Berry Curvature as a Multi-Band Effect in Boltzmann Equations

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To my stove that keeps me warm and well fed

Abstract

In this thesis we want to find a Boltzmann equation describing the kinematics in the surface states of a topological insulator. We start by using a variational method to get a semi-classical Boltzmann equation, which includes an anomalous velocity term, caused by a non-vanishing Berry curvature. Having established the Boltzmann equation we showed that we could get the anomalous Hall effect by solving the equation in a special chase. With a phenomenological result at hand we turned to the challenge of deriving the same result form the non-equilibrium approach of the Keldysh formalism. The main problem it posed was the non-trivial matrix structure of the Hamiltonian of a topological insulator, after we neglect collision terms. These difficulties were resolved by perturbatively diagonalizing the inverse Green's function, introducing minimal coupling of the Berry connection to both space and momentum. The minimal coupling eventually lead to a quantum Boltzmann equation in each band, with different Berry curvature terms in the equation. Finally we integrate, with respect to the energy yielding a renormalized semi-classical Boltzmann equation, which could be restricted to the same limit in which we calculated the anomalous Hall effect.

Contents

Chapter 1

Introduction

1.1 Electronic Transport in Topological Insulators

In recent years a whole new type of conductive materials has been discovered; the so called topological insulators. Topological insulators are, in the ideal case a material which has the bulk properties of an insulator, meaning a large energy gap above the last full band, in its interior, while on their surface the gap closes, giving rise to conducting surface states. A sketch for the band structure of such a system is shown in figure 1.1. Theoretical predictions of materials with such a band structure have a long history.

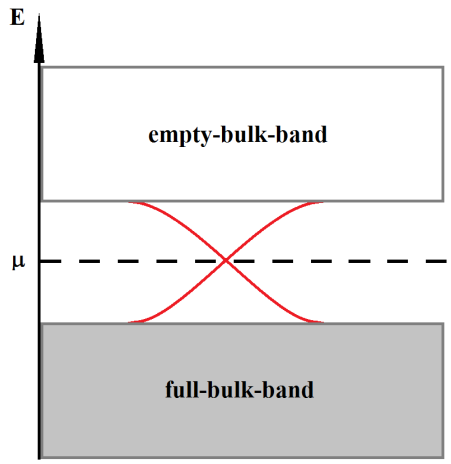

Figure 1.1: A sketch of the band structure of a topological insulator: On the first axis we have momentum and on the second axis we have energy, the stippled line is the chemical potential denoted by μ. The two boxes represent the bulk bands where the grey filling means that the band is full . Lastly, the red lines are the so called surface states, with a typical Dirac-cone.

They where first predicted in 1987 by Pankratov, Pakhomov and Volkov in Mercury-Telluride MgTe compounds, using super-symmetry, to show that they have symmetry protected surface states. However the fact that these surface states of Mercury-Telluride are indeed a topological property was not emphasized until Bernevig, Hughes and Zhang in 2006[1] rediscovered the result of Pankratov, Pakhomov and Volkov using a different approach. The first experimental observation of the surface sates in HgTe was done by Köning et. al. [4] ,in 2007. The same year Fu and Kane[2] found that some bismuth compounds where promising candidates to be strong 3-dimensional topological insulators. That a hand full of bismuth compounds in fact had the supposed surface band structure was observed in the following years using ARPES[1] on such samples[5]. While band structure measurements were obtained quit rapidly after their prediction, measurements of the transport in the surface sates has turned out to be much harder. The reason is that due to impurities in the bulk, the bulk also becomes conducting, hence it is difficult

[1] **A**ngle **R**esolved **P**hoto**E**mission **S**pectroscopy

to get an isolated measurement of the surface current. Recently, due to refinement in crystal growth, Cao et. al.[17] have been able to measure and control surfaces currents in Bismuth-Telluride-Selenide (Bi_2Te_2Se). Measurements like these raises the need for a theoretical prediction or understanding of the transport phenomena of the surface of a topological insulator.

Let us motivate what new transport phenomena one would expect on the surface of a topological insulator, compared to that of a normal 2 dimensional-Fermi liquid. In the bismuth compounds the electrons in the bands are prone to what is called spin-momentum locking, meaning that a specific momentum direction is locked to a specific spin direction. With this locking in mind, let us think what that might imply to a Boltzmann equation with an external force , like an electric field. The effect of an external electric field is a change in momentum of the electrons without changing its spin, but as momentum an spin are locked to each other one would imagine that electrons will changes their velocity to compensate for the change in momentum. Such corrections to the velocity is for historical reasons referred to as the anomalous velocity. It can be related to the Berry curvature. It turns out that if this effect should have a measurable effect on the electric current the band crossing of the surface sates have to be lifted by a Zeeman splitting which also tilts the spin slightly. The spin structure in both cases is sketched in figure1.2.

With the intuition that transport on the surface of a topological insulator is richer than in conven-

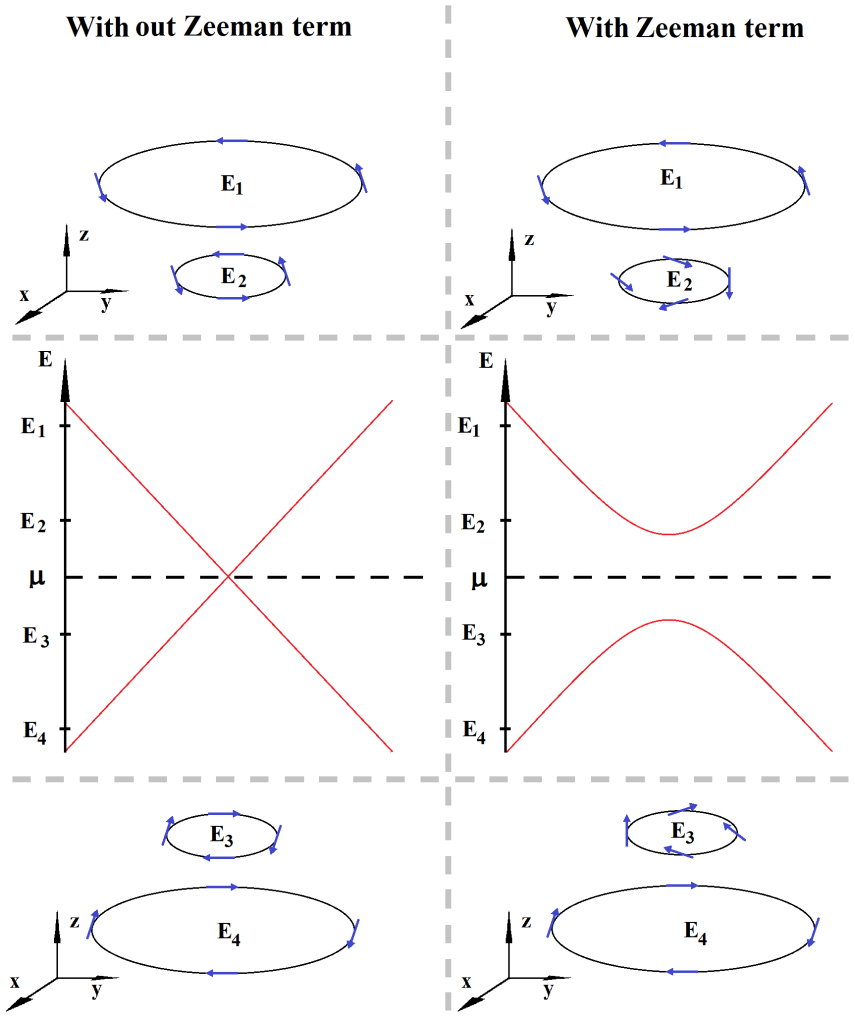

Figure 1.2: A sketch of the band structure and the spin structure of different energy contours. The circles are energy contours and should be thought of as being confined to the xy-plain in momentum space. The arrows lie in the plane for the none split chase(left side), but they rotate in different directions in the upper and lower band. In the split case (right side) the arrows have a projection along the z axis. In the lower band they point up, as the magnetic field is thought of as being in that direction, and in the upper band they point downwards. Note that for high momenta, the effect of the magnetic field is suppressed.

tional metals, and that this richness originates form the spin structure of the system, one can conclude that it is intrinsically a two band effect. This means that we can not hope to achieve a realistic result from standard one band calculations, as reviewed by Rammer and Smith[10]. So, in order to make the same kind of systematic derivation as Rammer and Smith, we need to consider a multi-band Keldysh-Dyson equation. Such equations have been considered before in the chase of superconductors [10] and in the case of semi-conductors by Haug and Jauho [27]. Since we are mainly interested in the electric properties at half filling, we can avoid some of the difficulties by projecting on to the bands, however this an approach need to be carry out carefully so one still active a systematic development of the resulting Boltzmann equation. Methods to derive such a band projecting equation form the Keldysh-Dyson equation have been studied for the past decade, first by Shindou and Balents in 2006[6] and 2008[7], later by Wong and Tserkovnyak in 2011[8] and finally Wickles and Belzing in 2013[9]. We would like to make it more accessible and establish the semi-classical limit with renormalization effects.

As the Keldysh approach to derive the Boltzmann equation is quite technical, results form a more phenomenological treatment have existed for some time. Such work was started in the modern context of Berry curvature by Change and Niu in 1996[14] and refined by Sundaram and Niu in 1999[13], however the anomalous term of the velocity had been noted by Karplus and Luttinger as early as 1954[12], in the context of ferromagnetics. The main problem of the method used by Niu and collaborators is that it can only capture effect allowed by the chosen wave function and it has no way of including renormalization effects. None the less the method gives a valuable intuition of the dynamics of the system as well as symmetries which become rather obvious in the calculatios. We will work through this method in order to get some insight before moving on to the previously mentioned Keldysh Derivation.
With this short introduction concerning the development of transport in systems of non-trivial topology, we will now give an outline of the structure of the thesis. The rest of the present chapter will concern the definition of the Berry connection and the Berry curvature as thy are used extensively in the calculations to come. An introduction the toy model we have used to perform simple calculations, along a brief comment on how to extend the definition of the Berry connection to a two band-calculation. The second chapter contains a phenomenological derivation of a Boltzmann equation for a multi-level system where the driving terms will be found through a variational method. The third chapter contains the full non-equilibrium quantum derivation of first a quantum Boltzmann equation, and then after an integrating out the energies, a semi-classical Boltzmann equation. The final chapter is reserved for summery and outlook. Let us turn to the definition of the Berry connection and the Berry curvature.

1.2 Definition of the Berry Connection and the Berry Curvature

As the concept of the Berry connection and the Berry curvature is used extensively throughout thesis, we will give the definitions on which we will rely on.

