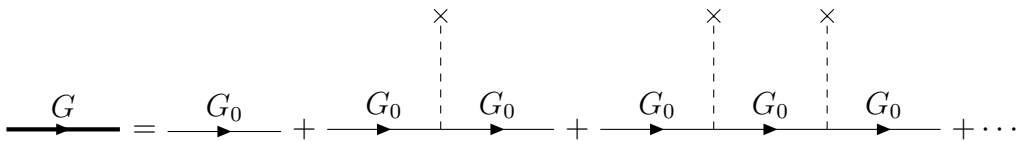and we will take perform the average over disorder for it.

Figure 1.1: Diagrammatic expression of Dyson's equation involving impurity scattering

1.4.2   Disorder average

Our goal now is to perform disorder average of the second order self-energy

$$\langle \Sigma(x_1, x_2) \rangle_{dis} = \langle v(x_1) G_0(x_1, x_2) v(x_2) \rangle_{dis}. \tag{1.83}$$

This means that we average over the positions of the impurities, which can be expressed as

$$\langle \Sigma(x_1, x_2) \rangle_{dis} = \frac{1}{\exp\left\{-\int dx \frac{v^2(x)}{v_0^2}\right\}} \int \mathcal{D}v\, \Sigma(x_1, x_2) \exp\left\{-\int dx \frac{v^2(x)}{v_0^2}\right\}, \tag{1.84}$$

where v_0 is the strength of the potential, or

$$\langle \Sigma(x_1, x_2) \rangle_{dis} = \frac{G_0(x_1, x_2)}{\exp\left\{-\int dx \frac{v^2(x)}{v_0^2}\right\}} \int \mathcal{D}v\, v(x_1) v(x_2) \exp\left\{-\int dx \frac{v^2(x)}{v_0^2}\right\}. \tag{1.85}$$

This is equivalent to adding sources, taking the second functional derivative and then setting the sources to zero

$$\langle \Sigma(x_1, x_2) \rangle_{dis} = \frac{G_0(x_1, x_2)}{\exp\left\{-\int dx \frac{v^2(x)}{v_0^2}\right\}} \frac{\delta^2}{\delta J(x_1) \delta J^*(x_2)} \int \mathcal{D}v\, \exp\left\{-\int dx \frac{v^2(x)}{v_0^2}\right\}$$
$$\exp\left\{\int dx J(x) v(x)\right\} \exp\left\{\int dx J^*(x) v(x)\right\} \Bigg|_{J=J^*=0}. \tag{1.86}$$

In the above we can complete the square, which leads to

$$\langle \Sigma(x_1, x_2) \rangle_{dis} = \frac{G_0(x_1, x_2)}{\exp\left\{-\int dx \frac{v^2(x)}{v_0^2}\right\}} \frac{\delta^2}{\delta J(x_1) \delta J^*(x_2)} \int \mathcal{D}v$$
$$\exp\left\{-\int dx \frac{(v(x) - v_0^2 J(x))^2}{v_0^2}\right\} \exp\left\{v_0^2 \int dx\, J^*(x) J(x)\right\} \Bigg|_{J=J^*=0}. \tag{1.87}$$

Now only the first exponential takes part in the integration, which is Gaussian and will cancel with the denominator, leading to just

$$\langle \Sigma(x_1, x_2) \rangle_{dis} = G_0(x_1, x_2) \frac{\delta^2}{\delta J(x_1) \delta J^*(x_2)} \exp\left\{v_0^2 \int dx\, J^*(x) J(x)\right\} \Bigg|_{J=J^*=0}. \tag{1.88}$$

Figure 1.2: Second order self-energy diagrams (a) before and (b) after disorder average.

Taking the functional derivatives and setting the sources to zero we end up with

$$\langle \Sigma(x_1, x_2)\rangle_{dis} = v_0^2 G_0(x_1, x_2)\delta(x_1 - x_2) \tag{1.89}$$

or in phase space

$$\langle \Sigma(x, p)\rangle_{dis} = v_0^2 \int \frac{\mathrm{d}^d q}{(2\pi)^d} G_0(q), \tag{1.90}$$

where d is the dimensionality of the system. This can be diagrammatically seen in figure 1.2, where 1.2a shows the self energy to second order in perturbation theory before the disorder average and 1.2b after averaging over disorder.

Chapter 2

Keldysh formalism

In section 1.1, we derived the Boltzmann equation using heuristic arguments for distribution functions and for an ensemble of classical particles, like an ideal gas. In condensed matter physics a system that is often of interest is that of electrons in a solid, and electrons are far from classical particles. For this reason, we will rederive the Boltzmann equation from a field theory approach. In a non-equilibrium situation, as is the case described by the Boltzmann equation, conventional equilibrium field theory, such as the Matsubara formalism, fails. For this reason, we have to use an out-of-equilibrium theory, also commonly known as Keldysh formalism. It was developed in the 60's by Schwinger [16], Konstantinov and Perel [17], Kadanoff and Baym [18] and Keldysh [19]. In this chapter, we will provide with the basics of the Keldysh formalism with the goal of deriveing a generic form of the quantum Boltzmann equation. The approach we will follow is similar to the one by Kamenev [15], while an alternative one can be found in lecture notes by Maciejko [20]. The whole derivation will be done for fermions, but the one for bosons is in principle similar with some changes and can be found in literature.

2.1 Closed time contour

To develop a non-equilibrium formulation we will start by considering a time-dependent Hamiltonian $\hat{H}(t)$. A system governed by $\hat{H}(t)$ will be described by a density matrix $\hat{\rho}(t)$. We assume that at time $t = -\infty$ the Hamiltonian is non-interacting and the density matrix $\hat{\rho}(-\infty)$ is known. At some point prior to any measurement, interactions are adiabatically switched on and then off again after the measurement. Until now the situation is the same as in equilibrium. However, the Hamiltonian can contain time-dependent perturbations that drive the system out of equilibrium.

The density matrix at time t can be expressed as

$$\hat{\rho}(t) = \hat{\mathcal{U}}(t, -\infty)\hat{\rho}(-\infty)\hat{\mathcal{U}}^{\dagger}(t, -\infty) = \hat{\mathcal{U}}(t, -\infty)\hat{\rho}(-\infty)\hat{\mathcal{U}}(-\infty, t), \qquad (2.1)$$

where $\hat{\mathcal{U}}(t, t')$ is the time-evolution operator defined as

$$\hat{\mathcal{U}}(t, t') = \mathcal{T} \exp\left(-i \int_{t'}^{t} dt_1\, \hat{H}(t_1)\right) \qquad (2.2)$$
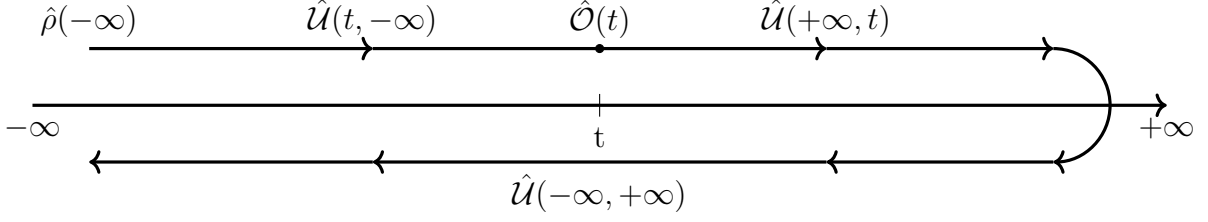
Figure 2.1: Evolution along the closed time contour $\mathcal{C}$.

and $\mathcal{T}$ stands for time-ordering. Something that is usually of interest is the expectation value of an operator defined as

$$\langle \hat{\mathcal{O}} \rangle(t) = \frac{\text{Tr}[\hat{\mathcal{O}}\hat{\rho}(t)]}{\text{Tr}\left[\hat{\rho}(t)\right]}. \tag{2.3}$$

Using eq. (2.1) we can write it as

$$\langle \hat{\mathcal{O}} \rangle(t) = \frac{\text{Tr}\left[\hat{\mathcal{O}}\hat{\mathcal{U}}(t, -\infty)\,\hat{\rho}(-\infty)\hat{\mathcal{U}}(-\infty, t)\right]}{\text{Tr}\left[\hat{\mathcal{U}}(t, -\infty)\,\hat{\rho}(-\infty)\hat{\mathcal{U}}(-\infty, t)\right]}$$

$$= \frac{1}{\text{Tr}\left[\hat{\rho}(-\infty)\right]}\,\text{Tr}\left[\hat{\mathcal{U}}(-\infty, t)\,\hat{\mathcal{O}}\hat{\mathcal{U}}(t, -\infty)\,\hat{\rho}(-\infty)\right] \tag{2.4}$$

where in the last step we performed cyclic permutation inside the trace and for the denominator used the unitarity of $\hat{\mathcal{U}}$.

The above equation states that to calculate an expectation value we follow the following procedure. We start at $t = -\infty$, where the density matrix is known, evolve to time t, calculate the expectation value of the operator and then go back to $t = -\infty$. In other words, time evolves forwards and then backwards. We can generalize this and extend the time evolution all the way to $t = +\infty$. This can be done by introducing the identity $\hat{1} = \hat{\mathcal{U}}(t, +\infty)\hat{\mathcal{U}}(+\infty, t)$. Then eq. (2.4) becomes

$$\langle \hat{\mathcal{O}} \rangle(t) = \frac{1}{\text{Tr}\left[\hat{\rho}(-\infty)\right]}\,\text{Tr}\left[\hat{\mathcal{U}}(-\infty, +\infty)\hat{\mathcal{U}}(+\infty, t)\,\hat{\mathcal{O}}\hat{\mathcal{U}}(t, -\infty)\,\hat{\rho}(-\infty)\right]. \tag{2.5}$$

This describes time evolution along a closed time contour $\mathcal{C}$, also called the Schwinger-Keldysh contour, that is depicted in figure 2.1, and consists of a forward and a backward branch.

This procedure of forward and backward time evolution is avoided in equilibrium. Assuming zero temperature, we are interested in expectation values $\langle \text{GS}|\hat{\mathcal{O}}|\text{GS}\rangle$, where $|\text{GS}\rangle$ is the ground state of the interacting system, given by $|\text{GS}\rangle = \hat{\mathcal{U}}(t, -\infty)|0\rangle$, where $|0\rangle$ is the ground state of the non-interacting system. Being in equilibrium means that the only time evolution allowed is adiabatically switching interactions on and off. By use of the adiabatic theorem, this implies that the system never transitions to an excited state, but only acquires a phase with respect to the initial state

$$\hat{\mathcal{U}}(+\infty, -\infty)|0\rangle = e^{iL}|0\rangle. \tag{2.6}$$

From the above equation, the relations $e^{iL} = \langle 0|\hat{\mathcal{U}}(+\infty, -\infty)|0\rangle$ and $\langle 0|\hat{\mathcal{U}}(+\infty, -\infty) = \langle 0|e^{iL}$ follow. Using these, we can calculate the expectation value

$$
\begin{aligned}
\langle \text{GS}|\hat{\mathcal{O}}|\text{GS}\rangle &= \langle 0|\hat{\mathcal{U}}(-\infty, t)\hat{\mathcal{O}}\hat{\mathcal{U}}(t, -\infty)|0\rangle \\
&= e^{-iL}\langle 0|e^{iL}\hat{\mathcal{U}}(-\infty, t)\hat{\mathcal{O}}\hat{\mathcal{U}}(t, -\infty)|0\rangle \\
&= \frac{\langle 0|\hat{\mathcal{U}}(+\infty, t)\hat{\mathcal{O}}\hat{\mathcal{U}}(t, -\infty)|0\rangle}{\langle 0|\hat{\mathcal{U}}(+\infty, -\infty)|0\rangle}.
\end{aligned}
\tag{2.7}
$$

It is now evident, that in equilibrium we only need to consider the forward time evolution. In the above we assumed zero temperature, but it can also be shown for finite temperature using the equilibrium density matrix and imaginary time.

The main difference that appears out of equilibrium is that eq. (2.6) does not hold anymore. Applying a non adiabatic perturbation can bring the system to an unpredictable superposition of excited states, that is not related to the initial state in a simple way. The closed time contour allows us to to bypass our ignorance of the state at $t = +\infty$. Evolution along this contour $\hat{\mathcal{U}}_{\mathcal{C}} = \hat{\mathcal{U}}(-\infty, +\infty)\hat{\mathcal{U}}(+\infty, -\infty) = \hat{1}$ unwinds everything back to the initial state $\hat{\rho}(-\infty)$, which allows us to develop functional integrals, similar to the equilibrium formalism.

2.2   Functional integration and Green's functions

We will now express the partition function for fermions out of equilibrium and develop a functional integral formalism along the closed time contour $\mathcal{C}$. As an example, we will use a single level Hamiltonian, which in second quantization is

$$
\hat{H} = \varepsilon_0 \hat{c}^\dagger \hat{c},
\tag{2.8}
$$

where $c^\dagger$ and c are fermionic creation and annihilation operators that obey canonical anti-commutation relations $\{c_i, c_j\} = \{c_i^\dagger, c_j^\dagger\} = 0$ and $\{c_i, c_j^\dagger\} = \delta_{ij}$. However, the main results of this and the next section are general and do not depend on this toy Hamiltonian.

The partition function is defined as

$$
\mathcal{Z} = \frac{\text{Tr}[\hat{\mathcal{U}}_{\mathcal{C}}\hat{\rho}(-\infty)]}{\text{Tr}[\hat{\rho}(-\infty)]}
\tag{2.9}
$$

The time evolution operator along the contour $\mathcal{C}$ is the identity $\hat{\mathcal{U}}_{\mathcal{C}} = \hat{1}$ which results in $\mathcal{Z} = 1$. Let us assume for simplicity that the initial density matrix is the equilibrium one denoted by ρ_0. Then

$$
\mathcal{Z} = \frac{\text{Tr}[\hat{\mathcal{U}}_{\mathcal{C}}\hat{\rho}_0]}{\text{Tr}[\hat{\rho}_0]}.
\tag{2.10}
$$

For the numerator we have

$$
\text{Tr}[\hat{\mathcal{U}}_{\mathcal{C}}\hat{\rho}_0] = \int \mathrm{d}\bar{\psi}\,\mathrm{d}\psi\, e^{-\bar{\psi}\psi} \langle \psi|\hat{\mathcal{U}}_{\mathcal{C}}\hat{\rho}_0\,|-\psi\rangle
\tag{2.11}
$$

Figure 2.2: Discretization of the closed time contour $\mathcal{C}$.

where ψ and $\bar{\psi}$ are Grassmann variables.

To express the partition function as a functional integral, we will discretize the time contour $\mathcal{C}$ in $2(N-1)$ intervals of length Δt, as shown in figure 2.2. At each discrete point, we introduce the identity expressed in the fermionic coherent state basis

$$\hat{1} = \int \mathrm{d}\bar{\psi}\,\mathrm{d}\psi e^{-\bar{\psi}\psi}|\psi\rangle\langle\psi|. \tag{2.12}$$

Doing that, the partition function contains the following sequence

$$\langle\psi_{2N}|\hat{\mathcal{U}}(-\Delta t)|\psi_{2N-1}\rangle\langle\psi_{2N-1}|\ldots|\psi_{N+1}\rangle\langle\psi_{N+1}|\hat{1}||\psi_N\rangle\langle\psi_N|$$
$$\ldots|\psi_2\rangle\langle\psi_2|\hat{\mathcal{U}}(+\Delta t)|\psi_1\rangle\langle\psi_1|\hat{\rho}(\varepsilon_0)|-\psi_{2N}\rangle, \tag{2.13}$$

where $\hat{\mathcal{U}}(\pm\Delta t)$ is the time evolution operator for a time interval Δt in the forward and backward part on the contour. It should also be pointed out that there is no time evolution between the points t_N and t_{N+1}. The matrix elements contained in the above equation are

$$\langle\psi_j|\hat{\mathcal{U}}(\pm\Delta t)|\psi_{j-1} = \langle\psi_j|e^{\mp i\hat{H}\Delta t}|\psi_{j-1}\rangle = \exp\left(\bar{\psi}_j\psi_{j-1} \mp i\varepsilon_0\bar{\psi}_j\psi_{j-1}\Delta t\right) \tag{2.14}$$

It can all be summed up to

$$\mathcal{Z} = \frac{1}{\mathrm{Tr}[\rho_0]} \int \prod_{j=1}^{2N} \mathrm{d}\bar{\psi}_j\,\mathrm{d}\psi_j\, \exp\left(i\sum_{j,j'=1}^{2N} \bar{\psi}_j G_{jj'}^{-1}\psi_{j'}\right), \tag{2.15}$$

where ψ, $\bar{\psi}$ are independent Grassmann variables and $G_{jj'}^{-1}$ is a $2N \times 2N$ matrix

$$iG_{jj'}^{-1} = \begin{pmatrix} -1 & & & & & & & & -\rho(\varepsilon_0) \\ h_- & -1 & & & & & & & \\ & h_- & -1 & & & & & & \\ & & \ddots & \ddots & & & & & \\ & & & h_- & -1 & & & & \\ & & & & 1 & -1 & & & \\ & & & & & h_+ & -1 & & \\ & & & & & & \ddots & \ddots & \\ & & & & & & & h_+ & -1 \\ & & & & & & & & h_+ & -1 \end{pmatrix} \tag{2.16}$$

with $h_\pm = 1 \pm i\varepsilon_0 \Delta t$.

The Green's function can be found by inverting the matrix (2.16). It is useful to separate the fields into ψ^+ that reside on the forward part of the contour and ψ^- that reside on the backward part. Then, the Green's function can be written as a 2×2 matrix

$$G = \begin{pmatrix} G^{\mathcal{T}} & G^< \\ G^> & G^{\tilde{\mathcal{T}}} \end{pmatrix}, \tag{2.17}$$

where

$$iG^<_{jj'} = \langle \psi^+_j \bar{\psi}^-_{j'} \rangle \qquad\qquad iG^>_{jj'} = \langle \psi^-_j \bar{\psi}^+_{j'} \rangle \tag{2.18}$$

$$iG^{\mathcal{T}}_{jj'} = \langle \psi^+_j \bar{\psi}^+_{j'} \rangle \qquad\qquad iG^{\tilde{\mathcal{T}}}_{jj'} = \langle \psi^-_j \bar{\psi}^-_{j'} \rangle \tag{2.19}$$

We can now take the continuum limit, meaning $N \to \infty$ and $\Delta t \to 0$. Then the four Green's functions for our example Hamiltonian (2.8) are given by

$$iG^<(t,t') = \langle \psi^+(t)\bar{\psi}^-(t') \rangle = -n_F e^{-i\varepsilon_0(t-t')} \tag{2.20a}$$

$$iG^>(t,t') = \langle \psi^-(t)\bar{\psi}^+(t') \rangle = (1-n_F)e^{-i\varepsilon_0(t-t')} \tag{2.20b}$$

$$iG^{\mathcal{T}}(t,t') = \langle \psi^+(t)\bar{\psi}^+(t') \rangle = \theta(t-t')iG^>(t,t') + \theta(t'-t)iG^<(t,t') \tag{2.20c}$$

$$iG^{\tilde{\mathcal{T}}}(t,t') = \langle \psi^-(t)\bar{\psi}^-(t') \rangle = \theta(t'-t)iG^>(t,t') + \theta(t-t')iG^<(t,t') \tag{2.20d}$$

where $n_F = \rho(\varepsilon_0)/(1+\rho(\varepsilon_0))$ is the fermionic occupation number of a single energy level.

We notice that the four Green's function are not all independent, but satisfy the equation

$$G^{\mathcal{T}}(t,t') + G^{\tilde{\mathcal{T}}}(t,t') = G^>(t,t') + G^<(t,t'). \tag{2.21}$$

This means that we can derive an equivalent formulation using only three Green's functions instead of three.

2.3 Keldysh rotation

To take advantage of eq. (2.21) Keldysh developed a formulation in his paper [19] that relies on a rotation of the basis and results in only three independent Green's functions. Due to its importance, we often refer to the whole non-equilibrium field theory as Keldysh formalism. The Keldysh rotation is performed by defining new fields

$$\psi_1(t) = \frac{1}{\sqrt{2}}\left(\psi^+(t) + \psi^-(t)\right) \qquad\qquad \psi_2(t) = \frac{1}{\sqrt{2}}\left(\psi^+(t) - \psi^-(t)\right) \tag{2.22}$$

and

$$\bar{\psi}_1(t) = \frac{1}{\sqrt{2}}\left(\bar{\psi}^+(t) - \bar{\psi}^-(t)\right) \qquad\qquad \bar{\psi}_2(t) = \frac{1}{\sqrt{2}}\left(\bar{\psi}^+(t) + \bar{\psi}^-(t)\right) \tag{2.23}$$

We should point out that the $\bar{\psi}$ fields transform in a different way than the ψ fields, which is possible because fermionic fields are independent Grassmann variables. It was

first introduced by Larkin and Ovchinnikov [21] and is convenient because, as we will see later, G^{-1}, G and Σ (the self energy) obtain the same matrix structure. However, for bosons $\bar{\phi}$ must be conjugate to ϕ.