The Berry connection and the Berry curvature can be defined[2] for any quantum mechanical system that depends on a continuous parameter. In some systems it gives rise to new physical phenomena, such as the anomalous Hall effect. In this thesis however we will not discuss when the Berry connection gives rise to such new physical effects, for treatment on that see Bernevig[18]. For a Hamiltonian H that depends on a set of continues parameters $\mathbf{R}$ eigenstates are defined as

$$H(\mathbf{R})\left|n(\mathbf{R})\right\rangle = \epsilon_n(\mathbf{R})\left|n(\mathbf{R})\right\rangle : \tag{1.2.1}$$

where the n refers to some band, spin or an other quantum number[3]. From here the Berry connection is defined as

$$\boldsymbol{\mathcal{A}}_n(\mathbf{R}) = i\left\langle n(\mathbf{R})\right|\partial_{\mathbf{R}}\left|n(\mathbf{R})\right\rangle, \tag{1.2.2}$$

where $\partial_{\mathbf{R}} \equiv \frac{\partial}{\partial \mathbf{R}}$. We note that the Berry connection is hermitian due to normalization of the eigenstates. This can be shown by

$$\partial_{\mathbf{R}}\left\langle n(\mathbf{R})\right|\left.n(\mathbf{R})\right\rangle = \left(\partial_{\mathbf{R}}\left\langle n(\mathbf{R})\right|\right)\left|n(\mathbf{R})\right\rangle + \left\langle n(\mathbf{R})\right|\partial_{\mathbf{R}}\left|n(\mathbf{R})\right\rangle = 0. \tag{1.2.3}$$

[2]For a more thoroughly discussion of Berry curvature see [11]

[3]We will use the term band and spin synonymous more ore less through the thesis as we are only considering non-degenerate eigenstate for the Hamiltonian, hence different spin just give raise to the double amount of bands.

Hence there exist the following relation:

$$\langle n(\mathbf{R})|\,\partial_{\mathbf{R}}\,|n(\mathbf{R})\rangle = -\left(\partial_{\mathbf{R}}\,\langle n(\mathbf{R})|\right)|n(\mathbf{R})\rangle\,. \tag{1.2.4}$$

So now taking the hermitian conjugate of $\boldsymbol{\mathcal{A}}_n(\mathbf{R})$ as it is defined in (1.2.2) gives

$$(\boldsymbol{\mathcal{A}}_n(\mathbf{R}))^\dagger = -i\left(\partial_{\mathbf{R}}\,\langle n(\mathbf{R})|\right)|n(\mathbf{R})\rangle = i\,\langle n(\mathbf{R})|\,\partial_{\mathbf{R}}\,|n(\mathbf{R})\rangle = \boldsymbol{\mathcal{A}}_n(\mathbf{R}). \tag{1.2.5}$$

Having showed that the Berry connection is hermitian, lets continue with noting that the Berry connection also transforms under gauge transformation of states. Transforming the states as

$$|n(\mathbf{R})\rangle \to e^{i\xi(\mathbf{R})}\,|n(\mathbf{R})\rangle \tag{1.2.6}$$

transforms the Berry connection as

$$\boldsymbol{\mathcal{A}}_n(\mathbf{R}) \to \boldsymbol{\mathcal{A}}_n(\mathbf{R}) - \partial_{\mathbf{R}}\xi(\mathbf{R}). \tag{1.2.7}$$

So the Berry connection is not a gauge invariant quantity in itself but it behaves like the electromagnetic vector potential. In the case of the electromagnetic vector potential we typically define the magnetic field in order to restore gauge invariance, and for the Berry connection we can analogously define the Berry curvature $\boldsymbol{\Omega}_n(\mathbf{R})$ is defined as

$$\Omega^n_{ij}(\mathbf{R}) = \partial_{R_i}\mathcal{A}^n_j(\mathbf{R}) - \partial_{R_j}\mathcal{A}^n_i(\mathbf{R}). \tag{1.2.8}$$

Which in 3-dimensions can be defined as the curl of the Berry connection

$$\boldsymbol{\Omega}_n(\mathbf{R}) = \partial_{\mathbf{R}} \times \boldsymbol{\mathcal{A}}_n(\mathbf{R}). \tag{1.2.9}$$

In the following section we will calculate the Berry curvature for a simple model:

1.3 The Rashba Hamiltonian with Zeeman-Splitting

One of the simplest examples of a model with none-trivial Berry curvature is the Rashba Hamiltonian model with Zeemann splitting. The Rashba Hamiltonian does in fact describe the low energy physic of surface states in bismuth selenide, and the Zeemann splitting can of course be induced by an external magnetic field. The Hamiltonian takes the form:

$$\underline{\underline{H}} = \sum_{k,\sigma'\sigma} c^\dagger{}_{\mathbf{k}\sigma'} h_{\sigma'\sigma}(\mathbf{k}) c_{\mathbf{k}\sigma} = \sum_k (c^\dagger_{\mathbf{k}\uparrow}\; c^\dagger_{\mathbf{k}\downarrow}) \begin{pmatrix} \Delta & v_f\,(k_x - ik_y) \\ v_f\,(k_x + ik_y) & -\Delta \end{pmatrix} \begin{pmatrix} c_{\mathbf{k}\uparrow} \\ c_{\mathbf{k}\downarrow} \end{pmatrix} \tag{1.3.1}$$

where v_f is the Fermi velocity and Δ is the Zeeman splitting. The energies for each point in momentum are

$$\epsilon_\pm = \pm\sqrt{v_f^2\left(k_x^2 + k_y^2\right) + \Delta^2}. \tag{1.3.2}$$

The normalized eigenvectors can be written as:

$$\psi_+ = \frac{1}{\sqrt{2}} \begin{pmatrix} u_+ e^{-i\theta} \\ u_- \end{pmatrix}, \tag{1.3.3}$$

$$\psi_- = \frac{1}{\sqrt{2}} \begin{pmatrix} u_- e^{-i\theta} \\ -u_+ \end{pmatrix}, \tag{1.3.4}$$

where $u_\pm$ is

$$u_\pm = \sqrt{1 \pm \frac{\Delta}{\sqrt{v_f^2\left(k_x^2 + k_y^2\right) + \Delta^2}}}, \tag{1.3.5}$$

with $\theta = \arctan(\frac{k_y}{k_x})$. The Berry connection in each band can be calculated to be

$$\boldsymbol{\mathcal{A}}_{\pm}(\mathbf{k}) = \frac{1}{2\left(k_x^2+k_y^2\right)}\left(1 \pm \frac{\Delta}{\sqrt{v_f^2\left(k_x^2+k_y^2\right)+\Delta^2}}\right)\begin{pmatrix}-k_y\\ k_x\end{pmatrix}. \tag{1.3.6}$$

Now, as we are considering a two-dimensional model, only the z-component of the Berry curvature is finite and is:

$$\boldsymbol{\Omega}_{+}(\mathbf{k}) = -\frac{v_f^2\Delta}{2(\Delta^2+v_f^2\left(k_x^2+k_y^2\right))^{3/2}}\hat{\mathbf{k}} \tag{1.3.7}$$

$$\boldsymbol{\Omega}_{-}(\mathbf{k}) = +\frac{v_f^2\Delta}{2(\Delta^2+v_f^2\left(k_x^2+k_y^2\right))^{3/2}}\hat{\mathbf{k}} \tag{1.3.8}$$

Note that the sum of the Berry curvatures is zero, which a general property of Berry curvatures[11, 18]. In the final section of this chapter we will discuss the unitary transformation that diagonalized Hamiltonians like the one in equation (1.3.1).

1.4 Unitary transformation

As advertised we will here discuss the unitary transformation that diagonalizes a Hamiltonian given in momentum space as

$$\underline{\underline{H}} = \sum_{\mathbf{k}} \mathbf{c}^{\dagger}{}_{\mathbf{k}}\,\underline{\underline{h}}_{\mathbf{k}}\mathbf{c}_{\mathbf{k}}, \tag{1.4.1}$$

where $\underline{\underline{h}}$ is a general finite dimensional hermitian matrix that depends on the continuous momentum $\mathbf{k}$ and has non-degenerate spectrum of every value of $\mathbf{k}$. $\mathbf{c}_{\mathbf{k}}$ is a vector of annihilation operators which annihilate a state with momentum $\mathbf{k}$ value in the discreet space of the Hamilton. Now as it often convenient to have the Hamiltonian in its diagonal basis we have to find the its eigenvectors. Such eigenvectors called $\psi_{(i)}$

$$\psi_{(i)}(\mathbf{k}) = (u_{(i)1}(\mathbf{k}), u_{(i)2}(\mathbf{k}), ..., u_{(i)n}(\mathbf{k})), \tag{1.4.2}$$

where $u_{(i)j}(\mathbf{k})$ is the jth component of the ith eigenvector which in general will depend on momentum and can be found using the eigenvector equation. After obtaining all the eigenvectors and normalizing them properly, the unitary transformation that diagonalizes the Hamiltonian is given as

$$\underline{\underline{U}}(\mathbf{k}) = \left(\psi_{(1)}(\mathbf{k}), \psi_{(2)}(\mathbf{k}), ..., \psi_{(n)}(\mathbf{k})\right), \tag{1.4.3}$$

along with its hermitian conjugate,

$$\underline{\underline{U}}^{\dagger}(\mathbf{k}) = \begin{pmatrix}\psi^{\dagger}_{(1)}(\mathbf{k})\\ \psi^{\dagger}_{(2)}(\mathbf{k})\\ \vdots\\ \psi^{\dagger}_{(n)}(\mathbf{k})\end{pmatrix}. \tag{1.4.4}$$

Now lets us look at the derivative of $\underline{\underline{U}}^{\dagger}\,\underline{\underline{U}}$ with respect to momentum

$$\partial_{\mathbf{k}}\,\underline{\underline{1}} = \partial_{\mathbf{k}}\left(\underline{\underline{U}}^{\dagger}\,\underline{\underline{U}}\right) = \left(\partial_{\mathbf{k}}\,\underline{\underline{U}}^{\dagger}\right)\underline{\underline{U}} + \underline{\underline{U}}^{\dagger}\left(\partial_{\mathbf{k}}\,\underline{\underline{U}}\right). \tag{1.4.5}$$

Obvious this implies the following identity

$$\underline{\underline{U}}^{\dagger}\left(\partial_{\mathbf{k}}\,\underline{\underline{U}}\right) = -\left(\partial_{\mathbf{k}}\,\underline{\underline{U}}^{\dagger}\right)\underline{\underline{U}}, \tag{1.4.6}$$

but it also suggests the following generalization of the Berry connection or equation (1.2.2)

$$\underline{\underline{\mathcal{A}}}(\mathbf{k}) = i\,\underline{\underline{U}}^{\dagger}\left(\partial_{\mathbf{k}}\,\underline{\underline{U}}\right) = -i\left(\partial_{\mathbf{k}}\,\underline{\underline{U}}^{\dagger}\right)\underline{\underline{U}} = \left(\underline{\underline{\mathcal{A}}}(\mathbf{k})\right)^{\dagger}. \tag{1.4.7}$$

First we see that $\underline{\underline{\mathcal{A}}}$ is Hermitian. $\underline{\underline{\mathcal{A}}}$ could be called the matrix Berry connection, however we will just call it the Berry connection. For the two level system, the Berry connection can formally be written as

$$\underline{\underline{\mathcal{A}}} = \begin{pmatrix} u^{\dagger}_{(1)1}\partial_{\mathbf{k}}u_{(1)1} + u^{\dagger}_{(1)2}\partial_{\mathbf{k}}u_{(1)2} & u^{\dagger}_{(1)1}\partial_{\mathbf{k}}u_{(2)1} + u^{\dagger}_{(1)2}\partial_{\mathbf{k}}u_{(2)2} \\ u^{\dagger}_{(2)1}\partial_{\mathbf{k}}u_{(1)1} + u^{\dagger}_{(2)2}\partial_{\mathbf{k}}u_{(1)2} & u^{\dagger}_{(2)2}\partial_{\mathbf{k}}u_{(2)2} + u^{\dagger}_{(2)1}\partial_{\mathbf{k}}u_{(2)1} \end{pmatrix}. \tag{1.4.8}$$

We note that the diagonal entries are the Berry connection as defined in equation (1.2.2). The off diagonal entries will only play a minor role an their physical interpretation are not clear. With this remark we conclude the introduction. In the next chapter we will derive a semi-classical transport equation form phase space arguments and the time dependent variational principle of quantum mechanics.

Chapter 2

Semi-classical Anomalous Transport

This chapter is centered on how to get the anomalous Hall response from semi-classical considerations. We will dissus the steps in the process of constructing a semi-classical Boltzmann equation, how to solve it in the cases where a anomalous velocity is perpendicular to the electric field, then use that solution to obtain the current density along with the conductivity.

2.1 Phenomenological Derivation of the Boltzmann Equation

The Boltzmann equation was originally developed to study transport in thin classical gases by Boltzmann in 1872, however it has also found wide application in transport phenomena of metals and semi-conductors. That electrons in metals can be treated as a non-interacting gas is not obvious, but due to the Fermi liquid picture provided by Landau in 1956 this is well justified. For completeness we give simple derivation of the Boltzmann equation from phase-space analysis. This is to set the basis for a further discussion of the Boltzmann equation. For a more detailed discussion of how to obtain the Boltzmann equation and its semi-classical use see Smith and Højgaard Jensen[20].

Lets consider the particle number $\mathrm{d}N(t,\mathbf{1})$ in a small region around a point called $(\mathbf{1})$ or $(\mathbf{r},\mathbf{k})$ in phase-space. We then can define a non-equilibrium distribution function $f(t,\mathbf{1})$ as

$$\mathrm{d}N(\mathbf{r},\mathbf{k},t) = f(\mathbf{r},\mathbf{k},t)\frac{\mathrm{d}\mathbf{r}\,\mathrm{d}\mathbf{k}}{8\pi^3}. \tag{2.1.1}$$

The continuity equation for f is obtained by considering the distribution function f at two infinitesimal separated times t and $t+\mathrm{d}t$

$$f(\mathbf{r},\mathbf{k},t)\mathrm{d}\mathbf{r}\,\mathrm{d}\mathbf{k} + I_{\mathrm{coll}}\mathrm{d}\mathbf{r}\,\mathrm{d}\mathbf{k}\,\mathrm{d}t = f(\mathbf{r}',\mathbf{k}',t+\mathrm{d}t)\mathrm{d}\mathbf{r}'\mathrm{d}\mathbf{k}', \tag{2.1.2}$$

where I_{coll} is the collision integral and is included to handle scattering effects the colloquial, interactions , etc.. The collision integarl will depend on the distribution function along with some explicit dependence on coordinates and time. One imported physical constraint on the collision integral is that its $\mathbf{k}$ integration must be zero to conserve particle number[1][27]. The evolution of the particles in phase-space has be sketched in figure 2.1. The primed and unprimed coordinates are connected by $\mathbf{1}' = \mathbf{1} + \dot{\mathbf{1}}dt$. Due Liouville's theorem[25] who states that the phase-space volume does not change, hence $\mathrm{d}\mathbf{r}'\mathrm{d}\mathbf{k}' = \mathrm{d}\mathbf{r}\,\mathrm{d}\mathbf{k}$. Applying this gives

$$f(\mathbf{r},\mathbf{k},t) + I_{\mathrm{coll}}\mathrm{d}t = f(\mathbf{r}+\dot{\mathbf{r}}\mathrm{d}t, \mathbf{k}+\dot{\mathbf{k}}\mathrm{d}t, t+\mathrm{d}t). \tag{2.1.3}$$

Now Taylor expanding the right side to linear order

$$f(\mathbf{r},\mathbf{k},t) + I_{\mathrm{coll}}\mathrm{d}t = f(\mathbf{r},\mathbf{k},t) + \frac{\mathrm{d}}{\mathrm{d}t}f(\mathbf{r},\mathbf{k},t)\mathrm{d}t. \tag{2.1.4}$$

[1]Note that in the case of a multi-band system, this is no longer true as scattering to another band is possible, while keeping the positions

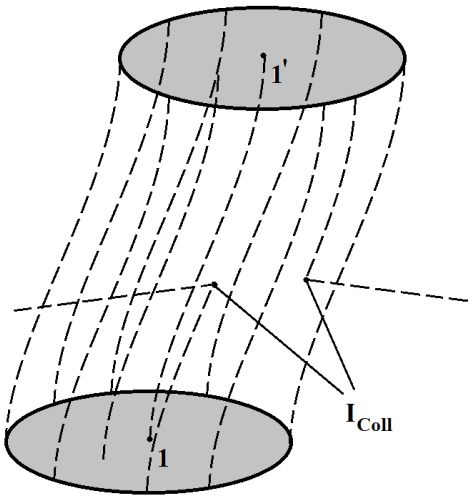

Figure 2.1: An sketched of phase-space evolution of a bunch of particles. Here the effect of the collision integral is illustrated by particles scattering in and out, note the thy only scatter to different $\mathbf{k}$ values as discontinuous parts in the space coordinate would violate causality.

Rearranging the terms, expanding the total derivative and suppressing the arguments in the distribution function, we finally arrive at the Boltzmann equation

$$I_{\text{coll}} = \frac{\partial}{\partial t} f + \dot{\mathbf{r}} \cdot \frac{\partial}{\partial \mathbf{r}} f + \dot{\mathbf{k}} \cdot \frac{\partial}{\partial \mathbf{k}} f. \tag{2.1.5}$$

By simple continuity arguments we where able to establish the Boltzmann equation, however we will need the equation of motion for $\mathbf{r}$ and $\mathbf{k}$. This will be done in the following section.

2.2 Semi-Classical Equation of Motion

In section 2.1 we derived the Boltzmann equation from phase-space consideration whicho has the form

$$\frac{\partial}{\partial t} f + \dot{\mathbf{r}} \cdot \frac{\partial}{\partial \mathbf{r}} f + \dot{\mathbf{k}} \cdot \frac{\partial}{\partial \mathbf{k}} f = I_{\text{coll}}. \tag{2.2.1}$$

However the phase-space consideration gives no equation of motion for $\mathbf{r}$ and $\mathbf{k}$. So one has to turn to the specific physical problem at hand. For example if we were to consider a charged classical gas we would have simply identified $\dot{\mathbf{k}}$ with the Lorentz force and $\dot{\mathbf{r}}$ with the velocity. However as we in general want to consider electrons with non-trivial spin structures a classical approach does not capture effects related to these degrees for freedom. Hence we have to use a method where we can include such quantum mechanical effects, but that raises the question on how to make sense of both well-defined position and momentum simultaneous with out violating the uncertainty principle. The answer to which would be some wave packet as they can be centred around point in both space and momentum, but at the same time satisfy the uncertainty principle. So let us restate the Boltzmann equation in terms of such centre of mass wave packet coordinates and denote them as $\mathbf{r}_c$ and $\mathbf{k}_c$. We then find the equation of motion of $\mathbf{r}_c$ and $\mathbf{k}_c$ which is usually done through the time dependent variational principle as discussed by Niu and collaborators [13, 14]. To do such calculation we will need to define the time dependent variational principle, which will be the subject of the next section.

2.2.1 The Time Dependent Variational Principle in Quantum Mechanics

In this section we will go through the arguments leading to the time dependent variational principle of quantum mechanics, which is based on the idea that by calculating the Lagrangian of quantum mechanics in a Hilbert space restricted by some parameters and do variational calculation one can obtain the equations of motion of those parameters.

Our starting point is Kramer and Saraceno[23] who define the following action for quantum mechanics

$$S = \int_{t_1}^{t_2} \mathrm{d}t L(\psi, \bar{\psi}; t), \tag{2.2.2}$$

where the Lagrangian $L(\psi, \bar{\psi})$ is:

$$L(\psi, \bar{\psi}; t) = \left\langle \psi(t) \left| i\frac{\partial}{\partial t} - H \right| \psi(t) \right\rangle, \tag{2.2.3}$$

$\langle \psi(t) |$ and $| \psi(t) \rangle$ have to be normalized at all times. Now let us show this is consistent with the Schrödinger equation. First note that $\langle \psi(t) |$ and $| \psi(t) \rangle$ are treated as they where independent, and think of them as fields [2]we vary the action in equation (2.2.2).

$$\begin{aligned} \delta S &= \int_{t_1}^{t_2} \mathrm{d}t \delta \left(\left\langle \psi(t) \left| i\frac{\partial}{\partial t} - H \right| \psi(t) \right\rangle \right) \\ &= \int_{t_1}^{t_2} \mathrm{d}t \left(i \left\langle \delta\psi(t) \right| \left. \partial_t \psi(t) \right\rangle + i \left\langle \psi(t) \right| \left. \partial_t \delta\psi(t) \right\rangle - \left\langle \delta\psi(t) \right| H \left| \psi(t) \right\rangle - \left\langle \psi(t) \right| H \left| \delta\psi(t) \right\rangle \right) \\ &= \int_{t_1}^{t_2} \mathrm{d}t \left(i \left\langle \delta\psi(t) \right| \left. \partial_t \psi(t) \right\rangle - i \left\langle \partial_t \psi(t) \right| \left. \delta\psi(t) \right\rangle - \left\langle \delta\psi(t) \right| H \left| \psi(t) \right\rangle - \left\langle \psi(t) \right| H \left| \delta\psi(t) \right\rangle \right), \end{aligned} \tag{2.2.4}$$

where in the second equality we used partial integration. Now as $| \psi(t) \rangle$ and $\langle \psi(t) |$ where treated as they were independent and $| \delta\psi(t) \rangle$ and $\langle \delta\psi(t) |$ can vary arbitrary except at the end points, the only way to get the variation of the action S to be zero, hence using Hamilton's principlem, is if the following two equation is zero

$$i\frac{\partial}{\partial t} \left| \psi(t) \right\rangle - H \left| \psi(t) \right\rangle = 0 \tag{2.2.5}$$

$$- \left\langle \psi(t) \right| i\frac{\partial}{\partial t} - \left\langle \psi(t) \right| H = 0, \tag{2.2.6}$$

which is precisely the Schrödinger equation and its complex conjugate.