Plugging eqs. (2.22) and (2.23) into (2.18) we get new Green's functions

$$G^R(t,t') = -i\langle\psi_1(t)\bar{\psi}_1(t')\rangle = \theta(t-t')\left(G^>(t,t') - G^<(t,t')\right) \tag{2.24a}$$

$$G^A(t,t') = -i\langle\psi_2(t)\bar{\psi}_2(t')\rangle = \theta(t'-t)\left(G^<(t,t') - G^>(t,t')\right) \tag{2.24b}$$

$$G^K(t,t') = -i\langle\psi_1(t)\bar{\psi}_2(t')\rangle = G^>(t,t') + G^<(t,t') \tag{2.24c}$$

and we can write the full Green's function in the matrix form

$$G(t,t') = \begin{pmatrix} G^R(t,t') & G^K(t,t') \\ 0 & G^A(t,t') \end{pmatrix}. \tag{2.25}$$

G^R and G^A are the retarded and advanced Green's functions, as is evident by the presence of θ-functions, similar to their equilibrium counterparts. G^K is a new Green's function, called Keldysh, that does not have an analog in equilibrium field theory, while $\langle\psi_2(t)\bar{\psi}_1(t')\rangle = 0$.

For our toy Hamiltonian (2.8), the three Green's functions obtain the forms

$$G^R(t,t') = -i\theta(t-t')e^{-i\varepsilon_0(t-t')} \tag{2.26a}$$

$$G^A(t,t') = i\theta(t'-t)e^{-i\varepsilon_0(t-t')} \tag{2.26b}$$

$$G^K(t,t') = -i(1-2n_F)e^{-i\varepsilon_0(t-t')}, \tag{2.26c}$$

and their Fourier transforms

$$G^R(E) = (E - \varepsilon_0 + i\eta)^{-1} \tag{2.27a}$$

$$G^A(E) = (E - \varepsilon_0 - i\eta)^{-1} \tag{2.27b}$$

$$G^K(E) = -2\pi i(1 - 2n_F)\delta(E - \varepsilon_0). \tag{2.27c}$$

We notice that the retarded and advanced Green's functions only contain information about the spectrum, but the Keldysh retains information about the occupation number. The following properties are now obvious

$$G^R = [G^A]^\dagger \qquad G^A = [G^R]^\dagger \qquad G^K = -[G^K]^\dagger. \tag{2.28}$$

They are general, however, and do not depend on the specific choice of Hamiltonian.

We can now generalize our study to fields depending on space-time coordinates $x = (t, \mathbf{r})$, instead of just time. Then we can write down the Keldysh fermionic action

$$S = \int dx_1 dx_2 \left(\bar{\psi}_1(x_1) \ \ \bar{\psi}_2(x_1)\right) G^{-1}(x_1, x_2) \begin{pmatrix} \psi_1(x_2) \\ \psi_2(x_2) \end{pmatrix} \tag{2.29}$$

with

$$G^{-1}(x_1, x_2) = \begin{pmatrix} [G^{-1}]^R(x_1, x_2) & [G^{-1}]^K(x_1, x_2) \\ 0 & [G^{-1}]^A(x_1, x_2) \end{pmatrix}. \tag{2.30}$$

Using the identity

$$\int \mathrm{d}x_3\, G^{-1}(x_1, x_3)G(x_3, x_2) = \delta(x_1 - x_2), \tag{2.31}$$

we find

$$\left[G^{-1}\right]^R = \left[G^R\right]^{-1} \qquad \left[G^{-1}\right]^A = \left[G^A\right]^{-1}. \tag{2.32}$$

For the Keldysh component, which is anti-Hermitian, it is useful to make a parametrization via a Hermitian function $F = F^\dagger$

$$G^K = G^R F - F\, G^A. \tag{2.33}$$

F is a two-point function $F(x_1, x_2)$ and products between two two-point functions imply integration over the intermediate variable, for example

$$G^R F = \int \mathrm{d}x_3\, G^R(x_1, x_3)F(x_3, x_2). \tag{2.34}$$

The Wigner transformation (see section 1.2) of F is the distribution function of the system. Specifically in our simple example, $F = 1 - 2n_F$ and its Wigner transformation will give the fermionic distribution function.

2.4 Quantum Boltzmann equation

Up until now we have looked at non-interacting systems. If the system is interacting, we can write the total action as the sum of the bare, or non-interacting action, and the term that contains the interactions

$$S = S_0 + S_{int}. \tag{2.35}$$

Then the full Green's function can be written as a functional integral

$$G_{ab}(x_1, x_2) = -i \int \mathcal{D}\bar{\psi}\mathcal{D}\psi\, \psi_a(x_1)\bar{\psi}_b(x_2)\, e^{i(S_0 + S_{int})} \tag{2.36}$$

where $a, b = (1, 2)$ is the Keldysh index.

The full Green's function can be calculated by expanding the exponent in powers of S_{int} and then using Wick's theorem. This results in an infinite series, where every term is represented by a Feynman diagram. Each diagram contains two external propagators accounting for $G_0(x_1, x_i)$ and $G_0(x_j, x_2)$. We can define the self-energy as the sum of all the irreducible diagrams, i.e. those that cannot be disconnected after cutting one internal line, after removing the external propagators. Then, the full Green's function can be written as

$$\begin{aligned} G &= G_0 + G_0 \Sigma G_0 + G_0 \Sigma G_0 \Sigma G_0 + \dots \\ &= G_0 + G_0 \Sigma \left(G_0 + G_0 \Sigma G_0 + \dots\right) \\ &= G_0 + G_0 \Sigma G \end{aligned} \tag{2.37}$$
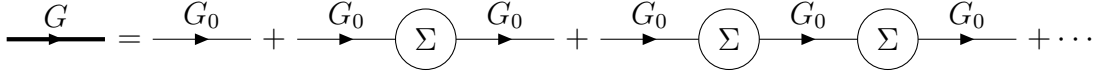
Figure 2.3: Diagrammatic expression of Dyson's equation

where products denote integration over the intermediate variable and multiplication of the 2×2 Keldysh matrices. This expansion can be seen diagrammatically in figure 2.3. Multiplying both sides of the equation with G_0^{-1} from the left we get

$$\left(G_0^{-1} - \Sigma\right) G = \mathbb{1} \tag{2.38}$$

This is Dyson's equation, also defined in equilibrium.

The difference is that, in contrast to the equilibrium case, G, G_0^{-1} and Σ are all 2×2 matrices. The self-energy has the same structure as the Green's function so we can write Dyson's equation in matrix form

$$\begin{pmatrix} G_0^{-1R} - \Sigma^R & -\Sigma^K \\ 0 & G_0^{-1A} - \Sigma^A \end{pmatrix} \begin{pmatrix} G^R & G^K \\ 0 & G^A \end{pmatrix} = \mathbb{1}, \tag{2.39}$$

where we took into account that $G_0^{-1K} \sim i\eta F$ and can be ignored compared to Σ^K.

For the retarded and advanced Green's functions we can write closed equations

$$\left(G_0^{-1R/A} - \Sigma^{R/A}\right) G^{R/A} = \delta(x_1 - x_2). \tag{2.40}$$

$G_0^{-1R/A}$ is known directly from the Hamiltonian and $\Sigma^{R/A}$ can be found up to some order in perturbation theory. Then, we can solve for the full retarded and advanced Green's function

$$G^{R/A} = \left(G_0^{-1R/A} - \Sigma^{R/A}\right)^{-1}. \tag{2.41}$$

From Dyson's equation an equation for the Keldysh component can also be found

$$\left(G_0^{-1R} - \Sigma^R\right) G^K - \Sigma^K G^A = 0. \tag{2.42}$$

Obviously, this is not a closed equation, but contains retarded and advanced components. We can use the parametrization (2.33) for the Keldysh Green's function and write

$$\left(G_0^{-1R} - \Sigma^R\right) \left(G^R F - F G^A\right) = \Sigma^K G^A. \tag{2.43}$$

Multiplying both sides of the equation from the right with $\left(G_0^{-1A} - \Sigma^A\right)$ and then using eq. (2.40) we get

$$F\left(G_0^{-1A} - \Sigma^A\right) - \left(G_0^{-1R} - \Sigma^R\right) F = \Sigma^K. \tag{2.44}$$

G_0^{-1R} and G_0^{-1A} differ only be a factor of $2i\eta$, which for our purposes can be ignore and simply write G_0^{-1}. However, this is not necessarily true for the corresponding self-energies. After some rearrangement we end up with

$$\left[F, G_0^{-1}\right] = \Sigma^K - \left(\Sigma^R F - F \Sigma^A\right), \tag{2.45}$$

where $[\,,\,]$ denotes a commutator. This is a generalized form of the quantum Boltzmann equation, or the kinetic equation for F. The left hand side contains only the bare Green's function and is the kinetic term of the equation. The right hand side contains self-energies and corresponds to the collision integral. However, this is not a very useful form for practical purposes. In practice, we will use Wigner transformation on the Boltzmann equation and find exact forms for specific systems with various properties. This will be the main topic of the rest of the thesis.

Chapter 3

Single-band systems

Having derived a generic form for the quantum Boltzmann equation, we will now go on to derive it for actual systems. In this chapter we will look at systems with dispersion that consists of only one band. The common feature of these systems is that they are described by a simple Hamiltonian, that is not a matrix, and all quantities involved in the Boltzmann equation, i.e. distribution function, Green's function, self-energy, commute among each other. We will start a simple electronic system and study its response to an extrnal electric field. Then, we will add a magnetic field to the previous system by performing minimal coupling. Finally, we will study the collision integral for a disordered system that involves impurity scattering.

3.1   Electrons in an electric field

The simplest non-trivial fermionic system one can study within the context of the Boltzmann equation is that of electrons in an electric field. For that, we will set the collision integral to zero. Then, the Boltzmann equation reduces to

$$[F, G_0^{-1}] = 0, \tag{3.1}$$

where G_0^{-1} is the inverse of the non-interacting, or bare, Green's function and the Wigner transformation of F is the distribution function. In other words, the distribution function is defined as

$$f(x, p) = \int dx' e^{-ipx'} F\left(x + \frac{x'}{2}, x - \frac{x'}{2}\right), \tag{3.2}$$

where x and x' are the center of mass and the relative coordinate respectively and we are using notation such that $x = (t, \mathbf{r})$ and $p = (E, \mathbf{k})$.

Eq. (3.1), though exact and general, does not contain much useful information. In order for the Boltzmann equation to include observable quantities and be expressed with respect to the actual distribution function $f(x, p)$, we will perform a Wigner transformation and products involving two-point functions will become Moyal products

$$[f, G_0^{-1}]^\star = 0. \tag{3.3}$$

Then, we can rewrite it by as an expansion over the gradients to first order, as introduced in section 1.2

$$\left[f, G_0^{-1}\right] + \frac{i}{2}\left\{\partial_x f, \partial_p G_0^{-1}\right\} - \frac{i}{2}\left\{\partial_p f, \partial_x G_0^{-1}\right\} = 0. \tag{3.4}$$

However, the above equation can be simplified since in the single-band case f and G_0^{-1} are 'simple' functions, i.e. not matrices, so they commute with each other. As a result, the Boltzmann equation for a collisionless single-band system to first order in the gradient expansion reduces to

$$i\left(\partial_x f \partial_p G_0^{-1} - \partial_p f \partial_x G_0^{-1}\right) = 0, \tag{3.5}$$

or after separating time and space coordinates

$$\partial_t f \partial_E G_0^{-1} - \nabla_{\mathbf{r}} f \nabla_{\mathbf{k}} G_0^{-1} - \partial_E f \partial_t G_0^{-1} + \nabla_{\mathbf{k}} f \nabla_{\mathbf{r}} G_0^{-1} = 0. \tag{3.6}$$

We can be more specific than that though. For a specific system, the bare Green's function is known, so in the end the kinetic equation contains only the distribution function as unknown. A very broad category of systems is that of those that possess translational invariance. They can be described by a Hamiltonian of the form $H(x_1, x_2) = H(x_1 - x_2) = H(x')$, where x' is the relative coordinate $x' = x_1 - x_2$. Then, the Wigner transformation of the Hamiltonian reduces simply to a Fourier transformation over x', which we write as $\varepsilon(\mathbf{k})$ and call it the dispersion relation of the system. This leads to the bare Green's function

$$G_0^{-1} = E - \varepsilon(\mathbf{k}). \tag{3.7}$$

If an electric field is applied to the system, the Hamiltonian acquires an extra term of $-e\,\mathbf{r}\cdot\mathbf{E}$, so the new Green's function is

$$G_0^{-1} = E - \varepsilon(\mathbf{k}) + e\,\mathbf{r}\cdot\mathbf{E}. \tag{3.8}$$

This can now be substituted into the Boltzmann equation eq. (3.6) to yield

$$\partial_t f + \nabla_{\mathbf{k}}\varepsilon(\mathbf{k})\cdot\nabla_{\mathbf{r}} f + e\,\nabla_{\mathbf{k}} f\cdot\mathbf{E} = 0. \tag{3.9}$$

This way, we have rederived the classical Boltzmann equation in the absence of collisions. This can be compared to (1.10) leading to the conclusion that a force $e\mathbf{E}$ acts on the system and the velocity is substituted by $\mathbf{v}(\mathbf{k}) = \nabla_{\mathbf{k}}\varepsilon(\mathbf{k})$. This is known as the group velocity and depends on the dispersion of each system.

A system of free electrons, also known as electron gas, is usually described by a Hamiltonian with a quadratic kinetic term. With the addition of an electric field, the Hamiltonian in second quantization is

$$H\left[\bar{\psi}, \psi\right] = \int d\mathbf{r}\,\bar{\psi}(t, \mathbf{r})\left(-\frac{\nabla_{\mathbf{r}}^2}{2m} - e\,\mathbf{r}\cdot\mathbf{E}\right)\psi(t, \mathbf{r}) \tag{3.10}$$

and the corresponding action

$$S\left[\bar{\psi}, \psi\right] = \int dt d\mathbf{r}\,\bar{\psi}(t, \mathbf{r})\left(i\partial_t + \frac{\nabla_{\mathbf{r}}^2}{2m} + e\,\mathbf{r}\cdot\mathbf{E}\right)\psi(t, \mathbf{r}), \tag{3.11}$$

where we have set $\hbar = 1$. From the action we can deduce the inverse Green's function

$$G_0^{-1}(t_1, \mathbf{r}_1, t_2, \mathbf{r}_2) = \delta(t_1 - t_2)\delta(\mathbf{r}_1 - \mathbf{r}_2)\left(i\partial_{t_2} + \frac{1}{2m}\partial_{\mathbf{r}_2}^2 + e\,\mathbf{r}_2 \cdot \mathbf{E}\right). \tag{3.12}$$

Since the system is translationally invariant, we can expect the Wigner transformation to be the same as the Fourier transformation, but let us show it formally. First, we go to the center of mass and relative coordinates $x = (x_1 + x_2)/2$ and $x' = x_1 - x_2$, which means that $x_{1,2} = x \pm x'/2$. Then, the derivatives transform as

$$\partial_{x_2} = \frac{1}{2}\partial_x - \partial_{x'} \tag{3.13}$$

and

$$\partial_{x_2}^2 = \frac{1}{4}\partial_x^2 - \partial_{xx'}^2 + \partial_{x'}^2. \tag{3.14}$$

In this new coordinate system the inverse Green's function is

$$G_0^{-1}(t, \mathbf{r}, t', \mathbf{r}') = \delta(t')\delta(\mathbf{r}')\left[i\left(\frac{1}{2}\partial_t - \partial_{t'}\right) + \frac{1}{2m}\left(\frac{1}{4}\partial_\mathbf{r}^2 - \partial_{\mathbf{rr'}}^2 + \partial_{\mathbf{r'}}^2\right)\right.$$
$$\left. + e\left(\mathbf{r} - \frac{1}{2}\mathbf{r}'\right)\cdot\mathbf{E}\right]. \tag{3.15}$$

The relative coordinate can now be Fourier transformed to give the Green's function in the Wigner representation.

$$G_0^{-1}(t, \mathbf{r}, E, \mathbf{k}) = \int \mathrm{d}t'\mathrm{d}\mathbf{r}'\,\delta(t')\delta(\mathbf{r}')\left[i\left(\frac{1}{2}\partial_t - \partial_{t'}\right) + \frac{1}{2m}\left(\frac{1}{4}\partial_\mathbf{r}^2 - \partial_{\mathbf{rr'}}^2 + \partial_{\mathbf{r'}}^2\right)\right.$$
$$\left. + e\left(\mathbf{r} - \frac{1}{2}\mathbf{r}'\right)\cdot\mathbf{E}\right]e^{-i(\mathbf{k}\cdot\mathbf{r}' - Et')} \tag{3.16}$$

Acting with the derivatives, only the ones with respect to the relative coordinate survive

$$G_0^{-1}(t, \mathbf{r}, E, \mathbf{k}) = \int \mathrm{d}t'\mathrm{d}\mathbf{r}'\,\delta(t')\delta(\mathbf{r}')\left[E - \frac{\mathbf{k}^2}{2m} + e\left(\mathbf{r} - \frac{1}{2}\mathbf{r}'\right)\cdot\mathbf{E}\right]e^{-i(\mathbf{k}\cdot\mathbf{r}' - Et')} \tag{3.17}$$

and performing the integrals with the use of the delta functions, we get the final form of the Wigner transformation of the Green's function

$$G_0^{-1}(t, \mathbf{r}, E, \mathbf{k}) = E - \frac{\mathbf{k}^2}{2m} + e\,\mathbf{r} \cdot \mathbf{E}. \tag{3.18}$$

This can now be plugged into the kinetic equation (3.6) to give

$$\partial_t f + \frac{\mathbf{k}}{m}\cdot\nabla_\mathbf{r}f + e\,\nabla_\mathbf{k}f\cdot\mathbf{E} = 0. \tag{3.19}$$

This is the same as eq. (3.9), but the velocity is now $\mathbf{v}(\mathbf{k}) = \mathbf{k}/m$. This is exactly what is expected for a system with quadratic dispersion, where electrons are treated as classical particles.