An equivalent, more transparent way to obtain the Schrödinger equation is to expand the wave function in a complete basis of eigenstates of the Hamiltonian and then do the variation with respect to the coefficient, hence complex numbers. First step is to rewrite the Lagrangian in equation (2.2.3) by expanding it in such a basis:

$$\begin{aligned} L(\psi, \bar{\psi}; t) = L(c_1^*, ..., c_\infty^*, c_1, ..., c_\infty) &= \sum_{n,m} c_m^*(t) \left\langle m \left| i\frac{\partial}{\partial t} - H \right| n \right\rangle c_n(t) \\ &= \sum_{n,m} i c_m^*(t) \left\langle m \right| \left. \dot{n} \right\rangle c_n(t) + i c_m^*(t) \left\langle m \right| \left. n \right\rangle \dot{c_n}(t) - c_m^*(t) \left\langle m \right| H \left| n \right\rangle c_n(t) \\ &= \sum_{n,m} i c_m^*(t) \left\langle m \right| \left. \dot{n} \right\rangle c_n(t) + i c_m^*(t) \delta_{mn} \dot{c}_n(t) - c_m^*(t) H_{mn} c_n(t). \end{aligned} \tag{2.2.7}$$

[2]Think of them being projected on to the position basis, if varying states in a Hilbert space seems strange.

Varying the action using this Lagrangian leads to

$$\delta S = \int_{t_1}^{t_2} \mathrm{d}t\, \delta \left(\sum_{n,m} i c_m^*(t) \langle m \mid \dot{n} \rangle c_n(t) + i c_m^*(t) \delta_{mn} \dot{c}_n(t) - c_m^*(t) H_{mn} c_n(t) \right) \tag{2.2.8}$$

$$\begin{aligned} &= \int_{t_1}^{t_2} \mathrm{d}t \sum_{n,m} \left(i\delta c_m^*(t) \langle m \mid \dot{n} \rangle c_n(t) + i c_m^*(t) \langle m \mid \dot{n} \rangle \delta c_n(t) + i\delta c_m^*(t) \delta_{mn} \dot{c}_n(t) \right. \\ &\quad \left. + i c_m^*(t) \delta_{mn} \delta \dot{c}_n(t) - \delta c_m^*(t) H_{mn} c_n(t) - c_m^*(t) H_{mn} \delta c_n(t) \right) \\ &= \int_{t_1}^{t_2} \mathrm{d}t \sum_{n,m} i \left(\delta c_m^*(t) \langle m \mid \dot{n} \rangle c_n(t) - i c_m^*(t) \langle \dot{m} \mid n \rangle \delta c_n(t) + i\delta c_m^*(t) \delta_{mn} \dot{c}_n(t) \right. \\ &\quad \left. - i\dot{c}_m^*(t) \delta_{mn} \delta c_n(t) - \delta c_m^*(t) H_{mn} c_n(t) - c_m^*(t) H_{mn} \delta c_n(t) \right), \end{aligned}$$

where we in the third equality we used partial integration on the fourth term. As c_m^* and c_n are treated as being independent the following two equations have to be zero:

$$\sum_n i \langle m \mid \dot{n} \rangle c_n(t) + i\delta_{mn} \dot{c}_n(t) - H_{mn} c_n(t) = 0, \tag{2.2.9}$$

$$\sum_m -i c_m^*(t) \langle \dot{m} \mid n \rangle - i\dot{c}_m^*(t) \delta_{mn} - c_m^*(t) H_{mn} = 0, \tag{2.2.10}$$

which is consistent with the result in equation (2.2.5) by making the same expansion on a complete set and taking the inner product with a specific sate from the same complete set. This gives explicitly the insight that one have to vary infinitely many parameters to get the Schrödinger equation, at least for a Hamiltonian that depends on a continues variable.
Now having shown that the variational principal can be used to derive quantum mechanics in general, we turn to the problem of getting equations of motion for parameters for a specific problem. These parameters can in principal be any ting, but if the reason for doing variational calculations is to get some semi-classical equations for motion, the parameter should in this case corespondet to classical variables. The process of getting an equation of motion for some parameter can be divided in to three steps:

Step

I Choose a trial wave function , written as $\psi(x_1(t), x_2(t), ..., x_n(t))$, depending on a finite number of time dependent parameters and with no other time dependences. The choice should be based on some physical reasoning, for example if we have a parameter that corresponds to position, the expectation value of the position operator should give that parameter.

II Calculate the Lagrangian given in equation (2.2.3) on the basis of the wave function chosen in I. Note that the Lagrangian will be a functional of $(x_1(t), x_2(t), ..., x_n(t))$ and $(\dot{x}_1(t), \dot{x}_2(t), ..., \dot{x}_n(t))$.

III Use the Euler-Lagrange equations to get equations of motion for $(x_1(t), x_2(t), ..., x_n(t))$. In general this will yield n, which is the number of parameters, coupled differential equations.

As pointed out in Step I, there is no formal way to choose the trial wave function. It is therefore up to intuition, symmetry considerations and that one should be able to calculate the Lagrangian in a closed form to choose the wave function. The arbitrariness of the trial wave function is also at the root of the problems with this method as there is no way to quantify how good the results from this method are. One should also note that this treatment relies heavily on Fermi liquid theory as we here relay on a one particle calculation. Having introduced the variational principle we will now use it in the context of a quantum system with a non-trivial spin structure.

2.2.2 Determination of $\dot{\mathbf{r}}$ and $\dot{\mathbf{p}}$ through Variational Principle

The following derivation is based on the book by Marder[24], but works along the same lines that was first made by Niu and collaborators [13, 14]. However we have simplified it in some respect to make it more compehedable and clarified some of the more involved steps.
In this subsection we will derive equations of motion for $\mathbf{r}$ and $\mathbf{p}$ though the method developed in

subsection 2.2.1. To make the process as transparent as possible the derivation will be carried out through the three steps introduced above.

Step I: The Trial Wave Function

Defining a trial wave function for the problem of transport is done through the following consideration. We first define a wave packet centred at a point in space. The form of the wave packet could for an example be Gaussian. The packet should have a width much larger than the atomic spacing but still much smaller that variation in the external fields. This also means that one can only use a small range of momentum space compared to the size of the Brillouin zone making the momentum distribution sharp. We have made a construction that enabled us to talk about a coordinates in both momentum space and real space at the same time in the sense of center of mass coordinates, called $\mathbf{r}_c$ and $\mathbf{k}_c$. It is important to note that $\mathbf{r}_c$ and $\mathbf{k}_c$ should not be considered variables, rather parameters with an explicit time dependence. The time dependence, however will be suppressed in the notation. With this in mind we define a wave packet $W_{\mathbf{r}_c\mathbf{k}_c}(\mathbf{r})$:

$$\langle\ \mathbf{r}\ |W_{\mathbf{r}_c\mathbf{k}_c}\rangle = W_{\mathbf{r}_c\mathbf{k}_c}(\mathbf{r}) = \frac{1}{\sqrt{\mathcal{V}}}\sum_{\mathbf{k}} w_{\mathbf{k}\mathbf{k}_c} e^{-i\chi(\mathbf{r})-i\mathbf{k}\cdot\mathbf{r}_c}\psi_{\mathbf{k}}(\mathbf{r}), \tag{2.2.11}$$

where $w_{\mathbf{k}\mathbf{k}_c}$ are the amplitudes of the Fourier transform, where the subscript specifies that the weight factors depends one the centre of mass coordinate, $\mathcal{V}$ is the volume of the system and $\psi_{\mathbf{k}}(\mathbf{r})$ is given as:

$$\psi_{\mathbf{k}}(\mathbf{r}) = u_{\sigma,\mathbf{k},n}e^{i\mathbf{k}\cdot\mathbf{r}}. \tag{2.2.12}$$

Where $u_{\sigma,\mathbf{k},n}$ is a normalized eigenspinor of the Hamiltonian of the problem studied, the σ is the spin index and n is the band [3], lastly $\chi(\mathbf{r})$ is a local gauge phase. The normalization of $W_{\mathbf{r}_c\mathbf{k}_c}(\mathbf{r})$ requires

$$\begin{aligned} 1 &= \langle W_{\mathbf{r}_c\mathbf{k}_c}\,|W_{\mathbf{r}_c\mathbf{k}_c}\rangle \\ &= \frac{1}{\mathcal{V}}\sum_{\mathbf{k}\mathbf{k}'}\int \mathrm{d}\mathbf{r} e^{i(\mathbf{k}'-\mathbf{k})\cdot\mathbf{r}_c} w^*_{\mathbf{k}'\mathbf{k}_c} w_{\mathbf{k}\mathbf{k}_c}\psi^*_{\mathbf{k}'}(\mathbf{r})\psi_{\mathbf{k}}(\mathbf{r}) \\ &= \sum_{\mathbf{k}\mathbf{k}'}\delta_{\mathbf{k}'\mathbf{k}} w^*_{\mathbf{k}'\mathbf{k}_c} w_{\mathbf{k}\mathbf{k}_c}. \end{aligned} \tag{2.2.13}$$

where we use that the eigenspinors are orthonormal and the exponential function gives a delta function when integrated. This gives the constrain on $w_{\mathbf{k}\mathbf{k}_c}$:

$$\sum_{\mathbf{k}} |w_{\mathbf{k}\mathbf{k}_c}|^2 = 1 \tag{2.2.14}$$

Now we require $W_{\mathbf{r}_c\mathbf{k}_c}(\mathbf{r})$ to be centered around $\mathbf{k}_c$ even when electromagnetic fields are present, where the kinetic momentum operator is given as $\hat{\mathbf{p}} = -i\partial_{\mathbf{r}} + e\mathbf{A}(\mathbf{r})$. So to get an equation for $\chi(\mathbf{r})$ let us calculate the expectation value of $-i\partial_{\mathbf{r}} + e\mathbf{A}(\mathbf{r})$ and require that it is equal to $\mathbf{k}_c$

$$\begin{aligned} \mathbf{k}_c &= \langle W_{\mathbf{r}_c\mathbf{k}_c}| - i\partial_{\mathbf{r}} + e\mathbf{A}(\mathbf{r})\,|W_{\mathbf{r}_c\mathbf{k}_c}\rangle \\ &= \frac{1}{\mathcal{V}}\int \mathrm{d}\mathbf{r}\sum_{\mathbf{k},\mathbf{k}'} w^*_{\mathbf{k}'\mathbf{k}_c} e^{i\chi(\mathbf{r})+i\mathbf{k}'\cdot\mathbf{r}_c-i\mathbf{k}\cdot\mathbf{r}} u^*_{\sigma,\mathbf{k}',n}\left(-i\partial_{\mathbf{r}} + e\mathbf{A}(\mathbf{r})\right) w_{\mathbf{k}\mathbf{k}_c} e^{-i\chi(\mathbf{r})-i\mathbf{k}\cdot\mathbf{r}_c+i\mathbf{k}\cdot\mathbf{r}} u_{\sigma,\mathbf{k},n} \\ &= \frac{1}{\mathcal{V}}\int \mathrm{d}\mathbf{r}\sum_{\mathbf{k},\mathbf{k}'} w^*_{\mathbf{k}'\mathbf{k}_c} e^{i\mathbf{k}'\cdot\mathbf{r}_c-i\mathbf{k}\cdot\mathbf{r}} u^*_{\sigma,\mathbf{k}',n}\left(\mathbf{k} + e\mathbf{A}(\mathbf{r}) - [\partial_{\mathbf{r}}\chi(\mathbf{r})]\right) w_{\mathbf{k}\mathbf{k}_c} e^{-i\mathbf{k}\cdot\mathbf{r}_c+i\mathbf{k}\cdot\mathbf{r}} u_{\sigma,\mathbf{k},n} \\ &= \mathbf{k}_c + \frac{1}{\mathcal{V}}\int \mathrm{d}\mathbf{r}\sum_{\mathbf{k},\mathbf{k}'} w^*_{\mathbf{k}'\mathbf{k}_c} e^{i\mathbf{k}'\cdot\mathbf{r}_c-i\mathbf{k}\cdot\mathbf{r}} u^*_{\sigma,\mathbf{k}',n}\left(e\mathbf{A}(\mathbf{r}) - [\partial_{\mathbf{r}}\chi(\mathbf{r})]\right) w_{\mathbf{k}\mathbf{k}_c} e^{-i\mathbf{k}\cdot\mathbf{r}_c+i\mathbf{k}\cdot\mathbf{r}} u_{\sigma,\mathbf{k},n}. \end{aligned} \tag{2.2.15}$$

[3] Marder for good reasons considers $\mathbf{u}_{\mathbf{k},n}$ to be dependent periodical (Bloch modulations) on space which gives a term in the final equation for the $\mathbf{r}_c$ concerning magnetisation of the magnetic unit cell.

Now we see that if

$$e\mathbf{A}(\mathbf{r}) = \partial_{\mathbf{r}}\chi(\mathbf{r}), \tag{2.2.16}$$

The expatiation value of the momentum operator is $\mathbf{k}_c$. Solving equation (2.2.16) for χ one gets

$$\chi(\mathbf{r}) = e\int^{\mathbf{r}} \mathbf{A}(\mathbf{r}')\mathrm{d}\mathbf{r}, \tag{2.2.17}$$

which is know as the Aharonov-Bohm phase. The Aharonov-Bohm phase can be simplified in our case, because the wave packet are required to be centered around $\mathbf{r}_c$ and the magnetic fields are required to be small. Therefor the vector potential can be viewed as constant in a region around $\mathbf{r}_c$ comparable to the spread of the wave pack, which means that the Aharonov-Bohm phase can be approximate as $e\mathbf{A}(\mathbf{r}_c)\cdot\mathbf{r}$. This means that our wave function should take on the form

$$\langle \mathbf{r}\,|W_{\mathbf{r}_c\mathbf{k}_c}\rangle = W_{\mathbf{r}_c\mathbf{k}_c}(\mathbf{r}) = \frac{1}{\sqrt{\mathcal{V}}}\sum_{\mathbf{k}} w_{\mathbf{k}\mathbf{k}_c} e^{-ie\mathbf{A}(\mathbf{r}_c)\cdot\mathbf{r}-i\mathbf{k}\cdot\mathbf{r}_c}\psi_{\mathbf{k}}(\mathbf{r}). \tag{2.2.18}$$

However we still need to make sure that $\mathbf{r}_c$ is the expectation value of the position operator $\mathbf{r}$. It turns out, in the presence of spinors that depends non-trivially on momentum, one has to choose the amplitudes $w_{\mathbf{k}\mathbf{k}_c}$ carefully, if the wave pack is to be centered around $\mathbf{r}_c$. To show this we will simply calculate the expectation value of the position operator $\mathbf{r}$ and observe which constraints on $w_{\mathbf{k}\mathbf{k}_c}$ this will lead to, if the expectation value is required to be $\mathbf{r}_c$:

$$\begin{aligned}
\mathbf{r}_c = \langle W_{\mathbf{r}_c\mathbf{k}_c}|\,\mathbf{r}\,|W_{\mathbf{r}_c\mathbf{k}_c}\rangle &= \frac{1}{N}\sum_{\mathbf{k}\mathbf{k}'}\int \mathrm{d}\mathbf{r} e^{i(\mathbf{k}'-\mathbf{k})\cdot\mathbf{r}_c} w^*_{\mathbf{k}'\mathbf{k}_c} w_{\mathbf{k}\mathbf{k}_c}\psi^*_{\mathbf{k}'}(\mathbf{r})\psi_{\mathbf{k}}(\mathbf{r})\mathbf{r} \qquad (2.2.19)\\
&= \frac{1}{N}\sum_{\mathbf{k}\mathbf{k}'}\int \mathrm{d}\mathbf{r} e^{i(\mathbf{k}'-\mathbf{k})\cdot(\mathbf{r}_c-\mathbf{r})} w^*_{\mathbf{k}'\mathbf{k}_c} w_{\mathbf{k}\mathbf{k}_c} u^*_{\sigma,\mathbf{k}',n} u_{\sigma,\mathbf{k},n}\mathbf{r}\\
&= \frac{1}{N}\sum_{\mathbf{k}\mathbf{k}'}\int \mathrm{d}\mathbf{r} w^*_{\mathbf{k}'\mathbf{k}_c} w_{\mathbf{k}\mathbf{k}_c} u^*{}_{\sigma,\mathbf{k}',n} u_{\sigma\mathbf{k},n}\left(\frac{\partial}{\partial i\mathbf{k}} e^{i(\mathbf{k}'-\mathbf{k})\cdot(\mathbf{r}_c-\mathbf{r})} + \mathbf{r}_c e^{i(\mathbf{k}'-\mathbf{k})\cdot(\mathbf{r}_c-\mathbf{r})}\right)\\
&= \mathbf{r}_c - \frac{1}{N}\sum_{\mathbf{k}\mathbf{k}'}\int \mathrm{d}\mathbf{r} w^*_{\mathbf{k}'\mathbf{k}_c} u^*{}_{\sigma,\mathbf{k}',n} e^{i(\mathbf{k}'-\mathbf{k})\cdot(\mathbf{r}_c-\mathbf{r})}\frac{\partial}{\partial i\mathbf{k}}\left[w_{\mathbf{k}\mathbf{k}_c} u_{\sigma,\mathbf{k},n}\right]\\
&= \mathbf{r}_c - \sum_{\mathbf{k}\mathbf{k}'} w^*_{\mathbf{k}'\mathbf{k}_c} u^*{}_{\sigma,\mathbf{k}',n}\delta_{\mathbf{k},\mathbf{k}'}\frac{\partial}{\partial i\mathbf{k}}\left[w_{\mathbf{k}\mathbf{k}_c} u_{\sigma,\mathbf{k},n}\right]\\
&= \mathbf{r}_c - \sum_{\mathbf{k}} |w_{\mathbf{k}\mathbf{k}_c}|^2 u^*{}_{\sigma,\mathbf{k},n}\frac{1}{w_{\mathbf{k}\mathbf{k}_c}}\frac{\partial}{\partial i\mathbf{k}}\left[w_{\mathbf{k}\mathbf{k}_c} u_{\sigma,\mathbf{k},n}\right]\\
&= \mathbf{r}_c + \sum_{\mathbf{k}} |w_{\mathbf{k}\mathbf{k}_c}|^2\left(i u^*{}_{\sigma,\mathbf{k},n}\frac{\partial}{\partial\mathbf{k}} u_{\sigma,\mathbf{k},n} - \frac{\partial}{\partial i\mathbf{k}}\ln w_{\mathbf{k}\mathbf{k}_c}\right) \qquad (2.2.20)
\end{aligned}$$

We see that the momentum sum must vanish. In order for that to happen we can assume a certain form for the amplitudes $w_{\mathbf{k}\mathbf{k}_c}$. First the norm should only depend one the relative coordinate written as $|w_{\mathbf{k}-\mathbf{k}_c}|$, more over we will also need that $|w_{\mathbf{k}-\mathbf{k}_c}|^2$ is sarply peaked at $\mathbf{k}_c$, where sarply peaked is used in the senses that we will treat it as a delta function for the sake of calculations. which meas that $|w_{\mathbf{k}-\mathbf{k}_c}|$ also have to has a maximum there. Lastly the phase of $w_{\mathbf{k}\mathbf{k}_c}$ is useful to specified as

$$w_{\mathbf{k}\mathbf{k}_c} = |w_{\mathbf{k}-\mathbf{k}_c}|\, e^{i(\mathbf{k}-\mathbf{k}_c)\cdot\boldsymbol{\mathcal{A}}_n(\mathbf{k}_c)}. \tag{2.2.21}$$