3.2   Electrons in a magnetic field

We will now add a magnetic field to the system that we studied before. Our starting point is the Boltzmann equation for a single-band system without collisions that we derived in the previous section

$$\partial_x f \partial_p G_0^{-1} - \partial_p f \partial_x G_0^{-1} = 0. \tag{3.20}$$

While before the electric field was taken into account by adding a term to the Hamiltonian, now it will be included together with the magnetic field by performing a minimal coupling, or in other words, going to the gauge-invariant momentum

$$p^\mu \to \Pi^\mu = p^\mu + eA^\mu, \tag{3.21}$$

where A^μ is the electromagnetic gauge field and e the electron charge. Doing this transformation though, also causes the derivatives to transform since $A^\mu = A^\mu(x)$.

$$\frac{\partial}{\partial x^\mu} \to \frac{\partial}{\partial x^\mu} + e\frac{\partial A^\nu}{\partial x^\mu}\frac{\partial}{\partial \Pi^\nu} \tag{3.22}$$

$$\frac{\partial}{\partial p^\mu} \to \frac{\partial}{\partial \Pi^\mu} \tag{3.23}$$

Applying these transformations to the Boltzmann equation we get

$$\left(\frac{\partial f}{\partial x^\mu} + e\frac{\partial f}{\partial \Pi^\nu}\frac{\partial A^\nu}{\partial x^\mu}\right)\frac{\partial G_0^{-1}}{\partial \Pi^\mu} - \frac{\partial f}{\partial \Pi^\mu}\left(\frac{\partial G_0^{-1}}{\partial x^\mu} + e\frac{\partial A^\nu}{\partial x^\mu}\frac{\partial G_0^{-1}}{\partial \Pi^\nu}\right) = 0. \tag{3.24}$$

Repeated indices can be renamed and, after rearranging, we end up with

$$\frac{\partial f}{\partial x^\mu}\frac{\partial G_0^{-1}}{\partial \Pi^\mu} - \frac{\partial f}{\partial \Pi^\mu}\frac{\partial G_0^{-1}}{\partial x^\mu} - e\frac{\partial f}{\partial \Pi^\mu}\left(\frac{\partial A^\nu}{\partial x^\mu} - \frac{\partial A^\mu}{\partial x^\nu}\right)\frac{\partial G_0^{-1}}{\partial \Pi^\nu} = 0, \tag{3.25}$$

or

$$\frac{\partial f}{\partial x^\mu}\frac{\partial G_0^{-1}}{\partial \Pi^\mu} - \frac{\partial f}{\partial \Pi^\mu}\left(\frac{\partial G_0^{-1}}{\partial x^\mu} + eF_{\mu\nu}\frac{\partial G_0^{-1}}{\partial \Pi^\nu}\right) = 0, \tag{3.26}$$

where we have identified the electromagnetic field strength tensor $F_{\mu\nu} = \partial_\mu A_\nu - \partial_\nu A_\mu$. Splitting the coordinates as $x = (t, \mathbf{r})$ and $\Pi = (\mathcal{E}, \mathbf{K})$ and taking into account that $F_{\mu\nu}$ is anti-symmetric we get

$$-\frac{\partial f}{\partial t}\frac{\partial G_0^{-1}}{\partial \mathcal{E}} + \frac{\partial f}{\partial r^i}\frac{\partial G_0^{-1}}{\partial K^i} + \frac{\partial f}{\partial \mathcal{E}}\left(\frac{\partial G_0^{-1}}{\partial t} + eF_{0i}\frac{\partial G_0^{-1}}{\partial K^i}\right)$$
$$-\frac{\partial f}{\partial K^i}\left(\frac{\partial G_0^{-1}}{\partial r^i} - eF_{i0}\frac{\partial G_0^{-1}}{\partial \mathcal{E}} + eF_{ij}\frac{\partial G_0^{-1}}{\partial K^j}\right) = 0. \tag{3.27}$$

We can now recognize the electric and magnetic fields as $F_{i0} = -F_{0i} = E_i$ and $F_{ij} = \epsilon_{ijk}B_k$. This leads to the gauge invariant equation

$$-\frac{\partial f}{\partial t}\frac{\partial G_0^{-1}}{\partial \mathcal{E}} + \frac{\partial f}{\partial r^i}\frac{\partial G_0^{-1}}{\partial K^i} + \frac{\partial f}{\partial \mathcal{E}}\left(\frac{\partial G_0^{-1}}{\partial t} - eE_i\frac{\partial G_0^{-1}}{\partial K^i}\right)$$
$$-\frac{\partial f}{\partial K^i}\left(\frac{\partial G_0^{-1}}{\partial r^i} - eE_i\frac{\partial G_0^{-1}}{\partial \mathcal{E}} + e\epsilon_{ijk}B_k\frac{\partial G_0^{-1}}{\partial K^j}\right) = 0, \tag{3.28}$$

or in vector notation

$$-\partial_t f \partial_{\mathcal{E}} G_0^{-1} + \nabla_{\mathbf{r}} f \cdot \nabla_{\mathbf{K}} G_0^{-1} + \partial_{\mathcal{E}} f \left(\partial_t G_0^{-1} - e\,\mathbf{E} \cdot \nabla_{\mathbf{K}} G_0^{-1}\right)$$
$$-\nabla_{\mathbf{K}} f \cdot \left(\nabla_{\mathbf{r}} G_0^{-1} - e\,\mathbf{E}\,\partial_{\mathcal{E}} G_0^{-1} + e\nabla_{\mathbf{K}} G_0^{-1} \times \mathbf{B}\right) = 0. \tag{3.29}$$

As mentioned in the previous section, the Green's function of translationally invariant system can be expressed as

$$G_0^{-1}(t, \mathbf{r}, \mathcal{E}, \mathbf{K}) = \mathcal{E} - \varepsilon(\mathbf{K}) \tag{3.30}$$

where now the dispersion is a function of the gauge invariant momentum. In this case, the Boltzmann equation reduces to

$$\partial_t f + \nabla_{\mathbf{r}} f \cdot \nabla_{\mathbf{K}} \varepsilon(\mathbf{K}) - e\,\partial_{\mathcal{E}} f\,\mathbf{E} \cdot \nabla_{\mathbf{K}} \varepsilon(\mathbf{K}) + e\nabla_{\mathbf{K}} f \cdot (\mathbf{E} + \nabla_{\mathbf{K}} \varepsilon(\mathbf{K}) \times \mathbf{B}) = 0. \tag{3.31}$$

In the last term, we can recognize the Lorentz force

$$\mathbf{F} = e\left(\mathbf{E} + \mathbf{v}(\mathbf{K}) \times \mathbf{B}\right) \tag{3.32}$$

that acts on a system when a magnetic field is present. We also observe a new "quantum" term $e\,\mathbf{E} \cdot \mathbf{v}(\mathbf{K})$. We notice that it includes only the electric field and not the magnetic field, accounting to the fact that the magnetic field produces no work. This term didn't show up in the previous case because of the gauge choice we made in the way we included the electric field. The classical Boltzmann equation can be retrieved by integrating out the energy $\mathcal{E}$, so this extra term vanishes.

3.3 Disordered electronic systems

So far, we have only studied the Boltzmann equation in the collisionless case. In this section, we will look at a disordered system, where electrons scatter with impurities. Therefore, we will go back to the full form of the Boltzmann equation in the Wigner representation

$$\left[f, G_0^{-1}\right]^{\star} = \Sigma^K - \left(\Sigma^R \star f - f \star \Sigma^A\right). \tag{3.33}$$

Performing the gradient expansion up to first order, keeping in mind that all functions commute with each other, we get

$$i\left(\partial_x f\,\partial_p G_0^{-1} - \partial_p f\,\partial_p G_0^{-1}\right) = \Sigma^K - \left(\Sigma^R f - f\,\Sigma^A\right)$$
$$-\frac{i}{2}\left(\partial_x \Sigma^R\,\partial_p f - \partial_x f\,\partial_p \Sigma^A\right) + \frac{i}{2}\left(\partial_p \Sigma^R\,\partial_x f - \partial_p f\,\partial_x \Sigma^A\right) \tag{3.34}$$

or

$$i\left(\partial_x f \partial_p G_0^{-1} - \partial_p f \partial_p G_0^{-1}\right) = \Sigma^K - f\left(\Sigma^R - \Sigma^A\right)$$
$$+\frac{i}{2}\partial_x f \partial_p\left(\Sigma^R + \Sigma^A\right) - \frac{i}{2}\partial_p f \partial_x\left(\Sigma^R + \Sigma^A\right). \tag{3.35}$$

In the Keldysh formalism, similar to the Green's functions, the retarded and advanced self-energies are mutually Hermitian, i.e. $\Sigma^{A\dagger}(x_1, x_2) = \Sigma^R(x_1, x_2)$. This implies that

$\Sigma^R(x, p) + \Sigma^A(x, p) = 2 \operatorname{Re}\Sigma^R(x, p)$ and $\Sigma^R(x, p) - \Sigma^A(x, p) = 2i \operatorname{Im}\Sigma^R(x, p)$. We can them rewrite the Boltzmann equation as

$$i\partial_x f \partial_p \left(G_0^{-1} - \operatorname{Re}\Sigma^R\right) - i\partial_p f \partial_x \left(G_0^{-1} - \operatorname{Re}\Sigma^R\right) = \Sigma^K - f \left(\Sigma^R - \Sigma^A\right). \tag{3.36}$$

The real part of the self-energy provides just a renormalization of the Green's function, while the imaginary part appears in the collision integral.

We will now focus on the collision integral. As explained in the section 1.4, since we do not know the exact location of the impurities, we perform disorder average and then the self-energies in second order of perturbation theory can be written as

$$\Sigma(t, \mathbf{r}, E, \mathbf{k}) = v_0^2 \int \frac{d^d\mathbf{q}}{(2\pi)^d} G_0(t, \mathbf{r}, E, \mathbf{q}), \tag{3.37}$$

where d is the dimensionality of the system. We can then write

$$\Sigma^R(t, \mathbf{r}, E, \mathbf{k}) - \Sigma^A(t, \mathbf{r}, E, \mathbf{k}) = v_0^2 \int \frac{d^d\mathbf{q}}{(2\pi)^d} \left(G_0^R(t, \mathbf{r}, E, \mathbf{q}) - G_0^A(t, \mathbf{r}, E, \mathbf{q})\right)$$
$$= -iv_0^2 \int \frac{d^d\mathbf{q}}{(2\pi)^d} A(t, \mathbf{r}, E, \mathbf{q}), \tag{3.38}$$

where $A(t, \mathbf{r}, E, \mathbf{q})$ is the spectral function $A = -2 \operatorname{Im} G_0^R = i \left(G_0^R - G_0^A\right)$. For the Keldysh component

$$\Sigma^K(t, \mathbf{r}, E, \mathbf{q}) = v_0^2 \int \frac{d^d\mathbf{q}}{(2\pi)^d} G_0^K(t, \mathbf{r}, E, \mathbf{q})$$
$$= v_0^2 \int \frac{d^d\mathbf{q}}{(2\pi)^d} f(t, \mathbf{r}, E, \mathbf{q}) \left(G_0^R(t, \mathbf{r}, E, \mathbf{q}) - G_0^A(t, \mathbf{r}, E, \mathbf{q})\right) \tag{3.39}$$
$$= -iv_0^2 \int \frac{d^d\mathbf{q}}{(2\pi)^d} f(t, \mathbf{r}, E, \mathbf{q}) A(t, \mathbf{r}, E, \mathbf{q}).$$

Finally, the collision integral is

$$I_{coll} = -iv_0^2 \int \frac{d^d\mathbf{q}}{(2\pi)^d} \left(f(t, \mathbf{r}, E, \mathbf{q}) - f(t, \mathbf{r}, E, \mathbf{k})\right) A(t, \mathbf{r}, E, \mathbf{q}) \tag{3.40}$$

The spectral function is sharply peaked and can be approximated by a delta function

$$A(t, \mathbf{r}, E, \mathbf{q}) = \delta(E - \varepsilon(\mathbf{k})), \tag{3.41}$$

which will facilitate integration of the Boltzmann equation over the energy E. This way, we require that the energy is uniquely defined by the systems spectrum $\varepsilon(\mathbf{k})$, or in other words take particles on-shell, and recover the classical Boltzmann equation.

Chapter 4

Multi-band systems

In section 1.3, we introduced the notions of the Berry phase and the Berry curvature. They arise from the dependence of the Hamiltonian on a general parameter $\mathbf{R}$ that can slowly vary in time. A translationally invariant system, however, is described by a momentum-dependent Hamiltonian $H(\mathbf{k})$. We can then make the reasonable choice to use momentum as parameter, and define the Berry phase, connection and curvature with respect to momentum. We also showed in eq. (1.54) that the Berry curvatures across all the energy levels sum up to zero. If the Hamiltonian $H(\mathbf{k})$ is a matrix, then its energy spectrum is organized in bands. Using momentum as a parameter, this is translated as the Berry curvature vanishing upon summation over all bands. We can then draw the conclusion that Berry phase effects can only appear in multi-band systems when we study one or some of the bands. This is what we will show in this chapter using the Boltzmann equation.

4.1   The matrix Boltzmann equation

For a multi-band system, the Hamiltonian is a matrix. The Boltzmann equation in the absence of disorder is

$$\left[f, G_0^{-1}\right]^\star = 0, \tag{4.1}$$

where both G_0^{-1} and f are matrices, making the Boltzmann equation itself a matrix. We will make an attempt to diagonalize it, using a unitary transformation U

$$U^\dagger \left[f, G_0^{-1}\right]^\star U = 0 \tag{4.2}$$

Specifically, we use the same transformation U that diagonalizes the Hamiltonian, that consists of the system's eigenstates. Then, U also diagonalizes the Green's function, namely

$$U^\dagger G_0^{-1} U = g_0^{-1}. \tag{4.3}$$

Acting with U on the distribution function transforms it as

$$U^\dagger f U = \tilde{f}, \tag{4.4}$$

but $\tilde{F}$ is not diagonal. In the following, we will rename $\tilde{f}$ back to f. The Boltzmann equation can then be written as

$$U^\dagger \left[U f U^\dagger, U g_0^{-1} U^\dagger\right]^\star U = 0. \tag{4.5}$$

The gradient expansion can now be performed, taking into account that g_0^{-1}, f and U are matrices that do not commute among each other, so the right expression for it is eq. (1.22). Applying it to the above equation we get

$$U^\dagger \left[U f U^\dagger, U g_0^{-1} U^\dagger \right] U + \frac{i}{2} U^\dagger \left\{ \partial_x \left(U f U^\dagger \right), \partial_p \left(U g_0^{-1} U^\dagger \right) \right\} U$$
$$- \frac{i}{2} U^\dagger \left\{ \partial_p \left(U f U^\dagger \right), \partial_x \left(U g_0^{-1} U^\dagger \right) \right\} U = 0. \tag{4.6}$$

We will now specify to translationally invariant systems described by a Hamiltonian $H(\mathbf{k})$ that is not diagonal on $\mathbf{k}$. Then, the Green's function is $G_0^{-1} = E \mathbb{1} - H(\mathbf{k})$. That means that the matrix that diagonalizes it depends on momentum, i.e. $U(\mathbf{k})$. However, for a more compact notation, we will write $U(p)$, where $p = (E, \mathbf{k})$, keeping in mind that it does not depend on E since the Green's function possesses only a trivial dependence on the energy. That way, $\partial_x U$ vanishes resulting in

$$\left[f, g_0^{-1} \right] + \frac{i}{2} U^\dagger \left\{ U \partial_x f U^\dagger, \partial_p U g_0^{-1} U^\dagger + U \partial_p g_0^{-1} U^\dagger + U g_0^{-1} \partial_p U^\dagger \right\} U$$
$$- \frac{i}{2} U^\dagger \left\{ \partial_p U f U^\dagger + U \partial_p f U^\dagger + U f \partial_p U^\dagger, U \partial_x g_0^{-1} U^\dagger \right\} U = 0, \tag{4.7}$$

where for the first term we used the fact that U is unitary, i.e. $U^\dagger U = \mathbb{1}$. As explained in section 1.3, the Berry connection can be defined as $A_p = i U^\dagger \partial_p U$. Due to it being Hermitian, it can also be expressed as $A_p = -i \partial_p U^\dagger U$. Exploiting this, we end up with the following form of the Boltzmann equation

$$\left[f, g_0^{-1} \right] + \frac{i}{2} \left\{ \partial_x f, \partial_p g_0^{-1} - i \left[A_p, g_0^{-1} \right] \right\} - \frac{i}{2} \left\{ \partial_p f - i \left[A_p, f \right], \partial_x g_0^{-1} \right\} = 0. \tag{4.8}$$

We can see that Berry phase effects appear naturally in the Boltzmann equation of multi-band systems. However, there is a big problem in the above equation. It is expressed with respect to the Berry connection, which, as explained in section 1.3, is not gauge invariant. This accounts for the fact that U is not uniquely defined, but there is an infinite number of matrices that can diagonalize the Hamiltonian that are related by a gauge transformation. Gauge-dependent quantities cannot correspond to observables, which makes the Boltzmann equation, under this representation, unable to account for any physical observables.

Comparing eq. (4.8) with the standard gradient expansion for non-commuting functions, eq. (1.22), we notice that ∂_p has been modified to a covariant type of derivative

$$D_p f / g_0^{-1} = \partial_p f / g_0^{-1} - i \left[A_p, f / g_0^{-1} \right] \tag{4.9}$$

containing the Berry connection.

4.2   Decoupling of the equation

In the previous section we wrote down the Boltzmann equation as a matrix. The diagonal elements of it represent evolution within a single band, while the off-diagonals

describe transitions between different bands. Since we are interested in Berry phase effects, by use of the adiabatic theorem we have to look at the diagonals. However, there can in principle contain both diagonal and non-diagonal elements of the distribution function. Because of that, we need to find a way to decouple the matrix Boltzmann equation. We will do this in a way similar to the one presented in [22].

We can assume that we can expand the distribution function in orders of the gradient expansion

$$f = f^{(0)} + f^{(1)} + \cdots + f^{(n)} \tag{4.10}$$

Assume that we can solve the off-diagonal elements of the Boltzmann equation in order n and find the off-diagonal elements of the distribution function f_{ij} in terms of the diagonals f_{ii}. Looking at the diagonal elements of the Boltzmann equation, we notice that the zero-th order vanishes, so what we are left with is at least first order in the gradient expansion. That means that if on that we substitute $f_{ij}^{(n)}$, we will have an equation that contains the diagonal elements of the distribution function up to order $(n+1)$.

Since we are interested in first order in the gradients, it is enough to examine the off-diagonal part of the Boltzmann equation in zero-th order, namely

$$\left[f, g_0^{-1} \right]_{ij} = 0. \tag{4.11}$$

Taking into account that g_0^{-1} is diagonal, we get

$$f_{ij}(g_0^{-1})_{jj} - (g_0^{-1})_{ii} f_{ij} = 0, \tag{4.12}$$

$$f_{ij} \left((g_0^{-1})_{ii} - (g_0^{-1})_{jj} \right) = 0. \tag{4.13}$$

For $i \neq j$, the above equation is solved by $f_{ij} = 0$.

As a result, the diagonal elements of the Boltzmann equation, will only contain the diagonal elements of the distribution function f_{ii}. Looking back at eq. (4.8), the commutator in the first term vanishes. For the first anti-commutator we have

$$\frac{i}{2} \left\{ \partial_x f_{ii}, \partial_p g_{0\,ii}^{-1} - i \left[A_p, g_0^{-1} \right]_{ii} \right\}, \tag{4.14}$$

where

$$\left[A_p, g_0^{-1} \right]_{ii} = A_{p\,ij} g_{0\,ji}^{-1} - g_{0\,ij}^{-1} A_{p\,ji} = 0 \tag{4.15}$$

since g_0^{-1} is diagonal. Then we are left with just $i\partial_x f \partial_p g_0^{-1}$, where both f and g_0^{-1} are diagonal. Similarly, the second anti-commutator reduces to $-i\partial_p f \partial_x g_0^{-1}$ resulting in the diagonal elements of the Boltzmann equation to be

$$i \left(\partial_x f \partial_p g_0^{-1} - \partial_p f \partial_x g_0^{1} \right) = 0. \tag{4.16}$$

This is the same as the Boltzmann equation to first order for a single-band system and is meant to describe evolution within one of the bands of the system. However, any Berry phase effects have vanished. This is because we have isolated one band and the Berry phase arises due to the effect of other bands.

4.3   Minimal coupling

In order to get a gauge invariant equation that includes the Berry phase effects, eq. (4.9) hints us to perform a minimal coupling, similar to the case of the magnetic field (see section 3.2). However, in the case of the magnetic field, the gauge field A lives in real space and we performed a minimal coupling on momentum. The Berry connection, however, lives in momentum space, so the minimal coupling has to be performed in real space by introducing a generalized, gauge invariant position

$$\xi^\mu = x^\mu - A_p^\mu. \tag{4.17}$$

Then, same as before, the derivatives appearing in the Boltzmann equation should transform as follows

$$\frac{\partial}{\partial x^\mu} \to \frac{\partial}{\partial \xi^\mu} \tag{4.18}$$

$$\frac{\partial}{\partial p^\mu} \to \frac{\partial}{\partial p^\mu} - \frac{\partial A_p^\nu}{\partial p^\mu} \frac{\partial}{\partial \xi^\nu}. \tag{4.19}$$

Starting from the equation of a single-band to first order

$$\partial_x f \partial_p g_0^{-1} - \partial_p f \partial_x g_0^{-1} = 0 \tag{4.20}$$

and performing the above transformation we obtain

$$\frac{\partial f}{\partial \xi^\mu} \left(\frac{\partial g_0^{-1}}{\partial p^\mu} - \frac{\partial A_p^\nu}{\partial p^\mu} \frac{\partial g_0^{-1}}{\partial \xi^\nu} \right) - \left(\frac{\partial f}{\partial p^\mu} - \frac{\partial f}{\partial \xi^\nu} \frac{\partial A_p^\nu}{\partial p^\mu} \right) \frac{\partial g_0^{-1}}{\partial \xi^\mu} = 0. \tag{4.21}$$

Repeated indices can be renamed leading to

$$\frac{\partial f}{\partial \xi^\mu} \frac{\partial g_0^{-1}}{\partial p^\mu} - \frac{\partial f}{\partial p^\mu} \frac{\partial g_0^{-1}}{\partial \xi^\mu} - \frac{\partial f}{\partial \xi^\mu} \left(\frac{\partial A_p^\nu}{\partial p^\mu} - \frac{\partial A_p^\mu}{\partial p^\nu} \right) \frac{\partial g_0^{-1}}{\partial \xi^\nu} = 0. \tag{4.22}$$

We can now recognize the definition of the Berry curvature in the Boltzmann equation and rewrite

$$\frac{\partial f}{\partial \xi^\mu} \left(\frac{\partial g_0^{-1}}{\partial p^\mu} - \Omega_{\mu\nu} \frac{\partial g_0^{-1}}{\partial \xi^\nu} \right) - \frac{\partial f}{\partial p^\mu} \frac{\partial g_0^{-1}}{\partial \xi^\mu} = 0. \tag{4.23}$$

The Berry curvature appeared in the Boltzmann equation in a similar manner as did the electromagnetic field strength tensor in section 3.2. The implications of this will become apparent in the following section.