Where $\mathcal{A}_n(\mathbf{k}_c)$ is a vector function to be specified later. Evaluating the last term in the sum in the last line of equation (2.2.20):

$$\begin{aligned}\sum_{\mathbf{k}} |w_{\mathbf{k}-\mathbf{k}_c}|^2 \frac{\partial}{\partial i\mathbf{k}} \ln w_{\mathbf{k}\mathbf{k}_c} &= \sum_{\mathbf{k}} |w_{\mathbf{k}-\mathbf{k}_c}|^2 \frac{\partial}{\partial i\mathbf{k}} \left(\ln |w_{\mathbf{k}-\mathbf{k}_c}| + i(\mathbf{k}-\mathbf{k}_c)\cdot \boldsymbol{\mathcal{A}}_n(\mathbf{k}_c)\right) \\ &= \sum_{\mathbf{k}} |w_{\mathbf{k}-\mathbf{k}_c}|^2 \left(\frac{1}{|w_{\mathbf{k}-\mathbf{k}_c}|}\frac{\partial}{\partial i\mathbf{k}} |w_{\mathbf{k}-\mathbf{k}_c}| + \boldsymbol{\mathcal{A}}_n(\mathbf{k}_c) + (\mathbf{k}-\mathbf{k}_c)\frac{\partial}{\partial \mathbf{k}}\boldsymbol{\mathcal{A}}_n(\mathbf{k}_c)\right) \\ &= \boldsymbol{\mathcal{A}}_n(\mathbf{k}_c),\end{aligned} \tag{2.2.22}$$

where we in the last equality used that $|w_{\mathbf{k}-\mathbf{k}_c}|$ does only depend on the relative coordinate $\mathbf{k}-\mathbf{k}_c$ and is peaked at $\mathbf{k}_c$. We now observe that if the expectation value of the position operator is to be $\mathbf{r}_c$, $\boldsymbol{\mathcal{A}}_n(\mathbf{k}_c)$ has to be

$$\boldsymbol{\mathcal{A}}_n(\mathbf{k}_c) = \sum_{\mathbf{k}} |w_{\mathbf{k}\mathbf{k}_c}|^2 \, i u^*_{\sigma,\mathbf{k},n} \frac{\partial}{\partial \mathbf{k}} u_{\sigma,\mathbf{k},n} = i u^*_{\sigma,\mathbf{k},n} \frac{\partial}{\partial \mathbf{k}} u_{\sigma,\mathbf{k},n}\Big|_{\mathbf{k}=\mathbf{k}_c}. \tag{2.2.23}$$

Now $\mathcal{A}_n$ can be recognized as the Berry curvature as it is of the form given in equation (1.2.2). We have now defined how a wave function centered in phase space around $(\mathbf{r}_c, \mathbf{k}_c)$ looks:

$$\langle \mathbf{r} | W_{\mathbf{r}_c\mathbf{k}_c} \rangle = \frac{1}{\sqrt{\mathcal{V}}} \sum_{\mathbf{k}} |w_{\mathbf{k}-\mathbf{k}_c}| \, e^{i(\mathbf{k}-\mathbf{k}_c)\cdot\boldsymbol{\mathcal{A}}_n(\mathbf{k}_c) - ie\mathbf{A}(\mathbf{r}_c)\cdot\mathbf{r} - i\mathbf{k}\cdot\mathbf{r}_c} \psi_{\mathbf{k}}(\mathbf{r}) \tag{2.2.24}$$

Note that the Berry connection enters in the same way as the vector potential, namely as Berry-"Aharonov-Bohm phase", but it depends on momentum instead of position hence we have a gauge phase which is local in phase space instead of real space

We have now defined a wave function $|W_{\mathbf{r}_c\mathbf{k}_c}\rangle$ that according to our intuition captures the important physical concepts of the type of systems we want to study, and that has a sufficiently simple form with respect to our goal of obtaining a closed expression of the Lagrangian. With a trial wave function at hand we can proceed to the next step.

Step II. Calculate the Lagrangian

Now we have to calculate the Lagrangian defined in (2.2.3), using the trail wave function found in the previous step. Note that this calculation takes place in the Hilbert space restricted by the two parameters $\mathbf{r}_c$ and $\mathbf{k}_c$ and the form of the wave function, and will there for only yield result that are achievable within this subspace. The Lagrangian in our specific case including the vector potential and the electric potential for including external fields is

$$\begin{aligned} L &= \langle W_{\mathbf{r}_c\mathbf{k}_c}| \, i\hbar \frac{\partial}{\partial t} |W_{\mathbf{r}_c\mathbf{k}_c}\rangle - \langle W_{\mathbf{r}_c\mathbf{k}_c}| \, H - e\varphi(\mathbf{r}) \, |W_{\mathbf{r}_c\mathbf{k}_c}\rangle, \\ H &= \frac{1}{2m}\left[p + e\mathbf{A}\right]^2, \\ \frac{p^2}{2m}\psi_{\mathbf{k}} &= \xi_{\mathbf{k}}\psi_{\mathbf{k}}, \end{aligned} \tag{2.2.25}$$

where φ is the electric potential. Note that we have take an explicit form of the Hamiltonian, the quadratic kinetic energy to simplify the calculations. However in some case one might want to consider other dispersions. The only change to the result will then be the terms derived from the Hamiltonian.

We start by treating the partial time derivative. Here we can use the explicit time dependence of $\mathbf{k}_c$ and $\mathbf{r}_c$ to expand it as

$$i\frac{\partial}{\partial t} = i\dot{\mathbf{r}}_c \cdot \frac{\partial}{\partial \mathbf{r}_c} + i\dot{\mathbf{k}}_c \cdot \frac{\partial}{\partial \mathbf{k}_c}. \tag{2.2.26}$$

Let us continue by evaluating the two resulting terms. We start with the $\dot{\mathbf{r}}_c$ term:

$$\begin{aligned}
&\langle W_{\mathbf{r}_c\mathbf{k}_c}|i\hbar\dot{\mathbf{r}}_c\cdot\frac{\partial}{\partial\mathbf{r}_c}|W_{\mathbf{r}_c\mathbf{k}_c}\rangle \qquad (2.2.27)\\
&=\frac{i\hbar}{\mathcal{V}}\int\mathrm{d}\mathbf{r}\sum_{\mathbf{k},\mathbf{k}'}w^*_{\mathbf{k}'\mathbf{k}_c}e^{ie\mathbf{A}(\mathbf{r}_c)\cdot\mathbf{r}+i\mathbf{k}'\cdot\mathbf{r}_c}\psi^*_{\mathbf{k}'}(\mathbf{r})\dot{\mathbf{r}}_c\cdot\frac{\partial}{\partial\mathbf{r}_c}w_{\mathbf{k}\mathbf{k}_c}e^{-ie\mathbf{A}(\mathbf{r}_c)\cdot\mathbf{r}-i\mathbf{k}\cdot\mathbf{r}_c}\psi_{\mathbf{k}}(\mathbf{r})\\
&=\frac{i\hbar}{\mathcal{V}}\int\mathrm{d}\mathbf{r}\sum_{\mathbf{k},\mathbf{k}'}w^*_{\mathbf{k}'\mathbf{k}_c}w_{\mathbf{k}\mathbf{k}_c}e^{i(\mathbf{k}'-\mathbf{k})\mathbf{r}_c}\psi^*_{\mathbf{k}_c}(\mathbf{r})\psi_{\mathbf{k}_c}(\mathbf{r})\dot{r}_{c,i}\cdot\left(-ie\frac{\partial}{\partial r_{c,i}}\left(r_jA(\mathbf{r}_c)_j\right)-ik_i\right)\\
&=er_j\left(\dot{r}_i\frac{\partial}{\partial r_i}\right)A(\mathbf{r}_c)_j+\sum_{\mathbf{k}}w^*_{\mathbf{k}\mathbf{k}_c}w_{\mathbf{k}\mathbf{k}_c}\left(\dot{r}_{c,i}k_i\right)\\
&=e\mathbf{r}_c\cdot\left(\dot{\mathbf{r}}_c\cdot\frac{\partial}{\partial\mathbf{r}_c}\right)\mathbf{A}(\mathbf{r}_c)+\dot{\mathbf{r}_c}\cdot\mathbf{k}_c,
\end{aligned}$$

where we have use Einstein's summing convention. The term proportional to the vector potential can be rewriting using symmetric gauge as $\mathbf{A}(\mathbf{r}_c)=-\mathbf{r}_c\times\mathbf{B}/2$.

$$e\mathbf{r}_c\cdot\left(\dot{\mathbf{r}}_c\cdot\frac{\partial}{\partial\mathbf{r}_c}\right)\mathbf{A}(\mathbf{r}_c)=\frac{e}{2}\mathbf{r}_c\cdot\left(\mathbf{B}\times\left(\dot{\mathbf{r}}_c\cdot\frac{\partial}{\partial\mathbf{r}_c}\right)\mathbf{r}_c\right)=-e\mathbf{A}\cdot\dot{\mathbf{r}}_c \qquad (2.2.28)$$

We proceed with the $\dot{\mathbf{k}}_c$ term:

$$\langle W_{\mathbf{r}_c\mathbf{k}_c}|\,i\dot{\mathbf{k}}_c\cdot\frac{\partial}{\partial\mathbf{k}_c}|W_{\mathbf{r}_c\mathbf{k}_c}\rangle=\frac{i\hbar}{\mathcal{V}}\int\mathrm{d}\mathbf{r}\sum_{\mathbf{k},\mathbf{k}'}w^*_{\mathbf{k}'\mathbf{k}_c}e^{-ie\mathbf{A}(\mathbf{r}_c)\cdot\mathbf{r}-i\mathbf{k}'\cdot\mathbf{r}_c}\psi^*_{\mathbf{k}_c}(\mathbf{r})\dot{\mathbf{k}}_c\cdot\frac{\partial}{\partial\mathbf{k}_c}w_{\mathbf{k}\mathbf{k}_c}e^{-ie\mathbf{A}(\mathbf{r}_c)\cdot\mathbf{r}-i\mathbf{k}\cdot\mathbf{r}_c}\psi_{\mathbf{k}_c}(\mathbf{r}) \qquad (2.2.29)$$

$$\begin{aligned}
&=\frac{i}{\mathcal{V}}\int\mathrm{d}\mathbf{r}\sum_{\mathbf{k},\mathbf{k}'}w^*_{\mathbf{k}'\mathbf{k}_c}e^{i(\mathbf{k}-\mathbf{k}')\mathbf{r}_c}\psi^*_{\mathbf{k}_c}(\mathbf{r})\psi_{\mathbf{k}_c}(\mathbf{r})\dot{\mathbf{k}}_c\cdot\frac{\partial}{\partial\mathbf{k}_c}w_{\mathbf{k}\mathbf{k}_c}\\
&=i\sum_{\mathbf{k}}\left|w_{\mathbf{k}-\mathbf{k}_c}\right|^2\frac{1}{\left|w_{\mathbf{k}-\mathbf{k}_c}\right|}\dot{\mathbf{k}}_c\cdot\frac{\partial}{\partial\mathbf{k}_c}w_{\mathbf{k}\mathbf{k}_c}\\
&=i\sum_{\mathbf{k}}\left|w_{\mathbf{k}-\mathbf{k}_c}\right|^2\frac{1}{\left|w_{\mathbf{k}-\mathbf{k}_c}\right|}e^{i(\mathbf{k}-\mathbf{k}_c)\cdot\boldsymbol{\mathcal{A}}_n(\mathbf{k}_c)}\dot{\mathbf{k}}_c\cdot\left[\frac{\partial}{\partial\mathbf{k}_c}\left|w_{\mathbf{k}-\mathbf{k}_c}\right|\right.\\
&\qquad\left.+\,i\left|w_{\mathbf{k}-\mathbf{k}_c}\right|\left(-\boldsymbol{\mathcal{A}}_n(\mathbf{k}_c)+(\mathbf{k}-\mathbf{k}_c)\frac{\partial}{\partial\mathbf{k}_c}\boldsymbol{\mathcal{A}}_n(\mathbf{k}_c)\right)\right]\\
&=\dot{\mathbf{k}}_c\cdot\boldsymbol{\mathcal{A}}_n(\mathbf{k}_c),
\end{aligned}$$

where we have used that $|w_{\mathbf{k}-\mathbf{k}_c}|^2$ is delta function i momentum in order to preform the last integration. Hence we have now determined the time derivative term in the Lagrangian, which is:

$$\langle W_{\mathbf{r}_c\mathbf{k}_c}|\,i\frac{\partial}{\partial t}|W_{\mathbf{r}_c\mathbf{k}_c}\rangle=-e\mathbf{A}\cdot\dot{\mathbf{r}}_c+\dot{\mathbf{r}_c}\cdot\mathbf{k}_c+\dot{\mathbf{k}}_c\cdot\mathcal{A}_n(\mathbf{k}_c) \qquad (2.2.30)$$

Now we turn our attention toward the Hamiltonian term in the Lagrangian. For this calculation one can reduce the trouble by first noting that the following equation holds for arbitrary polynomial f

$$\begin{aligned}
&f(-i\partial_{\mathbf{r}}+e\mathbf{A}(\mathbf{r}))e^{-ie\mathbf{A}(\mathbf{r}_c)\cdot\mathbf{r}-i\mathbf{k}\cdot\mathbf{r}_c}\psi_{\mathbf{k}}(\mathbf{r}) \qquad (2.2.31)\\
&\quad=e^{-ie\mathbf{A}(\mathbf{r}_c)\cdot\mathbf{r}-i\mathbf{k}\cdot\mathbf{r}_c}e^{i\mathbf{k}\cdot\mathbf{r}}f\left(-i\partial_{\mathbf{r}}+\mathbf{k}+e\left[+\mathbf{A}(\mathbf{r})-\mathbf{A}(\mathbf{r}_c)\right]\right)\mathbf{u}_{\mathbf{k},n}
\end{aligned}$$

From this relation we see that

$$\begin{aligned}
\langle W_{\mathbf{r}_c\mathbf{k}_c}|\,H-e\varphi(\mathbf{r})\,|W_{\mathbf{r}_c\mathbf{k}_c}\rangle=\frac{i}{\mathcal{V}}\int\mathrm{d}\mathbf{r}\sum_{\mathbf{k},\mathbf{k}'}w^*_{\mathbf{k}'\mathbf{k}_c}e^{i(\mathbf{k}-\mathbf{k}')\cdot(\mathbf{r}_c-\mathbf{r})}\mathbf{u}^*_{\mathbf{k},n} \qquad (2.2.32)\\
\times\left(\frac{1}{2m}\left[-i\partial_{\mathbf{r}}+\mathbf{k}+\frac{e}{c}\left(+\mathbf{A}(\mathbf{r})-\mathbf{A}(\mathbf{r}_c)\right)\right]^2-e\varphi(\mathbf{r})\right)w_{\mathbf{k}\mathbf{k}_c}\mathbf{u}_{\mathbf{k},n}.
\end{aligned}$$

Let us now expand the squared terms:

$$\left[-i\partial_{\mathbf{r}}+\mathbf{k}+\frac{e}{c}\left(+\mathbf{A}(\mathbf{r})-\mathbf{A}(\mathbf{r}_c)\right)\right]^2=-\partial_{\mathbf{r}}^2+\mathbf{k}^2-2i\partial_{\mathbf{r}}\mathbf{k}+\frac{e}{c}\left(-i\partial_{\mathbf{r}}+\mathbf{k}\right)\left(+\mathbf{A}(\partial_{\mathbf{r}})-\mathbf{A}(\mathbf{r}_c)\right) \tag{2.2.33}$$
$$+\frac{e}{c}\left(+\mathbf{A}(\mathbf{r})-\mathbf{A}(\mathbf{r}_c)\right)\left(-i\partial_{\mathbf{r}}+\mathbf{k}\right)+\frac{e^2}{c^2}\left(+\mathbf{A}(\mathbf{r})-\mathbf{A}(\mathbf{r}_c)\right)^2,$$

then integrate the terms without the vector potentials along with the electric potential $\varphi(\mathbf{r})$ term. To ease the calculation we will Taylor expand the electric potential around $\mathbf{r}_c$

$$\varphi(\mathbf{r})\approx\varphi(\mathbf{r}_c)+(\mathbf{r}-\mathbf{r}_c)\frac{\partial}{\partial\mathbf{r}_c}\varphi(\mathbf{r}_c), \tag{2.2.34}$$

note that we could have expanded to infinite order and achieved the same result because the expectation value of $\mathbf{r}$ is $\mathbf{r}_c$. So the integral of the terms with no vector potentials becomes

$$\begin{aligned}
&\frac{1}{\mathcal{V}}\int\mathrm{d}\mathbf{r}\sum_{\mathbf{k},\mathbf{k}'}w^*_{\mathbf{k}'\mathbf{k}_c}e^{i(\mathbf{k}-\mathbf{k}')\cdot(\mathbf{r}_c-\mathbf{r})}u^*_{\sigma,\mathbf{k},n}\left(-\frac{1}{2m}\partial_{\mathbf{r}}^2+\frac{1}{2m}{}^2\,\mathbf{k}^2-\frac{i}{m}\partial_{\mathbf{r}}\mathbf{k}\right.\\
&\left.-e\left(\varphi(\mathbf{r}_c)+(\mathbf{r}-\mathbf{r}_c)\frac{\partial}{\partial\mathbf{r}_c}\varphi(\mathbf{r}_c)\right)\right)w_{\mathbf{k}\mathbf{k}_c}u_{\sigma,\mathbf{k},n}\\
&=\frac{i}{\mathcal{V}}\int\mathrm{d}\mathbf{r}\sum_{\mathbf{k},\mathbf{k}'}w^*_{\mathbf{k}'\mathbf{k}_c}e^{i(\mathbf{k}-\mathbf{k}')\cdot(\mathbf{r}_c-\mathbf{r})}u^*_{\sigma,\mathbf{k},n}\left(\frac{1}{2m}\mathbf{k}^2-e\left(\varphi(\mathbf{r}_c)+(\mathbf{r}-\mathbf{r}_c)\frac{\partial}{\partial\mathbf{r}_c}\varphi(\mathbf{r}_c)\right)\right)w_{\mathbf{k}\mathbf{k}_c}u_{\sigma,\mathbf{k},n}\\
&=\frac{\mathbf{k}_c^2}{2m}-e\varphi(\mathbf{r}_c)=\xi_{\mathbf{k}_c}-e\varphi(\mathbf{r}_c).
\end{aligned} \tag{2.2.35}$$

Where At last we will calculate the reaming terms. However term proportional to $\left(+\mathbf{A}(\mathbf{r})-\mathbf{A}(\mathbf{r}_c)\right)^2$ will be discarded as thy are small for small magnetic fields, as they can be view as the gradient for the vector potential squared. Lastly remember that we chose the vector potential to be $\mathbf{A}=-\mathbf{r}\times\mathbf{B}/2$:

$$\begin{aligned}
&\frac{1}{2m\mathcal{V}}\int\mathrm{d}\mathbf{r}\sum_{\mathbf{k},\mathbf{k}'}w^*_{\mathbf{k}'\mathbf{k}_c}e^{i(\mathbf{k}-\mathbf{k}')\cdot(\mathbf{r}_c-\mathbf{r})}u^*_{\sigma,\mathbf{k},n}e\left(\left(-i\partial_{\mathbf{r}}+\mathbf{k}\right)\left(\mathbf{A}(\mathbf{r})-\mathbf{A}(\mathbf{r}_c)\right)\right.\\
&\left.+\left(\mathbf{A}(\mathbf{r})-\mathbf{A}(\mathbf{r}_c)\right)\left(-i\partial_{\mathbf{r}}+\mathbf{k}\right)\right)w_{\mathbf{k}\mathbf{k}_c}u_{\sigma,\mathbf{k},n}\\
&=\frac{-1}{4m\mathcal{V}}\int\mathrm{d}\mathbf{r}\sum_{\mathbf{k},\mathbf{k}'}w^*_{\mathbf{k}'\mathbf{k}_c}e^{i(\mathbf{k}-\mathbf{k}')\cdot(\mathbf{r}_c-\mathbf{r})}u^*_{\sigma,\mathbf{k},n}e\left((\mathbf{r}-\mathbf{r}_c)\times\mathbf{B}\right)\cdot\left(-i\partial_{\mathbf{r}}+\mathbf{k}\right)w_{\mathbf{k}\mathbf{k}_c}u_{\sigma,\mathbf{k},n}+\text{c.c.}\\
&=\frac{e\mathbf{B}}{4mN}\cdot\int\mathrm{d}\mathbf{r}\sum_{\mathbf{k},\mathbf{k}'}w^*_{\mathbf{k}'\mathbf{k}_c}e^{i(\mathbf{k}-\mathbf{k}')\cdot(\mathbf{r}_c-\mathbf{r})}u^*_{\sigma,\mathbf{k},n}\left((\mathbf{r}-\mathbf{r}_c)\times\left(-i\partial_{\mathbf{r}}+\mathbf{k}\right)\right)w_{\mathbf{k}\mathbf{k}_c}u_{\sigma,\mathbf{k},n}+\text{c.c.}\\
&=\frac{e\mathbf{B}}{4mN}\cdot\int\mathrm{d}\mathbf{r}\sum_{\mathbf{k},\mathbf{k}'}w^*_{\mathbf{k}'\mathbf{k}_c}u^*_{\sigma,\mathbf{k}',n}\left(-\frac{\partial}{\partial i\mathbf{k}'}e^{i(\mathbf{k}-\mathbf{k}')\cdot(\mathbf{r}_c-\mathbf{r})}\right)\times\left(-i\partial_{\mathbf{r}}+\mathbf{k}\right)w_{\mathbf{k}\mathbf{k}_c}u_{\sigma,\mathbf{k},n}+\text{c.c.}\\
&=\frac{e\mathbf{B}}{4mN}\cdot\int\mathrm{d}\mathbf{r}\sum_{\mathbf{k},\mathbf{k}'}e^{i(\mathbf{k}-\mathbf{k}')\cdot(\mathbf{r}_c-\mathbf{r})}\left(\frac{\partial}{\partial i\mathbf{k}'}w^*_{\mathbf{k}'\mathbf{k}_c}u^*_{\sigma,\mathbf{k}',n}\right)w_{\mathbf{k}\mathbf{k}_c}u_{\sigma,\mathbf{k},n}\times\left(-i\partial_{\mathbf{r}}+\mathbf{k}\right)+\text{c.c.}\\
&=\frac{e\mathbf{B}}{4m}\cdot\sum_{\mathbf{k}}\left(\frac{\partial\mathbf{u}^*_{\mathbf{k},n}}{\partial i\mathbf{k}}w^*_{\mathbf{k}\mathbf{k}_c}+u^*_{\sigma,\mathbf{k},n}w^*_{\mathbf{k}\mathbf{k}_c}\frac{\partial\ln(w^*_{\mathbf{k}\mathbf{k}_c})}{\partial i\mathbf{k}}\right)w_{\mathbf{k}\mathbf{k}_c}u_{\sigma,\mathbf{k},n}\times\left(-i\partial_{\mathbf{r}}+\mathbf{k}\right)+\text{c.c.}\\
&=\frac{e\mathbf{B}}{4m}\cdot\left(\frac{\partial\mathbf{u}^*_{\mathbf{k}_c,n}}{\partial i\mathbf{k}_c}-\mathbf{u}^*_{\mathbf{k}_c,n}\boldsymbol{\mathcal{A}}_n(\mathbf{k}_c)\right)\mathbf{u}_{\mathbf{k}_c,n}\times\mathbf{k}_c+\text{c.c.}\\
&=\frac{e\mathbf{B}}{4m}\cdot\left(-i\frac{\partial u^*_{\sigma,\mathbf{k}_c,n}}{\partial\mathbf{k}_c}u_{\sigma,\mathbf{k_c},n}-\boldsymbol{\mathcal{A}}_n(\mathbf{k}_c)\right)\times\mathbf{k}_c+\text{c.c.}\\
&=\frac{e\mathbf{B}}{4m}\cdot\left(iu^*_{\sigma,\mathbf{k}_c,n}\frac{\partial u_{\sigma,\mathbf{k}_c,n}}{\partial\mathbf{k}_c}-\boldsymbol{\mathcal{A}}_n(\mathbf{k}_c)\right)\times\mathbf{k}_c+\text{c.c.}=0,
\end{aligned} \tag{2.2.36}$$