For a simple translationally invariant system, its Green's function is given by

$$G_0^{-1} = E\mathbb{1} - H(\mathbf{k}) \tag{4.24}$$

and after diagonalizing

$$g_0^{-1} = E - \varepsilon(\mathbf{k}), \tag{4.25}$$

where $\varepsilon(\mathbf{k})$ is the energy dispersion of each band. Then, after splitting the space-time coordinates, the Boltzmann equation becomes

$$-\frac{\partial f}{\partial t} \frac{\partial g_0^{-1}}{\partial E} + \frac{\partial f}{\partial \xi^i} \left(\frac{\partial g_0^{-1}}{\partial k^i} - \Omega_{ij} \frac{\partial g_0^{-1}}{\partial \xi^j} \right) + \frac{\partial f}{\partial E} \frac{\partial g_0^{-1}}{\partial t} - \frac{\partial f}{\partial k^i} \frac{\partial g_0^{-1}}{\partial \xi^i} = 0. \tag{4.26}$$
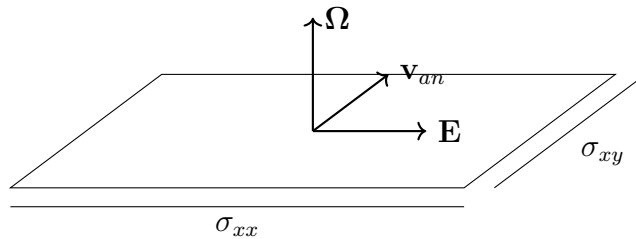
Figure 4.1: The setup for the anomalous Hall effect

When an electric field is added to the system, an extra $e\,\boldsymbol{\xi}\cdot\mathbf{E}$ term is added to the Green's function, so that $\nabla_{\boldsymbol{\xi}}g_0^{-1}=e\mathbf{E}$ and we end up with

$$\partial_t f + \nabla_{\boldsymbol{\xi}} f \cdot (\nabla_{\mathbf{k}}\varepsilon(\mathbf{k}) - e\mathbf{E}\times\boldsymbol{\Omega}) + e\nabla_{\mathbf{k}}f\cdot\mathbf{E} = 0, \qquad (4.27)$$

which is the Boltzmann equation for a multi-band system with translational invariance under the effect of an electric field.

4.4 The anomalous Hall effect

Having derived the Boltzmann equation (4.27), we can compare it with the phenomenological one eq. (1.10). The main observation is that we obtain a velocity term

$$\mathbf{v}(\mathbf{k}) = \nabla_{\mathbf{k}}\varepsilon(\mathbf{k}) - e\mathbf{E}\times\boldsymbol{\Omega}(\mathbf{k}). \qquad (4.28)$$

The first term $\nabla_{\mathbf{k}}\varepsilon(\mathbf{k})$ is attributed to the band dispersion and is present also in single-band systems, as seen in section 3.1. The second term exists due to the Berry curvature, so it appears only in multi-band systems. It goes by the name of anomalous velocity and is perpendicular both to the electric field and the Berry curvature.

In 2-dimensional systems, the Berry curvature will point along the axis perpendicular to the system, say the x-axis. If an electric field is applied along the x-direction, then there will be an anomalous velocity along the y-direction, a sketch of which can be seen in figure 4.1. That, under the right circumstances, has the potential of producing a Hall-like current, where the Berry curvature will act as an effective magnetic field. This phenomenon that a Hall current is observed without a magnetic field is known as the anomalous Hall effect.

In general, when an electric field is applied to a system, the induced current is

$$\mathbf{j} = -e\int\frac{\mathrm{d}\mathbf{k}}{(2\pi)^d}\mathbf{v}(\mathbf{k})f, \qquad (4.29)$$

where d is the dimensionality of the system and f the distribution function. In the case of multi-band systems with anomalous velocity, the current will reduce to

$$\mathbf{j} = -e\int\frac{\mathrm{d}\mathbf{k}}{(2\pi)^d}\nabla_{\mathbf{k}}\varepsilon(\mathbf{k})f + e^2\int\frac{\mathrm{d}\mathbf{k}}{(2\pi)^d}\left(\mathbf{E}\times\boldsymbol{\Omega}\right)f. \qquad (4.30)$$

Let us now look at what happens in the case of two big categories of systems, insulators and metals.

An insulator, or more specifically a band insulator, consists of two or more bands that are separated by a gap. Also, the Fermi energy lies in the gap, meaning that the bands below it are completely filled and the bands above it completely empty. We assume that the electric field is weak enough so that it cannot excite electrons to a higher band. Then, the distribution function is just the equilibrium distribution function, i.e. the Fermi-Dirac distribution. Then the first term vanishes, leaving us with

$$\mathbf{j} = e^2 \sum_n \int \frac{\mathrm{d}\mathbf{k}}{(2\pi)^d} \left(\mathbf{E} \times \mathbf{\Omega} \right) \tag{4.31}$$

where $\sum_n$ denotes the sum over all the filled bands. The conductivity in general can be found from

$$\sigma_{ij} = \frac{\partial j_i}{\partial E_j}. \tag{4.32}$$

Going back to the 2-dimensional case, we get $\sigma_{xx} = 0$, as expected for an insulator, while

$$\sigma_{xy} = e^2 \sum_n \int_{BZ} \frac{\mathrm{d}^2 k}{(2\pi)^2} \mathbf{\Omega}^n. \tag{4.33}$$

We ended up with a Hall conductivity for a band insulator without a magnetic field. The integration is performed over the Brillouin zone, which under periodic boundary conditions and in 2 dimensions is a torus. The integral of the Berry curvature over a closed surface is the Chern number, as we have seen in section 1.3, so we can rewrite

$$\sigma_{xy} = \frac{e^2}{2\pi} \sum_n C^n \tag{4.34}$$

This results in a Hall conductivity that is quantuzed in units of $e^2/2\pi$, which was first shown by Thouless [3]. Summing up, a Hall effect can be observed in a band insulator with a non-zero Chern number. We will look at what these systems can be in the next chapter in the case of graphene.

The other big category of systems with respect to their band structure is metals. In metals, energy bands can cross or overlap, but the main feature is that at least one band is partially filled. Then a weak electric field can excite electrons above the Fermi energy with an infinitesimal energy cost. However, when bands cross, the berry connections are not well-defined. For this reason, we will be concerned with what we described before as a band insulator, but set up the chemical potential such that the Fermi energy runs across one of the bands, leaving it partially filled. In this case the Hall conductivity is

$$\sigma_{xy} = e^2 \sum_n \int_{BZ} \frac{\mathrm{d}^2 k}{(2\pi)^2} \mathbf{\Omega}^n + e^2 \int_{BZ} \frac{\mathrm{d}^2 k}{(2\pi)^2} \mathbf{\Omega}^m f, \tag{4.35}$$

where $\sum_n$ is the sum over all filled bands and m signifies the band that is partially filled. f is the non-equilibrium distribution function, that can be found by solving the Boltzmann equation. This expression for the Hall conductivity means that even if a system has zero Chern number, a Hall current can still be induced due to the partially filled band, the conductivity however, is not quantized.

Chapter 5

Anomalous Hall effect in graphene

In the previous chapter, we saw how Berry phase effects appear in the Boltzmann equation of multi-band systems resulting in the anomalous velocity. This has the potential of inducing a Hall effect. In this chapter we will study under which conditions this is possible. As shown in section 4.4 calculating the Hall conductivity for metals requires knowledge of the distribution, which can be found by solving the Boltzmann equation. However, this is not an easy task, so we will restrict ourselves to insulators. First, we will look at some general properties that have to be obeyed in order to get a Hall current. Then, we will look at graphene as an example, starting from a simple model and increasing the complexity step by step.

5.1 Symmetries of the Berry curvature

We saw in section 4.4 that the Hall conductivity in the case of a band insulator is given by the Chern number, or the integral of the Berry curvature over the Brillouin zone. For simplicity, we will consider a two-band system, with the Fermi energy lying in the gap. Then

$$\sigma_{xy} = e^2 \int_{BZ} \frac{\mathrm{d}^2 k}{(2\pi)^2} \boldsymbol{\Omega}(\mathbf{k}), \tag{5.1}$$

where $\boldsymbol{\Omega}(\mathbf{k})$ is the Berry curvature of the lower band. Since, integration is performed over the Brillouin zone, it useful to examine some symmetries of the Berry curvature.

First, let us see what happens if the system has time-reversal symmetry. we assume the time-reversal operator $\mathcal{T}$ that reverses the arrow of time. Under time-reversal, the momentum changes sign $\mathcal{T}\mathbf{k} = -\mathbf{k}$, as it is proportional to the velocity. However, the position remains invariant $\mathcal{T}\mathbf{r} = \mathbf{r}$. Position and momentum satisfy a commutation relation $[\mathbf{r}, \mathbf{k}] = i\hbar$. Acting on it with the time-reversal operator we get $\mathcal{T}[\mathbf{r}, \mathbf{k}] = -[\mathbf{r}, \mathbf{k}] = -i\hbar$. This leads to $\mathcal{T}i = -i$, which means that time-reversal involves complex conjugation. Having verified that, we can act with time-reversal on the Berry curvature eq. (1.50) where we replace the general parameter $\mathbf{R}$ with momentum $\mathbf{k}$

$$\begin{aligned}
\mathcal{T}\boldsymbol{\Omega}(\mathbf{k}) &= i \left\langle \frac{\partial n(-\mathbf{k})}{\partial k^\nu} \bigg| \frac{\partial n(-\mathbf{k})}{\partial k^\mu} \right\rangle - i \left\langle \frac{\partial n(-\mathbf{k})}{\partial k^\mu} \bigg| \frac{\partial n(-\mathbf{k})}{\partial k^\nu} \right\rangle \\
&= -\boldsymbol{\Omega}(-\mathbf{k}).
\end{aligned} \tag{5.2}$$

If a system has time-reversal invariance, we demand that $\mathcal{T}\boldsymbol{\Omega}(\mathbf{k}) = \boldsymbol{\Omega}(\mathbf{k})$, which means that

$$\boldsymbol{\Omega}(\mathbf{k}) = -\boldsymbol{\Omega}(-\mathbf{k}). \tag{5.3}$$

In other words, the Berry curvature of a time-reversal invariant system is an odd function. We can then expect it to vanish upon integration over the Brillouin zone, leading to zero Hall conductance.

Another important symmetry is spatial inversion. We denote the spatial inversion operator $\mathcal{I}$, which changes the sign of position $\mathcal{I}\mathbf{r} = -\mathbf{r}$. Momentum will also change sign $\mathcal{I}\mathbf{k} = -\mathbf{k}$, which makes their commutator invariant $\mathcal{I}[\mathbf{r}, \mathbf{k}] = [\mathbf{r}, \mathbf{k}]$. Therefore, spatial inversion does not include complex conjugation. Then the Berry curvature will transform as

$$\begin{aligned}\mathcal{I}\boldsymbol{\Omega}(\mathbf{k}) &= i\left\langle\frac{\partial n(-\mathbf{k})}{\partial k^\mu}\bigg|\frac{\partial n(-\mathbf{k})}{\partial k^\nu}\right\rangle - i\left\langle\frac{\partial n(-\mathbf{k})}{\partial k^\nu}\bigg|\frac{\partial n(-\mathbf{k})}{\partial k^\mu}\right\rangle \\ &= \boldsymbol{\Omega}(-\mathbf{k}).\end{aligned} \tag{5.4}$$

In a system with spatial inversion symmetry $\mathcal{I}\boldsymbol{\Omega}(\mathbf{k}) = \boldsymbol{\Omega}(\mathbf{k})$, so

$$\boldsymbol{\Omega}(\mathbf{k}) = \boldsymbol{\Omega}(-\mathbf{k}) \tag{5.5}$$

the Berry curvature is an even function.

Combining eqs. (5.3) and (5.5), we can deduce that, if a system remains invariant under both time-reversal and spatial inversion, then its Berry curvature vanishes identically for all $\mathbf{k}$.

5.2 Tight-binding model for graphene

Graphene has the structure of a honeycomb lattice, consisting of two sublattices A (blue) and B (red), that can be seen in figure 5.1. A simple description can be given by a tight-binding Hamiltonian

$$H = -t\sum_{\langle ij\rangle}\left(a^\dagger(\mathbf{x}_i)b(\mathbf{x}_j) + h.c.\right) \tag{5.6}$$

where $a^\dagger$, a and $b^\dagger$, b are fermionic creation and annihilation operators for the sublattices A and B respectively, t is the real hopping amplitude and $\langle ij\rangle$ denotes nearest neighbours. As seen in figure 5.1, every lattice site has three neighbours denoted by the vectors $\mathbf{a}_1 = (0, 1)$, $\mathbf{a}_2 = (-\sqrt{3}/2, -1/2)$ and $\mathbf{a}_3 = (\sqrt{3}/2, -1/2)$.

The system is translationally invariant, so the Wigner transformation of the Hamiltonian is equivalent to Fourier transforming the creation and annihilation operators. Then we can write

$$H = \begin{pmatrix} a^\dagger(\mathbf{k}) & b^\dagger(\mathbf{k}) \end{pmatrix} H(\mathbf{k}) \begin{pmatrix} a(\mathbf{k}) \\ b(\mathbf{k}) \end{pmatrix} \tag{5.7}$$

where

$$H(\mathbf{k}) = \begin{pmatrix} 0 & t\sum_{i=1}^{3} e^{-i\mathbf{k}\cdot\mathbf{a}_i} \\ t\sum_{i=1}^{3} e^{i\mathbf{k}\cdot\mathbf{a}_i} & 0 \end{pmatrix}, \tag{5.8}$$
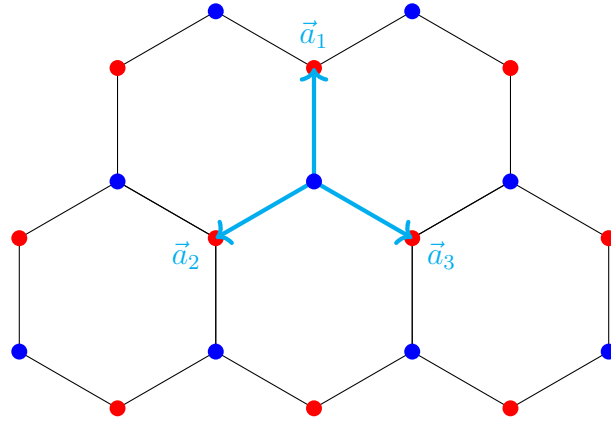
Figure 5.1: Honeycomb lattice structure of graphene, consisting of two sublattices A (blue) and B (red). $\vec{a}_1$, $\vec{a}_2$ and $\vec{a}_3$ signify the nearest neighbours.
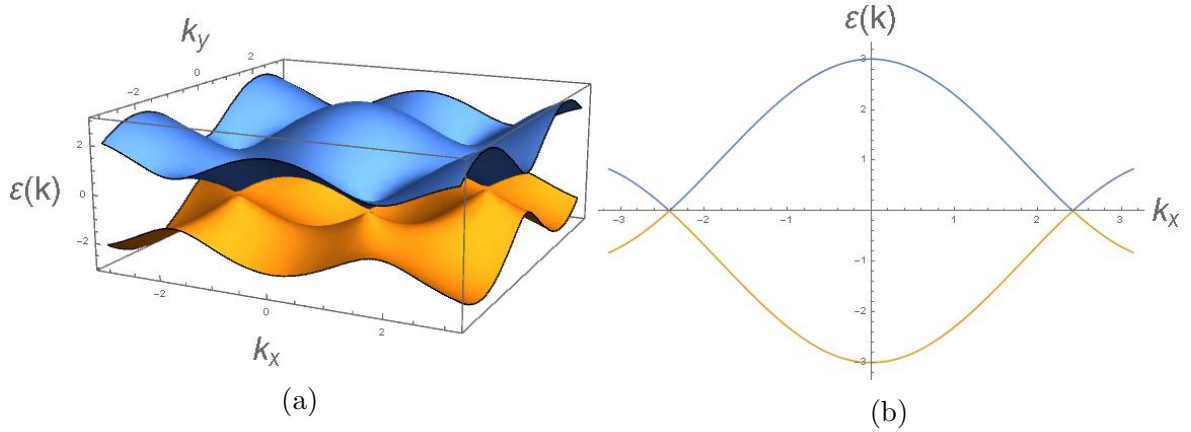

(a)

(b)

Figure 5.2: The energy spectrum of the tight-binding model for graphene (a) over the full Brillouin zone and (b) over the Brillouin zone for $k_y = 0$.

or with respect to Pauli matrices

$$H(\mathbf{k}) = t \sum_{i=1}^{3} \left[\cos\left(\mathbf{k} \cdot \mathbf{a}_i\right) \sigma_x + \sin\left(\mathbf{k} \cdot \mathbf{a}_i\right) \sigma_y \right]. \tag{5.9}$$

From now on, we will simply write $\sum_i$ and the summation will always run from 1 to 3, unless stated otherwise.

The energy spectrum of this Hamiltonian is

$$\varepsilon(\mathbf{k}) = \pm t \sqrt{\sum_{ij} e^{-i\mathbf{k}(\mathbf{a}_i - \mathbf{a}_j)}}, \tag{5.10}$$

or

$$\varepsilon(\mathbf{k}) = \pm t \sqrt{3 + 2\cos\left(\sqrt{3}k_x\right) + 4\cos\left(\frac{\sqrt{3}}{2}k_x\right)\cos\left(\frac{3}{2}k_y\right)} \tag{5.11}$$

and is shown in figure 5.2. We can see that the spectrum consists of two bands that touch for $\varepsilon(\mathbf{k}) = 0$. This happens at the two corners of the Brillouin zone, $\mathbf{K} = (4\pi/3\sqrt{3})$ and $\mathbf{K}' = (-4\pi/3\sqrt{3})$, that are known as the valleys of graphene. Close to these points the spectrum is linear and the Hamiltonian can be approximated by a Dirac Hamiltonian. For this reason, they are also called Dirac points.

In this simple tight-binding model for graphene, the two sublattices are treated as equivalent, so that they can be exchanged. This means that the Hamiltonian has spatial inversion symmetry and, on top of that, it also possesses time reversal symmetry. Then, according to the discussion in section 5.1, we expect the Berry curvature to vanish across the Brillouin zone, apart from the points that the two bands meet, where it will diverge giving rise to monopoles with opposite "charge", similar to the example of a spin in a magnetic field.

5.3 Graphene with a mass term

In an attempt to get a non-trivial Berry curvature, we will take the model one level of complexity higher by breaking the spatial inversion symmetry. This was done by Semenoff [23] by including opposite "mass" terms for the two sublattices, or, in other words, coupling a mass term to the third Pauli matrix. The resulting Hamiltonian is

$$H(\mathbf{k}) = t \sum_i \left[\cos\left(\mathbf{k} \cdot \mathbf{a}_i\right) \sigma_x + \sin\left(\mathbf{k} \cdot \mathbf{a}_i\right) \sigma_y \right] + M\sigma_z. \tag{5.12}$$

or explicitly

$$H(\mathbf{k}) = \begin{pmatrix} M & t \sum_i e^{-i\mathbf{k} \cdot \mathbf{a}_i} \\ t \sum_i e^{i\mathbf{k} \cdot \mathbf{a}_i} & -M \end{pmatrix}. \tag{5.13}$$

This Hamiltonian has energy spectrum

$$\varepsilon_\pm(\mathbf{k}) = \pm\sqrt{M^2 + t^2 \sum_{ij} e^{-i\mathbf{k} \cdot (\mathbf{a}_i - \mathbf{a}_j)}} \tag{5.14}$$

which can be seen in figures 5.3a and 5.3b. The bands now do not touch and the gap between the acquires its minimum value $2M$ at the Dirac points.

The eigenstates of the Hamiltonian are

$$|\psi_\pm(\mathbf{k})\rangle = \frac{1}{\sqrt{2}N_\pm} \begin{pmatrix} M \pm \sqrt{M^2 + t^2 \sum_{ij} e^{-i\mathbf{k} \cdot (\mathbf{a}_i - \mathbf{a}_j)}} \\ t \sum_i e^{i\mathbf{k} \cdot \mathbf{a}_i} \end{pmatrix} \tag{5.15}$$

where $\pm$ refers to the two bands and $N_\pm$ is a factor coming from the normalization of the eigenstates and is defined as

$$N_\pm^2 = \left(\frac{M}{2} \pm \sqrt{M^2 + t^2 \sum_{ij} e^{-i\mathbf{k} \cdot (\mathbf{a}_i - \mathbf{a}_j)}} \right)^2 - \frac{M^2}{4}. \tag{5.16}$$
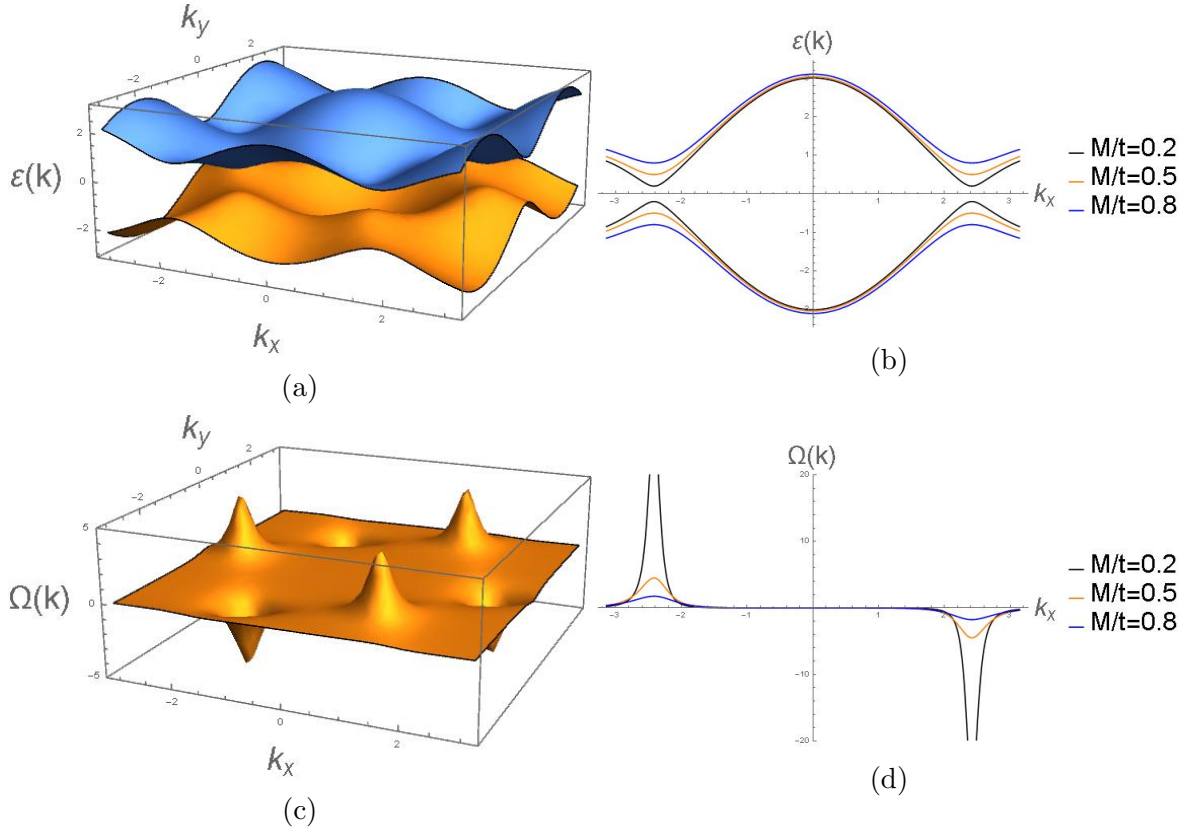
Figure 5.3: Plots for graphene with a mass term: (a) spectrum, (b) spectrum for $k_y = 0$ and different values of M/t, (c) Berry curvature of the lower band and (d) Berry curvature of the lower band for $k_y = 0$ and different values of M/t.

Details about the diagonalization procedure can be found in Appendix B.1.

We will now assume that the Fermi energy lies in the gap of the spectrum, so that the system is an insulator, and compute the Berry curvature for the lower band. The Berry connection is given by

$$\mathbf{A_k^-} = i \langle \psi_-(\mathbf{k})| \nabla_{\mathbf{k}} |\psi_-(\mathbf{k}) \rangle \tag{5.17}$$

which, for our model, results in the following two components

$$A_{k_x}^- = -\frac{\sqrt{3}t^2}{2N_-^2} \sin\left(\frac{\sqrt{3}}{2}k_x\right) \sin\left(\frac{3}{2}k_y\right) \tag{5.18}$$

and

$$A_{k_y}^- = \frac{t^2}{2N_-^2} \left[\cos\left(\sqrt{3}k_x\right) - \cos\left(\frac{\sqrt{3}}{2}k_x\right)\cos\left(\frac{3}{2}k_y\right)\right]. \tag{5.19}$$

The Berry curvature is then a vector pointing in the direction perpendicular to the two-dimensional Brillouin zone

$$\mathbf{\Omega}^- = \Omega_{k_x k_y}^- = \frac{\partial A_{k_y}^-}{\partial k_x} - \frac{\partial A_{k_x}^-}{\partial k_y}, \tag{5.20}$$

which in our model is

$$\mathbf{\Omega}^-(\mathbf{k}) = \frac{\sqrt{3}Mt^2 \sin\left(\frac{\sqrt{3}}{2}k_x\right)\left[\cos\left(\frac{\sqrt{3}}{2}k_x\right) - \cos\left(\frac{3}{2}k_y\right)\right]}{2\left\{M^2 + 3t^2 + 2t^2\left[\cos\left(\sqrt{3}k_x\right) + 2\cos\left(\frac{\sqrt{3}}{2}k_x\right)\cos\left(\frac{3}{2}k_y\right)\right]\right\}^{3/2}} \tag{5.21}$$

and can be seen in figure 5.3c. We can observe that the Berry curvature is highly concentrated around the Dirac points and spreads out as the energy gap becomes larger, which is depicted in figures 5.3b and 5.3d. This is a direct result of eq. (1.53).

It is also worth noticing that the Berry curvatures around the two Dirac points have opposite signs, due to the remaining time-reversal symmetry. This raises suspicions about the total Hall current. Indeed, as explained in section 4.4, the Hall conductivity of an insulator is given by integrating the Berry curvature of the lower band over the Brillouin zone, which in this case

$$\sigma_{xy} = e^2 \int_{BZ} \frac{\mathrm{d}^2\mathbf{k}}{(2\pi)^2} \, \mathbf{\Omega}^-(\mathbf{k}) = 0. \tag{5.22}$$

As a result, we cannot observe an anomalous Hall effect in this model, when it is an insulator. This was expected as, following the discussion in section 5.1, the Berry curvature in a system with time-reversal invariance is an odd function. Then it follows that is should vanish upon integration over the Brillouin zone.

However, if we force the Fermi energy to cross the upper band, the system becomes a metal and its behaviour changes. The Hall conductivity will then be given by eq. (4.35). Since it vanishes in the lower band, only the second term will contribute, namely

$$\sigma_{xy} = e^2 \int_{BZ} \frac{\mathrm{d}^2\mathbf{k}}{(2\pi)^2} \, \mathbf{\Omega}^+(\mathbf{k})f, \tag{5.23}$$

where $\mathbf{\Omega}^+(\mathbf{k})$ is the Berry curvature of the upper band and f is the non-equilibrium distribution function. $\mathbf{\Omega}^+(\mathbf{k})$ will also change sign between the two Dirac points, but since is it weighted by the non-equilibrium distribution function, the overall integral will not vanish and a Hall current will be present. We will not do such a calculation though.

5.4 Haldane model

We saw that breaking spatial inversion symmetry in graphene is not enough to induce a Hall current when the Fermi energy lies in the band gap. The next step would be to also break time-reversal symmetry which was done by Haldane [2]. It was done by introducing a complex second-nearest neighbour hopping between sites of the same sublattice. This breaks time-reversal invariance because hopping from one site to another has amplitude t, but hopping back has amplitude t^*. We can choose it so that if the hopping has a clockwise direction it will be $t_2 e^{i\phi}$ and $t_2 e^{-i\phi}$ for counter-clockwise. Each lattice site has six second-nearest neighbours, however, we will parametrize the Hamiltonian using only three of those, the ones that have a hopping with a clockwise direction. They are defined by the vectors $\mathbf{b}_1 = \mathbf{a}_2 - \mathbf{a}_3$, $\mathbf{b}_2 = \mathbf{a}_3 - \mathbf{a}_1$ and $\mathbf{b}_3 = \mathbf{a}_1 - \mathbf{a}_2$,
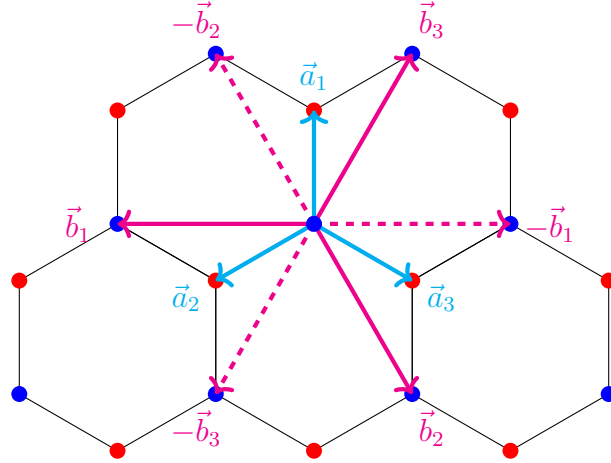
Figure 5.4: Honeycomb lattice structure of graphene, consisting of two sublattices A (blue) and B (red). $\vec{a}_i$ (light blue) signify the nearest neighbours. $\vec{b}_i$ (solid pink) are the second-nearest neighbours with hopping $t_2 e^{i\phi}$, while $-\vec{b}_i$ (dashed pink) those with $t_2 e^{-i\phi}$.

or $\mathbf{b}_1 = (-\sqrt{3}, 0)$, $\mathbf{b}_2 = (\sqrt{3}/2, -3/2)$, $\mathbf{b}_3 = (\sqrt{3}/2, 3/2)$, and can be seen in figure 5.4 as the pink solid vectors. With all that into account, the Hamiltonian is

$$H(\mathbf{k}) = \begin{pmatrix} 2t_2 \sum_i \cos\left(\phi + \mathbf{k} \cdot \mathbf{b}_i\right) + M & t_1 \sum_i e^{-i\mathbf{k} \cdot \mathbf{a}_i} \\ t_1 \sum_i e^{i\mathbf{k} \cdot \mathbf{a}_i} & 2t_2 \sum_i \cos\left(\phi - \mathbf{k} \cdot \mathbf{b}_i\right) - M \end{pmatrix} \quad (5.24)$$

or

$$H(\mathbf{k}) = 2t_2 \cos\phi \sum_i \cos\left(\mathbf{k} \cdot \mathbf{b}_i\right) \mathbb{1} + t_1 \sum_i \left[\cos\left(\mathbf{k} \cdot \mathbf{a}_i\right)\sigma_x + \sin\left(\mathbf{k} \cdot \mathbf{a}_i\right)\sigma_y\right]$$
$$+ \left[M - 2t_2 \sin\phi \sum_i \sin\left(\mathbf{k} \cdot \mathbf{b}_i\right)\right]\sigma_z. \quad (5.25)$$

The spectrum of this Hamiltonian is

$$\varepsilon_{\pm}(\mathbf{k}) = 2t_2 \cos\phi \sum_i \cos\left(\mathbf{k} \cdot \mathbf{b}_i\right) \pm \sqrt{\Delta^2(\mathbf{k}) + t_1^2 \left(3 + 2\sum_i \cos\left(\mathbf{k} \cdot \mathbf{b}_i\right)\right)}, \quad (5.26)$$

where

$$\Delta(\mathbf{k}) = M - 2t_2 \sin\phi \sum_i \sin\left(\mathbf{k} \cdot \mathbf{b}_i\right). \quad (5.27)$$

This new term $\Delta(\mathbf{k})$ plays the role that the mass used to play in the previous model, in the sense that it measures the gap between the bands. The gap can still only close at the Dirac points when $\Delta(\mathbf{k}) = 0$. At those points

$$\Delta(\mathbf{K}) = M - 3\sqrt{3}\, t_2 \sin\phi \quad (5.28)$$

and

$$\Delta(\mathbf{K}') = M + 3\sqrt{3}\, t_2 \sin\phi. \tag{5.29}$$

This means that the gap can only close for

$$M = \pm 3\sqrt{3}\, t_2 \sin\phi. \tag{5.30}$$

In figure 5.5a we can see the spectrum for different values of the parameters. In the region where $|M/t_2| > 3\sqrt{3}|\sin\phi|$, it shows a similar behaviour to the model with time-reversal symmetry. However, when $|M/t_2| < 3\sqrt{3}|\sin\phi|$ the gap on one of the Dirac points opens up significantly.

The eigenstates of the Hamiltonian can be expressed as

$$|\psi_\pm(\mathbf{k})\rangle = \frac{1}{\sqrt{2}N_\pm} \left(\begin{array}{c} \Delta(\mathbf{k}) \pm \sqrt{\Delta^2(\mathbf{k}) + t_1^2\left(3 + 2\sum_i \cos(\mathbf{k}\cdot\mathbf{b}_i)\right)} \\ t_1\sum_i e^{i\mathbf{k}\cdot\mathbf{a}_i} \end{array} \right), \tag{5.31}$$

where

$$N_\pm^2 = \left(\frac{\Delta(\mathbf{k})}{2} \pm \sqrt{\Delta^2(\mathbf{k}) + t^2\sum_{ij} e^{-i\mathbf{k}\cdot(\mathbf{a}_i - \mathbf{a}_j)}} \right)^2 - \frac{\Delta^2(\mathbf{k})}{4}. \tag{5.32}$$

Details of this derivation can be found in Appendix B.2. In the following, we will study the case when there is a clear gap in the spectrum and the bands never overlap, which is true for $|t_2/t_1| < 1/3$. We will also assume that the Fermi energy lies in the gap between the bands, so we will be concerned with the properties of the lower band. For that, we can calculate the Berry curvature as

$$\mathbf{\Omega}_-(\mathbf{k}) = i\left\langle \frac{\partial\psi_-(\mathbf{k})}{\partial k_x} \middle| \frac{\partial\psi_-(\mathbf{k})}{\partial k_y} \right\rangle - i\left\langle \frac{\partial\psi_-(\mathbf{k})}{\partial k_y} \middle| \frac{\partial\psi_-(\mathbf{k})}{\partial k_x} \right\rangle \tag{5.33}$$

and the result and can be seen in figures 5.5d and 5.5b for a few different values of the parameters. When $|M/t_2| > 3\sqrt{3}|\sin\phi|$, the situation is similar to the previous model of graphene with time-reversal symmetry. The Berry curvature is concentrated around the two Dirac points with opposite sign for each one, and vanishes upon integration over the Brillouin zone. In contrast, when $|M/t_2| < 3\sqrt{3}|\sin\phi|$, the Berry curvature possesses a unique positive or negative sign across the Brillouin zone. It is also worth mentioning that it is highly concentrated around one of the Dirac points, where the gap is still small, and quite spread out around the other, where the gap is larger. Integrating over the Brillouin zone, we get the Chern number in the following situations

$$C = \frac{1}{2\pi}\int_{BZ} \mathrm{d}^2\mathbf{k}\,\mathbf{\Omega}_-(\mathbf{k}) = \begin{cases} -1, & |M/t_2| < 3\sqrt{3}|\sin\phi|, \quad -\pi < \phi < 0 \\ 0, & |M/t_2| > 3\sqrt{3}|\sin\phi| \\ +1, & |M/t_2| < 3\sqrt{3}|\sin\phi|, \quad\ \ 0 < \phi < \pi \end{cases} \tag{5.34}$$

that can be summed up in a phase diagram in figure 5.5c. As a result, an anomalous Hall effect can be observed for parameters in the domain $|M/t_2| < 3\sqrt{3}|\sin\phi|$, with
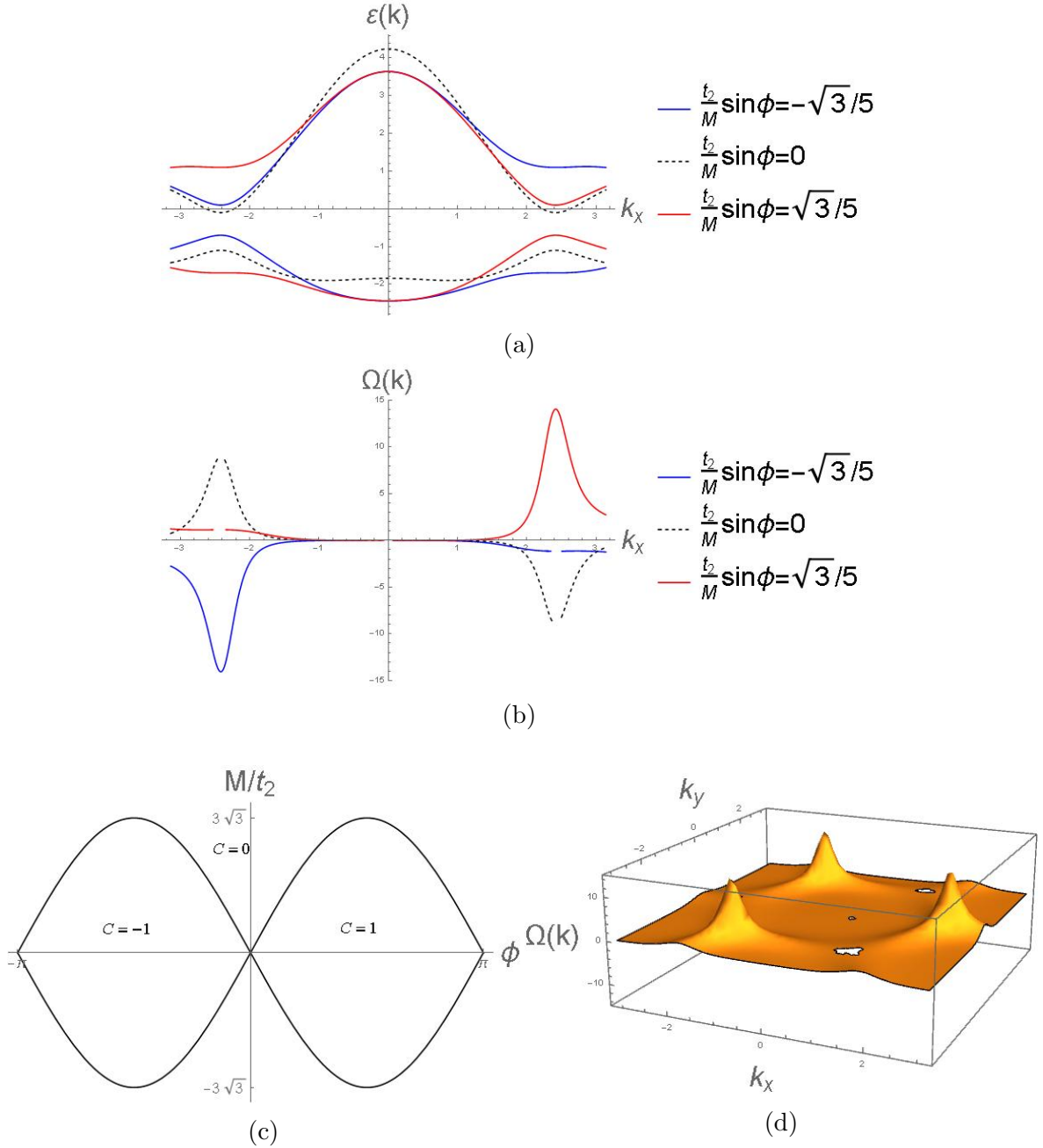
(a)

(b)

(c)

(d)

Figure 5.5: Plots for Haldane's model for graphene: (a) spectrum and (b) Berry curvature of the lower band for $k_y = 0$ and different values of the parameters, (c) phase diagram and (d) 3D plot of the Berry curvature of the lower band in the region of the phase diagram where $C = +1$.

Hall conductivity

$$\sigma_{xy} = \begin{cases} -\dfrac{e^2}{2\pi}, & -\pi < \phi < 0 \\[2mm] +\dfrac{e^2}{2\pi}, & 0 < \phi < \pi. \end{cases} \tag{5.35}$$

Chapter 6

Open problems

In the previous chapters we have studied how the Berry phase effects in momentum space enter the Boltzmann equation and their implications on electronic transport. In this chapter, possible extensions to this problem will be presented, that in one way or another remain unresolved. The common feature of these problems is that they combine the Berry phase with other phenomena, proving that interplay between different phenomena is not a trivial task in physics. First, we will add disorder in a multi-band system, then a magnetic field, and finally we will attempt to study a system that exhibits a Berry phase in both momentum and real space.

6.1 Disordered multi-band systems

As a first extension to the problems already studied, we will attempt to add disorder to a multi-band system and derive the Boltzmann equation. When we apply an electric field, the Berry curvature will enter the Boltzmann equation of a multi-band system, resulting in an anomalous velocity and a Hall current. Whenever there is a current in a disordered system, electrons scatter with impurities, which tend to relax the system towards its equilibrium state. Therefore, we would like to examine if there is any interplay between the Berry phase and disorder.

Our starting point is the the quantum Boltzmann equation with collisions

$$\left[f, G_0^{-1}\right]^\star = \Sigma^K - \left(\Sigma^R \star f - f \star \Sigma^A\right) \tag{6.1}$$

where all quantities involved in this equation are matrices. Similar to section 4.1, we will act on the Boltzmann equation with the unitary transformation that diagonalizes the Hamiltonian

$$U^\dagger \left[f, G_0^{-1}\right]^\star U = U^\dagger \Sigma^K U - U^\dagger \left(\Sigma^R \star f - f \star \Sigma^A\right) U. \tag{6.2}$$

Acting on the Green's function $U^\dagger G_0^{-1} U = g_0^{-1}$ makes it diagonal. When averaging over disorder $\Sigma(x, p) = \int \mathrm{d}^d q/(2\pi)^d \, G_0(x, q)$, so as a result, the self-energies $U^\dagger \Sigma U = \sigma$ also become diagonal. However, the distribution function $U^\dagger f U = \tilde{f}$ does not. In the

following we will rename $\tilde{f}$ back to f and rewrite the Boltzmann equation as

$$U^\dagger \left[UfU^\dagger, Ug_0^{-1}U^\dagger \right]^\star U = \sigma^K - U^\dagger \Big(\left(U\sigma^R U^\dagger \right) \star \left(UfU^\dagger \right)$$
$$- \left(UfU^\dagger \right) \star \left(U\sigma^A U^\dagger \right) \Big) U. \tag{6.3}$$

Now the gradient expansion can be performed up to first order, resulting in

$$\left[f, \left(g_0^{-1} - \operatorname{Re}\sigma^R \right) \right] + \frac{i}{2} \left\{ \partial_x f, \partial_p \left(g_0^{-1} - \operatorname{Re}\sigma^R \right) - i \left[A_p, g_0^{-1} - \operatorname{Re}\sigma^R \right] \right\}$$
$$- \frac{i}{2} \left\{ \partial_p f - i \left[A_p, f \right], \partial_x \left(g_0^{-1} - \operatorname{Re}\sigma^R \right) \right\} = \sigma^K - \left(\sigma^R f - f\sigma^A \right), \tag{6.4}$$

where A_p is the Berry connection defined as $A_p = iU^\dagger \partial_p U$. We notice that the berry connection appears only in the kinetic term, where the Green's function has become renormalized by a factor $\operatorname{Re}\sigma^R$.

As explained in section 4.1, we are interested in the diagonal elements of the Boltzmann equation. But first, we have to solve the off-diagonals for the off-diagonal terms of the distribution function f_{ij}. It is sufficient to only look at the zero-th order terms, namely

$$f_{ij} \left(g_0^{-1} - \operatorname{Re}\sigma^R \right)_{jj} - \left(g_0^{-1} - \operatorname{Re}\sigma^R \right)_{ii} f_{ij} = - \left(\sigma_{ii}^R f_{ij} - f_{ij}\sigma_{jj}^A \right) \tag{6.5}$$

or

$$f_{ij} \left(\left(g_0^{-1} - \operatorname{Re}\sigma^R \right)_{jj} - \left(g_0^{-1} - \operatorname{Re}\sigma^R \right)_{ii} \right) = f_{ij} \left(\sigma_{jj}^A - \sigma_{ii}^R \right). \tag{6.6}$$

For $i \neq j$, this is solved by $f_{ij} = 0$. Substituting this into the diagonals of the Boltzmann equation, we are left with

$$\partial_x f \partial_p \left(g_0^{-1} - \operatorname{Re}\sigma^R \right) - \partial_p f \partial_x \left(g_0^{-1} - \operatorname{Re}\sigma^R \right) = -i\sigma^K - 2f\operatorname{Im}\sigma^R, \tag{6.7}$$

which is the same as of r a single-band system with disorder and the Berry phase has been decoupled.

In order to include the Berry phase, we will perform minimal coupling in real space, as in section 4.3, given by

$$x^\mu \to \xi^\mu = x^\mu - A_p^\mu. \tag{6.8}$$

Therefore, derivatives present in the Boltzmann equation will transform as

$$\frac{\partial}{\partial x^\mu} \to \frac{\partial}{\partial \xi^\mu} \tag{6.9}$$

$$\frac{\partial}{\partial p^\mu} \to \frac{\partial}{\partial p^\mu} - \frac{\partial A_p^\nu}{\partial p^\mu} \frac{\partial}{\partial \xi^\nu}. \tag{6.10}$$

When this transformation is applied to the Boltzmann equation, it affects the kinetic term resulting in

$$\frac{\partial f}{\partial \xi^\mu} \left(\frac{\partial}{\partial p^\mu} \left(g_0^{-1} - \operatorname{Re}\sigma^R \right) - \Omega_{\mu\nu} \frac{\partial}{\partial \xi^\nu} \left(g_0^{-1} - \operatorname{Re}\sigma^R \right) \right)$$
$$- \frac{\partial f}{\partial p^\mu} \frac{\partial}{\partial \xi^\mu} \left(g_0^{-1} - \operatorname{Re}\sigma^R \right) = -i\sigma^K - 2f\operatorname{Im}\sigma^R. \tag{6.11}$$

The Berry curvature has appeared as in the case without disorder, with the difference that the Green's function is renormalized by the self-energies.

Let us look at the collision integral now. As explained previously, the disorder averaged self-energy in second order of perturbation theory is

$$\sigma(t, \mathbf{r}, E, \mathbf{k}) = \int \frac{\mathrm{d}^d q}{(2\pi)^d} \, g_0(t, \mathbf{r}, E, \mathbf{q}) \tag{6.12}$$

for the retarded, advanced or Keldysh components. Now, there are two possibilities. The first one is that the above remains unchanged and we can continue to express the collision integral in the same way as for the single-band case. This would mean that the Berry phase and disorder are two independent effects that do not affect each other. The other possibility is that, upon performing the minimal coupling, $\int \mathrm{d}^d q$ will transform. Potentially, the right transformation could create terms involving the Berry curvature in the collision integral. That would mean that the Berry phase and disorder are not independent, but there is an interplay between them. However, the question remains open and we do not know yet if there is any interplay between the two phenomena.

6.2 A multi-band system in a magnetic field

We have seen that the Berry curvature can act in a similar manner to a magnetic field, to the point that it can cause a Hall effect. The question that naturally arises is whether the Berry curvature and the magnetic field behave independently, each one creating a Hall current that are simply added for the combined effect, or if there is an interplay between them, each one of them affecting the system's response to the other. Both phenomena are formulated by a gauge field. The question can then be translated as whether the two gauge fields couple to each other or not.

As we have seen in section 4.3, we can include the Berry phase effects present in a multi-band system into the Boltzmann equation via minimal coupling in position space, while a magnetic field enters the Boltzmann equation via minimal coupling in momentum space, as seen in section 3.2. Reasonably, the first thought of including both effects would be to perform both substitutions at the same time

$$x^\mu \to \xi^\mu = x^\mu - A_\Pi^\mu \tag{6.13}$$
$$p^\mu \to \Pi^\mu = p^\mu + e A_e^\mu, \tag{6.14}$$

where A_Π in the Berry connection and A_e the electromagnetic gauge field. It is important to notice that the gauge fields now depend on the new variables, namely $A_\Pi^\mu = A_\Pi^\mu(\Pi^\nu)$ and $A_e^\mu = A_e^\mu(\xi^\nu)$. This leads to the following transformation for the derivatives

$$\frac{\partial}{\partial x^\mu} \to \frac{\partial}{\partial \xi^\mu} + e \frac{\partial A_e^\nu}{\partial \xi^\mu} \frac{\partial}{\partial \Pi^\nu} \tag{6.15}$$

$$\frac{\partial}{\partial p^\mu} \to \frac{\partial}{\partial \Pi^\mu} - \frac{\partial A_\Pi^\nu}{\partial \Pi^\mu} \frac{\partial}{\partial \xi^\nu} \tag{6.16}$$

Our starting point is again the diagonal elements of the quantum Boltzmann equation to first order in the gradient expansion

$$\partial_x f \partial_p g_0^{-1} - \partial_p f \partial_x g_0^{-1} = 0. \tag{6.17}$$

Applying the above transformations we get

$$\left(\frac{\partial f}{\partial \xi^\mu} + e \frac{\partial f}{\partial \Pi^\nu} \frac{\partial A_e^\nu}{\partial \xi^\mu} \right) \left(\frac{\partial g_0^{-1}}{\partial \Pi^\mu} - \frac{\partial A_\Pi^\lambda}{\partial \Pi^\mu} \frac{\partial g_0^{-1}}{\partial \xi^\lambda} \right)$$
$$- \left(\frac{\partial f}{\partial \Pi^\mu} - \frac{\partial f}{\partial \xi^\nu} \frac{\partial A_\Pi^\nu}{\partial \Pi^\mu} \right) \left(\frac{\partial g_0^{-1}}{\partial \xi^\mu} + e \frac{\partial A_e^\lambda}{\partial \xi^\mu} \frac{\partial g_0^{-1}}{\partial \Pi^\lambda} \right) = 0. \tag{6.18}$$

We can rename some repeated indices and rearrange the terms to acquire a more convenient form

$$\frac{\partial f}{\partial \xi^\mu} \left(\frac{\partial g_0^{-1}}{\partial \Pi^\mu} - \frac{\partial A_\Pi^\nu}{\partial \Pi^\mu} \frac{\partial g_0^{-1}}{\partial \xi^\nu} + \frac{\partial A_\Pi^\mu}{\partial \Pi^\nu} \frac{\partial g_0^{-1}}{\partial \xi^\nu} + e \frac{\partial A_\Pi^\mu}{\partial \Pi^\lambda} \frac{\partial A_e^\nu}{\partial \xi^\lambda} \frac{\partial g_0^{-1}}{\partial \Pi^\nu} \right)$$
$$- \frac{\partial f}{\partial \Pi^\mu} \left(\frac{\partial g_0^{-1}}{\partial \xi^\mu} + e \frac{\partial A_e^\nu}{\partial \xi^\mu} \frac{\partial g_0^{-1}}{\partial \Pi^\nu} - e \frac{\partial A_e^\mu}{\partial \xi^\nu} \frac{\partial g_0^{-1}}{\partial \Pi^\nu} + e \frac{\partial A_e^\mu}{\partial \xi^\lambda} \frac{\partial A_\Pi^\nu}{\partial \Pi^\lambda} \frac{\partial g_0^{-1}}{\partial \xi^\nu} \right) = 0, \tag{6.19}$$

where we can identify the electromagnetic field strength and the Berry curvature and end up with

$$\frac{\partial f}{\partial \xi^\mu} \left(\frac{\partial g_0^{-1}}{\partial \Pi^\mu} - \Omega_{\mu\nu} \frac{\partial g_0^{-1}}{\partial \xi^\nu} + e \frac{\partial A_\Pi^\mu}{\partial \Pi^\lambda} \frac{\partial A_e^\nu}{\partial \xi^\lambda} \frac{\partial g_0^{-1}}{\partial \Pi^\nu} \right)$$
$$- \frac{\partial f}{\partial \Pi^\mu} \left(\frac{\partial g_0^{-1}}{\partial \xi^\mu} + e F_{\mu\nu} \frac{\partial g_0^{-1}}{\partial \Pi^\nu} + e \frac{\partial A_e^\mu}{\partial \xi^\lambda} \frac{\partial A_\Pi^\nu}{\partial \Pi^\lambda} \frac{\partial g_0^{-1}}{\partial \xi^\nu} \right) = 0. \tag{6.20}$$

We observe that the electromagnetic field strength and the Berry curvature enter the Boltzmann equation independently and give rise to the Lorentz force and the anomalous velocity respectively. However, two new terms enter the equation, namely

$$e \frac{\partial A_\Pi^\mu}{\partial \Pi^\lambda} \frac{\partial A_e^\nu}{\partial \xi^\lambda} \frac{\partial g_0^{-1}}{\partial \Pi^\nu} \tag{6.21}$$

and

$$e \frac{\partial A_e^\mu}{\partial \xi^\lambda} \frac{\partial A_\Pi^\nu}{\partial \Pi^\lambda} \frac{\partial g_0^{-1}}{\partial \xi^\nu} \tag{6.22}$$

These terms seem to couple the two fields together, however, they are not gauge invariant. This causes a problem because, eventually, we would like to associate terms of the Boltzmann equation with physical observables.

The problem has been treated phenomenologically and the result is a set of two coupled equations of motion. Intuitively, an interplay of the two effects is expected, since the Berry phase is caused by a non-trivial band structure and the magnetic field changes the system's band structure. A modified minimal coupling that includes extra terms that couple the two gauge fields was proposed by Chang and Niu [24]. However, within our formulation, it has only managed to complicate the problem and create even more gauge-dependent terms. An alternative treatment involving the

Boltzmann equation has been done by Son and Yamamoto [25]. It is based on the fact that, when both the Berry curvature and a magnetic field are involved, the phase space is modified resulting to a modification in Liouville's theorem. The result is a Boltzmann equation that couples the Berry curvature with the magnetic field and is gauge invariant. However, it is still not clear how our approach could be modified to recreate these results.

6.3 Berry curvature in momentum and in real space

Surprisingly, some complications that are present in the previous problem could be resolved in a seemingly more complicated problem. That is, to replace the magnetic field with a Berry curvature in real space. Again, there are two gauge fields invloved, but the extra complication is due to the fact that now both of them depend on both variables of the phase space. On the other hand, this problem is simpler with regards to the nature of the two phenomena. Both gauge fields originate from diagonalizing the Hamiltonian and can be even viewed as components of the same field. They both stem from intrinsic properties of the system, while the magnetic field is an external field that acts on the system.

In order for a system to have a Berry curvature both in momentum and in real space, it has to be described by a Hamiltonian with a non-trivial matrix structure both in momentum and in real space. A Hamiltonian like that breaks translational invariance. An example can be a simple two band system that also contains a spin texture. The spin texture can be formulated by the local magnetization coupled to the Pauli matrices. We can also allow it to evolve in time, so that the Hamiltonian is

$$H(t, \mathbf{r}, \mathbf{k}) = h_0(\mathbf{k})\mathbb{1} + \mathbf{h}(\mathbf{k}) \cdot \boldsymbol{\sigma} + \mathbf{M}(t, \mathbf{r}) \cdot \boldsymbol{\sigma} \tag{6.23}$$

In general, a Hamiltonian like that is diagonalized by a unitary matrix $U(x, p)$ that depends on both coordinates. Usually, the Hamiltonians that we are interested in do not contain an explicit energy dependence, but for notational convenience we will use the 4-momentum p instead of $\mathbf{k}$. From the unitary matrix $U(x, p)$ two types of Berry connections can be defined, i.e. $A_p(x, p) = iU^\dagger \partial_p U$ and $A_x(x, p) = iU^\dagger \partial_x U$, that depend on both variables of phase space.

Our starting point is again the collisionless limit of the quantum Boltzmann equation in the Wigner representation

$$\left[f, G_0^{-1}\right]^\star = 0. \tag{6.24}$$

As in the case of only one Berry phase, we will apply the unitary transformation $U(x, p)$ and perform the gradient expansion up to first order for non-commuting functions

$$U^\dagger \left[UfU^\dagger, Ug_0^{-1}U^\dagger\right] U + \frac{i}{2}U^\dagger \left\{\partial_x \left(UfU^\dagger\right), \partial_p \left(Ug_0^{-1}U^\dagger\right)\right\} U$$
$$-\frac{i}{2}U^\dagger \left\{\partial_p \left(UfU^\dagger\right), \partial_x \left(Ug_0^{-1}U^\dagger\right)\right\} U = 0, \tag{6.25}$$

where g_0^{-1} is diagonal. The difference now is that both derivatives of U survive, resulting in the two Berry connections in the Boltzmann equation

$$
\begin{aligned}
&\left[f, g_0^{-1}\right] + \frac{i}{2}\left\{\partial_x f - i\left[A_x, f\right], \partial_p g_0^{-1} - i\left[A_p, g_0^{-1}\right]\right\} \\
&\quad - \frac{i}{2}\left\{\partial_p f - i\left[A_p, f\right], \partial_x g_0^{-1} - i\left[A_x, g_0^{-1}\right]\right\} = 0.
\end{aligned}
\tag{6.26}
$$

In order for Berry connections to be properly defined, we are interested in the diagonal elements of the Boltzmann equation that describe evolution within a band. The decoupling of the matrix equation is done exactly in the same way as for the case in chapter 4. The off-diagonal elements are solved by $f_{ij} = 0$ and substituting this into the diagonals, we are left with

$$
\partial_x f \partial_p g_0^{-1} - \partial_p f \partial_x g_0^{-1} = 0,
\tag{6.27}
$$

where the Berry connections have decoupled form the equation.

The Berry connections can be reincluded in the Boltzmann equation via a simultaneous minimal coupling in both coordinates, namely

$$
x^\mu \rightarrow \xi^\mu = x^\mu - A_\Pi^\mu
\tag{6.28}
$$
$$
p^\mu \rightarrow \Pi^\mu = p^\mu + A_\xi^\mu.
\tag{6.29}
$$

This is similar to the case studied in the previous section, where A_ξ has replaced the electromagnetic gauge field. The main difference is that now $A_\Pi = A_\Pi(\xi, \Pi)$ and $A_\xi = A_\xi(\xi, \Pi)$. Because of this, the derivatives present in the Boltzmann equation will transform as

$$
\frac{\partial}{\partial x^\mu} \rightarrow \frac{\partial}{\partial \xi^\mu} - \frac{\partial A_\Pi^\nu}{\partial \xi^\mu}\frac{\partial}{\partial \xi^\nu} + \frac{\partial A_\xi^\nu}{\partial \xi^\mu}\frac{\partial}{\partial \Pi^\nu}
\tag{6.30}
$$
$$
\frac{\partial}{\partial p^\mu} \rightarrow \frac{\partial}{\partial \Pi^\mu} + \frac{\partial A_\xi^\nu}{\partial \Pi^\mu}\frac{\partial}{\partial \Pi^\nu} - \frac{\partial A_\Pi^\nu}{\partial \Pi^\mu}\frac{\partial}{\partial \xi^\nu}.
\tag{6.31}
$$

Applying the transformation to the Boltzmann equation we get

$$
\begin{aligned}
&\left(\frac{\partial f}{\partial \xi^\mu} - \frac{\partial f}{\partial \xi^\nu}\frac{\partial A_\Pi^\nu}{\partial \xi^\mu} + \frac{\partial f}{\partial \Pi^\nu}\frac{\partial A_\xi^\nu}{\partial \xi^\mu}\right)\left(\frac{\partial g_0^{-1}}{\partial \Pi^\mu} + \frac{\partial A_\xi^\lambda}{\partial \Pi^\mu}\frac{\partial g_0^{-1}}{\partial \Pi^\lambda} - \frac{\partial A_\Pi^\lambda}{\partial \Pi^\mu}\frac{\partial g_0^{-1}}{\partial \xi^\lambda}\right) \\
&- \left(\frac{\partial f}{\partial \Pi^\mu} + \frac{\partial f}{\partial \Pi^\nu}\frac{\partial A_\xi^\nu}{\partial \Pi^\mu} - \frac{\partial f}{\partial \xi^\nu}\frac{\partial A_\Pi^\nu}{\partial \Pi^\mu}\right)\left(\frac{\partial g_0^{-1}}{\partial \xi^\mu} - \frac{\partial A_\Pi^\lambda}{\partial \xi^\mu}\frac{\partial g_0^{-1}}{\partial \xi^\lambda} + \frac{\partial A_\xi^\lambda}{\partial \xi^\mu}\frac{\partial g_0^{-1}}{\partial \Pi^\lambda}\right) = 0.
\end{aligned}
\tag{6.32}
$$

We can rearranging and renaming some repeated indices

$$
\begin{aligned}
&\frac{\partial f}{\partial \xi^\mu}\left(\frac{\partial g_0^{-1}}{\partial \Pi^\mu}+\frac{\partial A_\xi^\nu}{\partial \Pi^\mu}\frac{\partial g_0^{-1}}{\partial \Pi^\nu}-\frac{\partial A_\Pi^\nu}{\partial \Pi^\mu}\frac{\partial g_0^{-1}}{\partial \xi^\nu}\right)\\
&-\frac{\partial f}{\partial \xi^\mu}\frac{\partial A_\Pi^\mu}{\partial \xi^\nu}\left(\frac{\partial g_0^{-1}}{\partial \Pi^\nu}+\frac{\partial A_\xi^\lambda}{\partial \Pi^\nu}\frac{\partial g_0^{-1}}{\partial \Pi^\lambda}-\frac{\partial A_\Pi^\lambda}{\partial \Pi^\nu}\frac{\partial g_0^{-1}}{\partial \xi^\lambda}\right)\\
&+\frac{\partial f}{\partial \Pi^\mu}\frac{\partial A_\xi^\mu}{\partial \xi^\nu}\left(\frac{\partial g_0^{-1}}{\partial \Pi^\nu}+\frac{\partial A_\xi^\lambda}{\partial \Pi^\nu}\frac{\partial g_0^{-1}}{\partial \Pi^\lambda}-\frac{\partial A_\Pi^\lambda}{\partial \Pi^\nu}\frac{\partial g_0^{-1}}{\partial \xi^\lambda}\right)\\
&-\frac{\partial f}{\partial \Pi^\mu}\left(\frac{\partial g_0^{-1}}{\partial \xi^\mu}-\frac{\partial A_\Pi^\nu}{\partial \xi^\mu}\frac{\partial g_0^{-1}}{\partial \xi^\nu}+\frac{\partial A_\xi^\nu}{\partial \xi^\mu}\frac{\partial g_0^{-1}}{\partial \Pi^\nu}\right)\\
&-\frac{\partial f}{\partial \Pi^\mu}\frac{\partial A_\xi^\mu}{\partial \Pi^\nu}\left(\frac{\partial g_0^{-1}}{\partial \xi^\nu}-\frac{\partial A_\Pi^\lambda}{\partial \xi^\nu}\frac{\partial g_0^{-1}}{\partial \xi^\lambda}+\frac{\partial A_\xi^\lambda}{\partial \xi^\nu}\frac{\partial g_0^{-1}}{\partial \Pi^\lambda}\right)\\
&+\frac{\partial f}{\partial \xi^\mu}\frac{\partial A_\Pi^\mu}{\partial \Pi^\nu}\left(\frac{\partial g_0^{-1}}{\partial \xi^\nu}-\frac{\partial A_\Pi^\lambda}{\partial \xi^\nu}\frac{\partial g_0^{-1}}{\partial \xi^\lambda}+\frac{\partial A_\xi^\lambda}{\partial \xi^\nu}\frac{\partial g_0^{-1}}{\partial \Pi^\lambda}\right)=0
\end{aligned}
\tag{6.33}
$$

and regroup some terms to get

$$
\begin{aligned}
&\frac{\partial f}{\partial \xi^\mu}\left\{\frac{\partial g_0^{-1}}{\partial \Pi^\mu}-\left(\frac{\partial A_\Pi^\nu}{\partial \Pi^\mu}-\frac{\partial A_\Pi^\mu}{\partial \Pi^\nu}-\frac{\partial A_\Pi^\mu}{\partial \xi^\lambda}\frac{\partial A_\Pi^\nu}{\partial \Pi^\lambda}+\frac{\partial A_\Pi^\mu}{\partial \Pi^\lambda}\frac{\partial A_\Pi^\nu}{\partial \xi^\lambda}\right)\frac{\partial g_0^{-1}}{\partial \xi^\nu}\right.\\
&\qquad\left.+\left(\frac{\partial A_\xi^\nu}{\partial \Pi^\mu}-\frac{\partial A_\Pi^\mu}{\partial \xi^\nu}-\frac{\partial A_\Pi^\mu}{\partial \xi^\lambda}\frac{\partial A_\xi^\nu}{\partial \Pi^\lambda}+\frac{\partial A_\Pi^\mu}{\partial \Pi^\lambda}\frac{\partial A_\xi^\nu}{\partial \xi^\lambda}\right)\frac{\partial g_0^{-1}}{\partial \Pi^\nu}\right\}\\
&-\frac{\partial f}{\partial \Pi^\mu}\left\{\frac{\partial g_0^{-1}}{\partial \xi^\mu}+\left(\frac{\partial A_\xi^\nu}{\partial \xi^\mu}-\frac{\partial A_\xi^\mu}{\partial \xi^\nu}-\frac{\partial A_\xi^\mu}{\partial \xi^\lambda}\frac{\partial A_\xi^\nu}{\partial \Pi^\lambda}+\frac{\partial A_\xi^\mu}{\partial \Pi^\lambda}\frac{\partial A_\xi^\nu}{\partial \xi^\lambda}\right)\frac{\partial g_0^{-1}}{\partial \Pi^\nu}\right.\\
&\qquad\left.-\left(\frac{\partial A_\Pi^\nu}{\partial \xi^\mu}-\frac{\partial A_\xi^\mu}{\partial \Pi^\nu}-\frac{\partial A_\xi^\mu}{\partial \xi^\lambda}\frac{\partial A_\Pi^\nu}{\partial \Pi^\lambda}+\frac{\partial A_\xi^\mu}{\partial \Pi^\lambda}\frac{\partial A_\Pi^\lambda}{\partial \xi^\nu}\right)\frac{\partial g_0^{-1}}{\partial \xi^\nu}\right\}=0.
\end{aligned}
\tag{6.34}
$$

We can recognize the quantities in the parentheses and treat them like generalized berry curvatures defined as

$$
\Omega_{\Pi\Pi}^{\mu\nu}=\partial_\Pi^\mu A_\Pi^\nu-\partial_\Pi^\nu A_\Pi^\mu-\left\{A_\Pi^\mu,A_\Pi^\nu\right\}
\tag{6.35}
$$

$$
\Omega_{\Pi\xi}^{\mu\nu}=\partial_\Pi^\mu A_\xi^\nu-\partial_\xi^\nu A_\Pi^\mu-\left\{A_\Pi^\mu,A_\xi^\nu\right\}
\tag{6.36}
$$

$$
\Omega_{\xi\xi}^{\mu\nu}=\partial_\xi^\mu A_\xi^\nu-\partial_\xi^\nu A_\xi^\mu-\left\{A_\xi^\mu,A_\xi^\nu\right\}
\tag{6.37}
$$

$$
\Omega_{\xi\Pi}^{\mu\nu}=\partial_\xi^\mu A_\Pi^\nu-\partial_\Pi^\nu A_\xi^\mu-\left\{A_\xi^\mu,A_\Pi^\nu\right\},
\tag{6.38}
$$

where $\{\,,\}$ denotes the Poisson bracket and rewrite the Boltzmann equation in a compact way

$$
\begin{aligned}
&\frac{\partial f}{\partial \xi^\mu}\left(\frac{\partial g_0^{-1}}{\partial \Pi^\mu}-\Omega_{\Pi\Pi}^{\mu\nu}\frac{\partial g_0^{-1}}{\partial \xi^\nu}+\Omega_{\Pi\xi}^{\mu\nu}\frac{\partial g_0^{-1}}{\partial \Pi^\nu}\right)\\
&-\frac{\partial f}{\partial \Pi^\mu}\left(\frac{\partial g_0^{-1}}{\partial \xi^\mu}+\Omega_{\xi\xi}^{\mu\nu}\frac{\partial g_0^{-1}}{\partial \Pi^\nu}-\Omega_{\xi\Pi}^{\mu\nu}\frac{\partial g_0^{-1}}{\partial \xi^\nu}\right)=0.
\end{aligned}
\tag{6.39}
$$

The first thing to observe is that there are four types of Berry curvature involved, one in momentum space, one in real space, and two that mix the real and momentum space. Even more importantly, the Berry curvatures now contain an extra term consisting of a Poisson bracket that is not present in the usual definition of the Berry curvature. However, this is reminiscent of a non-abelian Berry curvature, which contains a commutator. A commutator becoming a Poisson bracket can be justified in the context of the Wigner transformation being a semi-classical approximation. As explained in section 1.3, a non-abelian Berry curvature arises when there are degeneracies in the system. In the type of systems we are studying though, it is unclear where the non-abelian nature stems from.

A more important problem is that a non-abelian Berry curvature, containing either a commutator or a Poisson bracket, is not gauge invariant. This is in contradiction with results from a phenomenological derivation as in [4] and further research is required to find out where this contradiction originates from and which result is the correct one. In the case that a system like this is indeed described by non-abelian berry curvatures, we have to take a step back and ask whether the Boltzmann equation has to necessarily be gauge invariant. What is definitely true is that the Berry curvature cannot be directly measured. What can be measured is the current or conductivity caused by it. These have the possibility to be gauge invariant but it is not clear yet. Even if indeed the conductivity is gauge invariant and we allow for a gauge dependent Berry curvature, there are still problems concerning the distribution function. Can a gauge dependent Boltzmann equation have a gauge invariant solution for the distribution function? The distribution function is related to observable quantities like the definition of the current in metal for instance. This means that it has to either be gauge invariant, or its gauge dependence should cancel when entering formulas for observables. These are all questions that are yet to be resolved and require more research.

Conclusion

In this thesis, we have studied the transport properties of systems with a Berry phase using the Boltzmann equation.

The Boltzmann equation describes a system's behaviour out of equilibrium, so, apart from its phenomenological derivation, we have shown that it can also be derived from the Keldysh formalism. Then, the kinetic term is expressed with respect to the system's Green's function and the collision integral with respect to self-energies. To this a Wigner transformation can be applied that transforms two point functions to functions in phase space and results in a semi-classical expansion. Finally, taking particles on-shell, the classical Boltzmann equation can be rederived. This can be applied to single band systems that include effects like magnetic fields and disorder.

In multi-band systems Berry phases appear and the Boltzmann equation becomes a matrix. We have shown that after diagonalizing it, the Berry connection can enter via a minimal coupling in real space. The main result of this treatment is the anomalous velocity, a velocity perpendicular to the electric field. This can cause an anomalous Hall effect, a Hall effect without a magnetic field, where the Berry curvature plays the role of the magnetic field. The Hall conductivity in this case is quantized, given by Chern numbers, and it is non-zero for systems that break time-reversal symmetry. A famous example of a system with this property is Haldane's model for graphene.

Finally, we made an attempt to include various effects in multi-band systems and investigate their interplay with the Berry phase. The Berry phase and disorder are two opposing effects that should affect each other. Whether the Berry phase enters the collision integral is still an open question that is mostly stuck by technical difficulties. The Berry phase and a magnetic field are two effects with very similar results, namely each one creates a Hall current. Instead of just being add up, we expect each phenomenon will affect the system's response to the other. However, introducing the two effects with two simultaneous minimal couplings, has resulted in a gauge dependent result. The problem has been treated with different approaches and right now the most promising direction to follow would be to modify the minimal coupling by introducing a coupling between the two corresponding gauge fields. For a system with a Berry phase in both real and momentum space, as for instance in a multi-band system with a spin texture, a non-abelian Berry curvature has been derived, which contradicts the existing literature. There is again a problem with gauge invariance and in this case we have to check at which quantities in fact correspond to observables. All this enhances the idea that studying the interplay between different phenomena is in general a non trivial task in physics.

Appendix A

Derivation of the Moyal product

Let us consider a two-point function $C(x_1, x_2)$ that is given by a product of two other two-point functions while integrating over the intermediate variable

$$C(x_1, x_2) = \int \mathrm{d}x_3 \, A(x_1, x_3) B(x_3, x_2). \tag{A.1}$$

We are interested in finding its Wigner transformation $C(x, p)$. We should start by replacing $A(x_1, x_3)$ and $B(x_3, x_2)$ by their inverse Wigner transformations given by eq. (1.18). Then

$$C(x_1, x_2) = \int \mathrm{d}x_3 \sum_{p_1 p_2} e^{ip_1(x_1 - x_3)} A\left(\frac{x_1 + x_3}{2}, p_1\right) e^{ip_2(x_3 - x_2)} B\left(\frac{x_3 + x_2}{2}, p_2\right). \tag{A.2}$$

Now the Wigner transformation of C can be performed by shifting the coordinates to the center of mass and relative ones $x = (x_1 + x_2)/2$ and $x' = x_1 - x_2$, and Fourier transforming x', which results in

$$
\begin{aligned}
C(x, p) = \int \mathrm{d}x' \, e^{-ipx'} \int \mathrm{d}x_3 \sum_{p_1 p_2} e^{ip_1(x + x'/2 - x_3) + ip_2(x_3 - x + x'/2)} \\
A\left(\frac{x + x'/2 + x_3}{2}, p_1\right) B\left(\frac{x_3 + x + x'/2}{2}, p_2\right).
\end{aligned}
\tag{A.3}
$$

Eventually, the goal is to perform all integrals and sums and express everything in terms of x and p. As a first step, we perform a change of the coordinates and momenta that are integrated or summed over by defining new ones

$$x_{a,b} = x_3 - x \pm \frac{x'}{2} \tag{A.4}$$

and

$$p_{a,b} = p_{1,2} - p. \tag{A.5}$$

Then, the exponent of the previous expression simplifies significantly

$$
\begin{aligned}
p_1\left(x + \frac{x'}{2} - x_3\right) + p_2\left(x_3 - x + \frac{x'}{2}\right) - px' \\
= (p_a + p)\left(x + \frac{x'}{2} - x_3\right) + (p_b + p)\left(x_3 - x + \frac{x'}{2}\right) - px' \\
= p_b \, x_a - p_a \, x_b
\end{aligned}
\tag{A.6}
$$

and we end up with

$$C(x,p) = \iint \mathrm{d}x_a \mathrm{d}x_b \sum_{p_1 p_2} e^{i(p_b x_a - p_a x_b)} A\left(x + \frac{x_a}{2}, p + p_a\right) B\left(x + \frac{x_b}{2}, p + p_b\right). \quad (A.7)$$

The next step is to expand the functions A and B into separate Taylor series in the momenta p_a and p_b

$$C(x,p) = \iint \mathrm{d}x_a \mathrm{d}x_b \sum_n \sum_{p_a} \frac{1}{n!} \partial_p^n A\left(x + \frac{x_a}{2}, p\right) e^{-i p_a x_b} p_a^n$$
$$\times \sum_m \sum_{p_b} \frac{1}{m!} \partial_p^m B\left(x + \frac{x_b}{2}, p\right) e^{+i p_b x_b} p_b^m. \quad (A.8)$$

To proceed, a crucial observation has to be made, that is the n-th power of the momentum combined with an exponential can be in fact rewritten as the n-th derivative of a delta function

$$\sum_p e^{\pm i p x} p^n = (\mp)^n \delta^{(n)}(x). \quad (A.9)$$

This way, the sums over the momenta can be performed, leading to

$$C(x,p) = \iint \mathrm{d}x_a \mathrm{d}x_b \sum_n \frac{1}{n!} \partial_p^n A\left(x + \frac{x_a}{2}, p\right) (i)^n \delta^{(n)}(x_b)$$
$$\times \sum_m \frac{1}{m!} \partial_p^m B\left(x + \frac{x_b}{2}, p\right) (-i)^m \delta^{(m)}(x_a). \quad (A.10)$$

In order to evaluate the integrals over the coordinates, we perform partial integration n and m times in the two integrals that have decoupled

$$C(x,p) = \sum_{nm} \frac{1}{n!m!} (-i)^n (i)^m \int \mathrm{d}x_a\, \partial_{x_a}^m \partial_p^n A\left(x + \frac{x_a}{2}, p\right) \delta(x_a)$$
$$\times \int \mathrm{d}x_b\, \partial_{x_b}^n \partial_p^m B\left(x + \frac{x_b}{2}, p\right) \delta(x_b). \quad (A.11)$$

One last shift has to be performed before calculating the integrals, namely

$$\tilde{x}_{a,b} = x + \frac{x_{a,b}}{2}, \quad (A.12)$$

while taking advantage of the property of the delta function $\delta(ax) = \delta(x)/a$, resulting in

$$C(x,p) = \sum_{nm} \frac{1}{n!m!} (-i)^n (i)^m \int \mathrm{d}\tilde{x}_a \left(\frac{1}{2}\right)^m \partial_{\tilde{x}_a}^m \partial_p^n A(\tilde{x}_a, p)\, \delta(\tilde{x}_a - x)$$
$$\times \int \mathrm{d}\tilde{x}_b \left(\frac{1}{2}\right)^n \partial_{\tilde{x}_b}^n \partial_p^m B(\tilde{x}_b, p)\, \delta(\tilde{x}_b - x). \quad (A.13)$$

The integrals can now be performed by use of the delta functions and the result is

$$C(x,p) = \sum_{nm} \frac{1}{n!m!} \left(-\frac{i}{2}\right)^n \left(\frac{i}{2}\right)^m \partial_x^m \partial_p^n A(x,p)\, \partial_x^n \partial_p^m B(x,p). \quad (A.14)$$

This can be rearranged a bit, noting that the derivatives only act on either $A(x,p)$ and $B(x,p)$ and not on everything that is on their left or right

$$C(x,p) = A(x,p) \sum_m \frac{1}{m!} \left(\frac{i}{2}\right)^m \overleftarrow{\partial}_x^m \overrightarrow{\partial}_p^m \sum_n \frac{1}{n!} \left(-\frac{i}{2}\right)^n \overleftarrow{\partial}_p^n \overrightarrow{\partial}_x^n B(x,p). \qquad (A.15)$$

We can now recognize the Taylor expansions of two exponentials, which reproduce the final expression that we were after

$$C(x,p) = A(x,p)\, e^{\frac{i}{2}\left(\overleftarrow{\partial}_x \overrightarrow{\partial}_p - \overleftarrow{\partial}_p \overrightarrow{\partial}_x\right)} B(x,p). \qquad (A.16)$$

This is a product between two functions in phase space and is called the Moyal product, symbolically written as $C = A \star B$.

Appendix B

Diagonalization of graphene Hamiltonians

In this Appendix detailed calculations related to chapter 5 are presented. Specifically, the diagonalization procedure of Hamiltonians of the tight-binding model with real hopping and a mass term and the Haldane model is described to get the corresponding spectra and eigenstates.

B.1 Graphene with real hopping and mass term

In this section we will diagonalize the tight binding Hamiltonian for graphene with real hopping and a mass term, i.e.

$$H(\mathbf{k}) = \begin{pmatrix} M & t \sum_i e^{-i\mathbf{k}\cdot\mathbf{a}_i} \\ t \sum_i e^{i\mathbf{k}\cdot\mathbf{a}_i} & -M \end{pmatrix}. \tag{B.1}$$

The spectrum can be found by solving

$$\begin{vmatrix} M - \lambda & t \sum_i e^{-i\mathbf{k}\cdot\mathbf{a}_i} \\ t \sum_i e^{i\mathbf{k}\cdot\mathbf{a}_i} & -M - \lambda \end{vmatrix} = 0$$

$$- (M - \lambda)(M + \lambda) - t^2 \sum_{ij} e^{-i\mathbf{k}\cdot(\mathbf{a}_i - \mathbf{a}_j)} = 0$$

$$\lambda^2 - M^2 - t^2 \sum_{ij} e^{-i\mathbf{k}\cdot(\mathbf{a}_i - \mathbf{a}_j)} = 0$$

which results in the two band spectrum

$$\varepsilon_\pm(\mathbf{k}) = \pm \sqrt{M^2 + t^2 \sum_{ij} e^{-i\mathbf{k}\cdot(\mathbf{a}_i - \mathbf{a}_j)}} . \tag{B.2}$$

The eigenstates of the Hamiltonian $|\psi_-\rangle$ and $|\psi_+\rangle$ should satisfy the eigenvalue equation

$$H(\mathbf{k})|\psi_\pm\rangle = \varepsilon_\pm(\mathbf{k})|\psi_\pm\rangle. \tag{B.3}$$

To facilitate the calculation we will express the eigenstates as $|\psi_\pm\rangle = (u_\pm, v_\pm)^T$. Then the eigenvalue equation becomes

$$
\begin{pmatrix} M & t\sum_i e^{-i\mathbf{k}\cdot\mathbf{a}_i} \\ t\sum_i e^{i\mathbf{k}\cdot\mathbf{a}_i} & -M \end{pmatrix} \begin{pmatrix} u_\pm \\ v_\pm \end{pmatrix} = \pm\sqrt{M^2 + t^2\sum_{ij} e^{-i\mathbf{k}\cdot(\mathbf{a}_i-\mathbf{a}_j)}} \begin{pmatrix} u_\pm \\ v_\pm \end{pmatrix}.
\tag{B.4}
$$

Taking the second of the two equations defined in the above we get

$$
t\sum_i e^{i\mathbf{k}\cdot\mathbf{a}_i}\, u_\pm - Mv_\pm = \pm\sqrt{M^2 + t^2\sum_{ij} e^{-i\mathbf{k}\cdot(\mathbf{a}_i-\mathbf{a}_j)}}\, v_\pm
\tag{B.5}
$$

and after rearranging and squaring

$$
t^2\sum_{ij} e^{-i\mathbf{k}\cdot(\mathbf{a}_i-\mathbf{a}_j)}|u_\pm|^2 =
$$
$$
\left\{ 2M^2 + t^2\sum_{ij} e^{-i\mathbf{k}\cdot(\mathbf{a}_i-\mathbf{a}_j)} \pm 2M\sqrt{M^2 + t^2\sum_{ij} e^{-i\mathbf{k}\cdot(\mathbf{a}_i-\mathbf{a}_j)}} \right\} |v_\pm|^2.
\tag{B.6}
$$

The eigenstates should be normalized, meaning

$$
\langle\psi_\pm|\psi_\pm\rangle = 1 \Rightarrow |u_\pm|^2 + |v_\pm|^2 = 1
\tag{B.7}
$$

Using this, we have

$$
2\left\{ M^2 + t^2\sum_{ij} e^{-i\mathbf{k}\cdot(\mathbf{a}_i-\mathbf{a}_j)} \pm M\sqrt{M^2 + t^2\sum_{ij} e^{-i\mathbf{k}\cdot(\mathbf{a}_i-\mathbf{a}_j)}} \right\} |v_\pm|^2 = t^2\sum_{ij} e^{-i\mathbf{k}\cdot(\mathbf{a}_i-\mathbf{a}_j)}
\tag{B.8}
$$

We can define the quantity inside the bracket as

$$
N_\pm^2 = \left(\frac{M}{2} \pm \sqrt{M^2 + t^2\sum_{ij} e^{-i\mathbf{k}\cdot(\mathbf{a}_i-\mathbf{a}_j)}} \right)^2 - \frac{M^2}{4}
\tag{B.9}
$$

and solve for

$$
|v_\pm|^2 = \frac{t^2}{2N_\pm^2}\sum_{ij} e^{-i\mathbf{k}\cdot(\mathbf{a}_i-\mathbf{a}_j)}.
\tag{B.10}
$$

Then it follows from the normalization condition that

$$
|u_\pm|^2 = \frac{1}{2N_\pm^2}\left(M \pm \sqrt{M^2 + t^2\sum_{ij} e^{-i\mathbf{k}\cdot(\mathbf{a}_i-\mathbf{a}_j)}} \right)^2
\tag{B.11}
$$

Since the eigenstates are not uniquely defined, we can choose $u_\pm$ to be real and $v_\pm$ to acquire a phase, resulting in the following eigenstates

$$
|\psi_\pm(\mathbf{k})\rangle = \frac{1}{\sqrt{2}N_\pm}\begin{pmatrix} M \pm \sqrt{M^2 + t^2\sum_{ij} e^{-i\mathbf{k}\cdot(\mathbf{a}_i-\mathbf{a}_j)}} \\ t\sum_i e^{i\mathbf{k}\cdot\mathbf{a}_i} \end{pmatrix}
\tag{B.12}
$$

B.2 Haldane model

In this section we will provide with the steps to diagonalizing the Hamiltonian for the Haldane model, namely

$$H(\mathbf{k}) = \begin{pmatrix} 2t_2 \sum_i \cos(\phi + \mathbf{k} \cdot \mathbf{b}_i) + M & t_1 \sum_i e^{-i\mathbf{k} \cdot \mathbf{a}_i} \\ t_1 \sum_i e^{i\mathbf{k} \cdot \mathbf{a}_i} & 2t_2 \sum_i \cos(\phi - \mathbf{k} \cdot \mathbf{b}_i) - M \end{pmatrix}. \tag{B.13}$$

The first step to diagonalizing this Hamiltonian is to find the eigenvalues by solving

$$\begin{vmatrix} 2t_2 \sum_i \cos(\phi + \mathbf{k} \cdot \mathbf{b}_i) + M - \lambda & t_1 \sum_i e^{-i\mathbf{k} \cdot \mathbf{a}_i} \\ t_1 \sum_i e^{i\mathbf{k} \cdot \mathbf{a}_i} & 2t_2 \sum_i \cos(\phi - \mathbf{k} \cdot \mathbf{b}_i) - M - \lambda \end{vmatrix} = 0, \tag{B.14}$$

$$\left(2t_2 \sum_i \cos(\phi + \mathbf{k} \cdot \mathbf{b}_i) + M - \lambda \right) \left(2t_2 \sum_i \cos(\phi - \mathbf{k} \cdot \mathbf{b}_i) - M - \lambda \right)$$
$$- t_1^2 \sum_{ij} e^{-i\mathbf{k} \cdot (\mathbf{a}_i - \mathbf{a}_j)} = 0. \tag{B.15}$$

From the definition of $\mathbf{b}_i = \epsilon_{ijk}(\mathbf{a}_j - \mathbf{a}_k)$, we have that

$$\sum_{ij} e^{-i\mathbf{k} \cdot (\mathbf{a}_i - \mathbf{a}_j)} = 3 + \sum_i \left(e^{-i\mathbf{k} \cdot \mathbf{b}_i} + e^{-i\mathbf{k} \cdot \mathbf{b}_i} \right) = 3 + 2 \sum_i \cos(\mathbf{k} \cdot \mathbf{b}_i), \tag{B.16}$$

which leads to

$$\lambda^2 - 2\lambda t_2 \sum_i \left[\cos(\phi + \mathbf{k} \cdot \mathbf{b}_i) + \cos(\phi - \mathbf{k} \cdot \mathbf{b}_i) \right]$$
$$- M^2 - 2Mt_2 \sum_i \left[\cos(\phi + \mathbf{k} \cdot \mathbf{b}_i) - \cos(\phi - \mathbf{k} \cdot \mathbf{b}_i) \right]$$
$$+ 4t_2^2 \sum_{ij} \cos(\phi + \mathbf{k} \cdot \mathbf{b_i}) \cos(\phi - \mathbf{k} \cdot \mathbf{b}_j) - t_1^2 \left(3 + 2 \sum_i \cos(\mathbf{k} \cdot \mathbf{b}_i) \right) = 0. \tag{B.17}$$

Completing the square for the first two terms

$$\left(\lambda - t_2 \sum_i \left[\cos(\phi + \mathbf{k} \cdot \mathbf{b}_i) + \cos(\phi - \mathbf{k} \cdot \mathbf{b}_i) \right] \right)^2$$
$$- t_2^2 \left(\sum_i \left[\cos(\phi + \mathbf{k} \cdot \mathbf{b}_i) + \cos(\phi - \mathbf{k} \cdot \mathbf{b}_i) \right] \right)^2 - M^2$$
$$- 2Mt_2 \sum_i \left[\cos(\phi + \mathbf{k} \cdot \mathbf{b}_i) - \cos(\phi - \mathbf{k} \cdot \mathbf{b}_i) \right]$$
$$+ 4t_2^2 \sum_{ij} \cos(\phi + \mathbf{k} \cdot \mathbf{b_i}) \cos(\phi - \mathbf{k} \cdot \mathbf{b}_j) - t_1^2 \left(3 + 2 \sum_i \cos(\mathbf{k} \cdot \mathbf{b}_i) \right) = 0 \tag{B.18}$$

and rearranging a bit

$$\left(\lambda - t_2 \sum_i \left[\cos\left(\phi + \mathbf{k} \cdot \mathbf{b}_i \right) + \cos\left(\phi - \mathbf{k} \cdot \mathbf{b}_i \right) \right] \right)^2 - M^2$$
$$- 2Mt_2 \sum_i \left[\cos\left(\phi + \mathbf{k} \cdot \mathbf{b}_i \right) - \cos\left(\phi - \mathbf{k} \cdot \mathbf{b}_i \right) \right]$$
$$- t_2^2 \left(\sum_i \left[\cos\left(\phi + \mathbf{k} \cdot \mathbf{b}_i \right) - \cos\left(\phi - \mathbf{k} \cdot \mathbf{b}_i \right) \right] \right)^2$$
$$- t_1^2 \left(3 + 2 \sum_i \cos\left(\mathbf{k} \cdot \mathbf{b}_i \right) \right) = 0, \tag{B.19}$$

we get a more convenient form of the initial equation

$$\left(\lambda - t_2 \sum_i \left[\cos\left(\phi + \mathbf{k} \cdot \mathbf{b}_i \right) + \cos\left(\phi - \mathbf{k} \cdot \mathbf{b}_i \right) \right] \right)^2$$
$$- \left(M + t_2 \sum_i \left[\cos\left(\phi + \mathbf{k} \cdot \mathbf{b}_i \right) - \cos\left(\phi - \mathbf{k} \cdot \mathbf{b}_i \right) \right] \right)^2 \tag{B.20}$$
$$- t_1^2 \left(3 + 2 \sum_i \cos\left(\mathbf{k} \cdot \mathbf{b}_i \right) \right) = 0.$$

Finally, using trigonometric identities we can rewrite

$$\sum_i \left[\cos\left(\phi + \mathbf{k} \cdot \mathbf{b}_i \right) + \cos\left(\phi - \mathbf{k} \cdot \mathbf{b}_i \right) \right] = 2 \cos\phi \sum_i \cos\left(\mathbf{k} \cdot \mathbf{b}_i \right) \tag{B.21}$$

and

$$\sum_i \left(\cos\left(\phi + \mathbf{k} \cdot \mathbf{b}_i \right) - \cos\left(\phi - \mathbf{k} \cdot \mathbf{b}_i \right) \right) = -2 \sin\phi \sum_i \sin\left(\mathbf{k} \cdot \mathbf{b}_i \right), \tag{B.22}$$

to eventually get the energy spectrum

$$\varepsilon(\mathbf{k}) = 2t_2 \cos\phi \sum_i \cos\left(\mathbf{k} \cdot \mathbf{b}_i \right)$$
$$\pm \left\{ \left(M - 2t_2 \sin\phi \sum_i \sin\left(\mathbf{k} \cdot \mathbf{b}_i \right) \right)^2 + t_1^2 \left(3 + 2 \sum_i \cos\left(\mathbf{k} \cdot \mathbf{b}_i \right) \right) \right\}^{1/2}. \tag{B.23}$$

For the eigenstates we have to solve the eigenvalue equation

$$H(\mathbf{k})|\psi_\pm\rangle = \varepsilon_\pm(\mathbf{k})|\psi_\pm\rangle. \tag{B.24}$$

If we express the eigenstates as $\psi_\pm(\mathbf{k}) = (u_\pm, v_\pm)^T$, we can write it as

$$\begin{pmatrix} 2t_2 \sum_i \cos\left(\phi + \mathbf{k} \cdot \mathbf{b}_i \right) + M & t_1 \sum_i e^{-i\mathbf{k}\cdot\mathbf{a}_i} \\ t_1 \sum_i e^{i\mathbf{k}\cdot\mathbf{a}_i} & 2t_2 \sum_i \cos\left(\phi - \mathbf{k} \cdot \mathbf{b}_i \right) - M \end{pmatrix} \begin{pmatrix} u_\pm \\ v_\pm \end{pmatrix} = \varepsilon(\mathbf{k}) \begin{pmatrix} u_\pm \\ v_\pm \end{pmatrix}. \tag{B.25}$$

Since the eigenstates are not uniquely defined, we can use any of the two equations defined in the above, say the lower one

$$
t_1 \sum_i e^{i\mathbf{k}\cdot\mathbf{a}_i} u_\pm + \left(2t_2 \sum_i \cos\left(\phi - \mathbf{k}\cdot\mathbf{b}_i\right) - M \right) v_\pm = \left[2t_2 \cos\phi \sum_i \cos\left(\mathbf{k}\cdot\mathbf{b}_i\right) \right.
$$
$$
\left. \pm \left\{ \left(M - 2t_2 \sin\phi \sum_i \sin\left(\mathbf{k}\cdot\mathbf{b}_i\right) \right)^2 + t_1^2 \left(3 + 2\sum_i \cos\left(\mathbf{k}\cdot\mathbf{b}_i\right) \right) \right\}^{1/2} \right] v_\pm .
$$
(B.26)

Using trigonometric identities we can rewrite

$$
\sum_i \cos\left(\phi - \mathbf{k}\cdot\mathbf{b}_i\right) = \cos\phi \sum_i \cos\left(\mathbf{k}\cdot\mathbf{b}_i\right) + \sin\phi \sum_i \sin\left(\mathbf{k}\cdot\mathbf{b}_i\right)
$$
(B.27)

which results in

$$
t_1 \sum_i e^{i\mathbf{k}\cdot\mathbf{a}_i} u_\pm = \left[M - 2t_2 \sin\phi \sum_i \sin\left(\mathbf{k}\cdot\mathbf{b}_i\right) \right.
$$
$$
\left. \pm \left\{ \left(M - 2t_2 \sin\phi \sum_i \sin\left(\mathbf{k}\cdot\mathbf{b}_i\right) \right)^2 + t_1^2 \left(3 + 2\sum_i \cos\left(\mathbf{k}\cdot\mathbf{b}_i\right) \right) \right\}^{1/2} \right] v_\pm .
$$
(B.28)

We can now square this equation

$$
t_1^2 \sum_{ij} e^{i\mathbf{k}\cdot(\mathbf{a}_i-\mathbf{a}_j)} |u_\pm|^2 = \left[2 \left(M - 2t_2 \sin\phi \sum_i \sin\left(\mathbf{k}\cdot\mathbf{b}_i\right) \right)^2 \right.
$$
$$
+ t_1^2 \left(3 + 2\sum_i \cos\left(\mathbf{k}\cdot\mathbf{b}_i\right) \right) \pm 2 \left(M - 2t_2 \sin\phi \sum_i \sin\left(\mathbf{k}\cdot\mathbf{b}_i\right) \right)
$$
$$
\left. \times \left\{ \left(M - 2t_2 \sin\phi \sum_i \sin\left(\mathbf{k}\cdot\mathbf{b}_i\right) \right)^2 + t_1^2 \left[3 + 2\sum_i \cos\left(\mathbf{k}\cdot\mathbf{b}_i\right) \right] \right\}^{1/2} \right] |v_\pm|^2
$$
(B.29)

and take advantage of the normalization of the eigenstates, i.e. $|u_\pm|^2 + |v_\pm|^2 = 1$. This results in an equation containing only one of the components of the eigenstates

$$
t_1^2 \sum_{ij} e^{i\mathbf{k}\cdot(\mathbf{a}_i-\mathbf{a}_j)} = 2 \left[\left(M - 2t_2 \sin\phi \sum_i \sin\left(\mathbf{k}\cdot\mathbf{b}_i\right) \right)^2 \right.
$$
$$
+ t_1^2 \left(3 + 2\sum_i \cos\left(\mathbf{k}\cdot\mathbf{b}_i\right) \right) \pm \left(M - 2t_2 \sin\phi \sum_i \sin\left(\mathbf{k}\cdot\mathbf{b}_i\right) \right)
$$
$$
\left. \times \left\{ \left(M - 2t_2 \sin\phi \sum_i \sin\left(\mathbf{k}\cdot\mathbf{b}_i\right) \right)^2 + t_1^2 \left[3 + 2\sum_i \cos\left(\mathbf{k}\cdot\mathbf{b}_i\right) \right] \right\}^{1/2} \right] |v_\pm|^2 .
$$
(B.30)

Similar to the previous model, we can define the factor

$$
N_\pm^2 = \left(\frac{\Delta(\mathbf{k})}{2} \pm \sqrt{\Delta^2(\mathbf{k}) + t^2 \sum_{ij} e^{-i\mathbf{k}\cdot(\mathbf{a}_i - \mathbf{a}_j)}} \right)^2 - \frac{\Delta^2(\mathbf{k})}{4}, \tag{B.31}
$$

where

$$
\Delta(\mathbf{k}) = M - 2t_2 \sin\phi \sum_i \sin\left(\mathbf{k}\cdot\mathbf{b}_i\right). \tag{B.32}
$$

Then

$$
|v_\pm|^2 = \frac{t_1^2}{2N_\pm^2} \sum_{ij} e^{i\mathbf{k}\cdot(\mathbf{a}_i - \mathbf{a}_j)}, \tag{B.33}
$$

and from the normalization

$$
|u_\pm|^2 = \frac{1}{2N_\pm^2} \left[\Delta^2(\mathbf{k}) \pm \sqrt{\Delta(\mathbf{k}) + t_1^2 \left(3 + 2\sum_i \cos\left(\mathbf{k}\cdot\mathbf{b}_i\right) \right)} \right]^2. \tag{B.34}
$$

Since the eigenstates are not uniquely defined, $u_\pm$ can be chosen to be real and $v_\pm$ to acquire a phase. Then, a solution for the eigenstates is

$$
|\psi_\pm(\mathbf{k})\rangle = \begin{pmatrix} u_\pm(\mathbf{k}) \\ v_\pm(\mathbf{k}) \end{pmatrix}, \tag{B.35}
$$

where

$$
u_\pm(\mathbf{k}) = \frac{1}{\sqrt{2}N_\pm} \left[\Delta^2(\mathbf{k}) \pm \sqrt{\Delta(\mathbf{k}) + t_1^2 \left(3 + 2\sum_i \cos\left(\mathbf{k}\cdot\mathbf{b}_i\right) \right)} \right] \tag{B.36}
$$

and

$$
v_\pm(\mathbf{k}) = \frac{t_1}{\sqrt{2}N_\pm} \sum_i e^{i\mathbf{k}\cdot\mathbf{a}_i}. \tag{B.37}
$$

Bibliography

[1] M. V. Berry, "Quantal phase factors accompanying adiabatic changes," *Proceedings of the Royal Society of London. A. Mathematical and Physical Sciences*, vol. 392, no. 1802, pp. 45–57, 1984.

[2] F. D. M. Haldane, "Model for a quantum hall effect without landau levels: Condensed-matter realization of the" parity anomaly"," *Physical Review Letters*, vol. 61, no. 18, p. 2015, 1988.

[3] D. J. Thouless, "Quantization of particle transport," *Phys. Rev. B*, vol. 27, pp. 6083–6087, May 1983.

[4] D. Xiao, M.-C. Chang, and Q. Niu, "Berry phase effects on electronic properties," *Reviews of modern physics*, vol. 82, no. 3, p. 1959, 2010.

[5] C. Kittel, *Introduction to Solid State Physics*. Wiley, 8 ed., 2004.

[6] D. Tong, "Lectures on kinetic theory," 2012.

[7] G. D. Mahan, *Many Particle Physics, Third Edition*. New York: Plenum, 2000.

[8] D. Tong, "Lectures on the quantum hall effect," 2016.

[9] X. Wen, *Quantum Field Theory of Many-Body Systems:From the Origin of Sound to an Origin of Light and Electrons: From the Origin of Sound to an Origin of Light and Electrons*. Oxford Graduate Texts, OUP Oxford, 2004.

[10] B. Bernevig and T. Hughes, *Topological Insulators and Topological Superconductors*. Princeton University Press, 2013.

[11] F. Wilczek and A. Zee, "Appearance of gauge structure in simple dynamical systems," *Phys. Rev. Lett.*, vol. 52, pp. 2111–2114, Jun 1984.

[12] W. Kohn and J. M. Luttinger, "Quantum theory of electrical transport phenomena," *Phys. Rev.*, vol. 108, pp. 590–611, Nov 1957.

[13] H. Bruus and K. Flensberg, *Many-body quantum theory in condensed matter physics - an introduction*. United States: Oxford University Press, 2004.

[14] A. Altland and B. D. Simons, *Condensed Matter Field Theory*. Cambridge University Press, 2 ed., 2010.

[15] A. Kamenev, *Field theory of non-equilibrium systems*. Cambridge University Press, 1 2011.

[16] J. Schwinger, "Brownian motion of a quantum oscillator," *Journal of Mathematical Physics*, vol. 2, no. 3, pp. 407–432, 1961.

[17] O. Konstantinov and V. Perel, "A graphical technique for computation of kinetic quantities," *Zhur. Eksptl'. i Teoret. Fiz.*, vol. 39, 1960.

[18] L. P. Kadanoff and G. Baym, "Quantum statistical mechanics," *American Journal of Physics*, vol. 31, no. 4, pp. 309–309, 1963.

[19] L. V. Keldysh *et al.*, "Diagram technique for nonequilibrium processes," *Sov. Phys. JETP*, vol. 20, no. 4, pp. 1018–1026, 1965.

[20] J. Maciejko, "An introduction to nonequilibrium many-body theory," *Lecture Notes, Springer*, 2007.

[21] A. Larkin and Y. Ovchinnikov, "Nonlinear conductivity of superconductors in the mixed state," *Sov. Phys. JETP*, vol. 41, no. 5, pp. 960–965, 1975.

[22] C. H. Wong and Y. Tserkovnyak, "Quantum kinetic equation in phase-space textured multiband systems," *Phys. Rev. B*, vol. 84, p. 115209, Sep 2011.

[23] G. W. Semenoff, "Condensed-matter simulation of a three-dimensional anomaly," *Phys. Rev. Lett.*, vol. 53, pp. 2449–2452, Dec 1984.

[24] M.-C. Chang and Q. Niu, "Berry curvature, orbital moment, and effective quantum theory of electrons in electromagnetic fields," *Journal of Physics: Condensed Matter*, vol. 20, no. 19, p. 193202, 2008.

[25] D. T. Son and N. Yamamoto, "Kinetic theory with berry curvature from quantum field theories," *Physical Review D*, vol. 87, no. 8, p. 085016, 2013.