where in the last equality we have used that $|u_{\sigma,\mathbf{k}_c,n}|^2=1$ to realize that $\left(\partial_{\mathbf{k_c}}u^*_{\sigma,\mathbf{k}_c,n}\right)u_{\sigma,\mathbf{k_c},n}=-u^*_{\sigma,\mathbf{k}_c,n}\left(\partial_{\mathbf{k_c}}u_{\sigma,\mathbf{k_c},n}\right)$. By combining equations (2.2.30),(2.2.35) and (2.2.36) the Lagrangian in our re-

stricted Hilbert space can be written as

$$L(\mathbf{r}_c, \dot{\mathbf{r}}_c; \mathbf{k}_c, \dot{\mathbf{k}}_c) = -e\dot{\mathbf{r}}_c \cdot \mathbf{A}(\mathbf{r}_c) + \dot{\mathbf{r}_c} \cdot \mathbf{k}_c + \dot{\mathbf{k}}_c \cdot \boldsymbol{\mathcal{A}}_n(\mathbf{k}_c) - \xi_{\mathbf{k}_c} + e\varphi(\mathbf{r}_c) \tag{2.2.37}$$

Note that this Lagrangian has the following "extend" gauge invariance under the transformation

$$\begin{aligned} \mathbf{A} &\mapsto \mathbf{A} + \frac{1}{e}\partial_{\mathbf{r}}\chi, \\ \mathcal{A}_n &\mapsto \boldsymbol{\mathcal{A}}_n - \partial_{\mathbf{k}}\chi, \\ \varphi &\mapsto \varphi - \dot{\chi}. \end{aligned} \tag{2.2.38}$$

Where χ is a differentiable function of space, momentum and time. Under this transformation the Lagrangian becomes:

$$\begin{aligned} \tilde{L}(\mathbf{r}_c, \dot{\mathbf{r}}_c; \mathbf{k}_c, \dot{\mathbf{k}}_c) &= -e\dot{\mathbf{r}}_c \cdot \left(\mathbf{A}(\mathbf{r}_c) + \frac{1}{e}\partial_{\mathbf{r}}\chi\right) + \dot{\mathbf{r}_c} \cdot \mathbf{k}_c + \dot{\mathbf{k}}_c \cdot (\boldsymbol{\mathcal{A}}_n(\mathbf{k}_c) - \partial_{\mathbf{k}}\chi) - \xi_{\mathbf{k}_c} + e\left(\varphi(\mathbf{r}_c) - \dot{\chi}\right) \\ &= L(\mathbf{r}_c, \dot{\mathbf{r}}_c; \mathbf{k}_c, \dot{\mathbf{k}}_c) - e\dot{\chi} - \dot{\mathbf{k}}_c \cdot \partial_{\mathbf{k}}\chi - e\dot{\mathbf{r}}_c \cdot \partial_{\mathbf{r}}\chi \\ &= L(\mathbf{r}_c, \dot{\mathbf{r}}_c; \mathbf{k}_c, \dot{\mathbf{k}}_c) - \frac{\mathrm{d}\chi}{\mathrm{d}t}, \end{aligned} \tag{2.2.39}$$

and as a total time derivative does not change the equation of motion, hence the $\tilde{L}$ contains the same physique as L. Having noted this peculiar 6-dimensional gauges invariance, we can proceed to the third and final step.

Step III. Apply the Euler-Lagrange's Equations

This step is straightforward. We only have to differentiate and remember some vector identities to get the result precedented in a nice reconcilable way. We start by noting the Euler-Lagrange equations of the two parameters:

$$\frac{\partial L}{\partial \mathbf{r}_c} = \frac{\mathrm{d}}{\mathrm{d}t}\frac{\partial \mathcal{L}}{\partial \dot{\mathbf{r}}_c}, \tag{2.2.40}$$

$$\frac{\partial L}{\partial \mathbf{k}_c} = \frac{\mathrm{d}}{\mathrm{d}t}\frac{\partial L}{\partial \dot{\mathbf{k}}_c}. \tag{2.2.41}$$

Let us first consider the centre of mass momentum through equation (2.2.40). For transparency we calculate each side separately

$$\frac{\partial \mathcal{L}}{\partial \mathbf{r}_c} = -e\left(\dot{\mathbf{r}}_c \cdot \frac{\partial}{\partial \mathbf{r}_c}\mathbf{A}(\mathbf{r}_c)\right) + e\frac{\partial}{\partial \mathbf{r}_c}\varphi(\mathbf{r}_c) \tag{2.2.42}$$

$$\frac{\mathrm{d}}{\mathrm{d}t}\frac{\partial \mathcal{L}}{\partial \dot{\mathbf{r}}_c} = -\frac{\mathrm{d}}{\mathrm{d}t}e\mathbf{A} - \frac{\mathrm{d}}{\mathrm{d}t}(\mathbf{k}_c) = -e\frac{\partial}{\partial t}\mathbf{A}(\mathbf{r}_c) - e\left(\dot{\mathbf{r}}_c \cdot \frac{\partial}{\partial \mathbf{r}_c}\right)\mathbf{A}(\mathbf{r}_c) + \dot{\mathbf{k}}_c. \tag{2.2.43}$$

Then solving for $\dot{\mathbf{k}}_c$, using that $\mathbf{E} = -\frac{\partial}{\partial \mathbf{r}_c}\varphi - \frac{\partial}{\partial t}\mathbf{A}$ and the general vector identity:

$$\mathbf{D} \times \left(\frac{\partial}{\partial \mathbf{x}} \times \mathbf{C}(\mathbf{x})\right) = \frac{\partial}{\partial \mathbf{x}}\left(\mathbf{D} \cdot \mathbf{C}(\mathbf{x})\right) - \left(\mathbf{D} \cdot \frac{\partial}{\partial \mathbf{x}}\right)\mathbf{C}(\mathbf{x}), \tag{2.2.44}$$

we obtain the familiar Lorentz force:

$$\dot{\mathbf{k}}_c = -e\left(\mathbf{E} + \dot{\mathbf{r}}_c \times \mathbf{B}\right). \tag{2.2.45}$$

We turn to the center of mass position through equation (2.2.41) and again calculate each side separately:

$$\frac{\partial \mathcal{L}}{\partial \mathbf{k}_c} = \dot{\mathbf{r}}_c + \frac{\partial}{\partial \mathbf{k}_c}(\dot{\mathbf{k}}_c \cdot \boldsymbol{\mathcal{A}}_n(\mathbf{k}_c)) - \frac{\partial}{\partial \mathbf{k}_c}\xi_{\mathbf{k}_c} \tag{2.2.46}$$

$$\frac{\mathrm{d}}{\mathrm{d}t}\frac{\partial \mathcal{L}}{\partial \dot{\mathbf{k}}_c} = \frac{\mathrm{d}}{\mathrm{d}t}\left(\boldsymbol{\mathcal{A}}_n(\mathbf{k}_c)\right) = \left(\dot{\mathbf{k}}_c \cdot \frac{\partial}{\partial \mathbf{k}_c}\right)\mathcal{A}_n(\mathbf{k}_c). \tag{2.2.47}$$

Remembering that the we defined the Berry curvature in equation (1.2.9), use equation (2.2.44) and solving for $\mathbf{k}_c$:

$$\dot{\mathbf{r}}_c = \frac{\partial}{\partial \mathbf{k}_c}\xi_{\mathbf{k}_c} - \dot{\mathbf{k}}_c \times \boldsymbol{\Omega}_n \tag{2.2.48}$$

Let us state the equation of motion for $\mathbf{r}$,$\mathbf{k}$ together.

$$\dot{\mathbf{r}}_c = \frac{\partial}{\partial \mathbf{k}_c}\xi_{\mathbf{k}_c} - \dot{\mathbf{k}}_c \times \boldsymbol{\Omega}_n \tag{2.2.49}$$

$$\hbar\dot{\mathbf{k}}_c = -e\left(\mathbf{E} + \dot{\mathbf{r}}_c \times \mathbf{B}\right) \tag{2.2.50}$$

The second term in equation (2.2.49) is known as the anomalous velocity and was first found by Karplus and Luttinger[12] in the context of the Hall effect in ferromagnetics and explained the derivation from the ordinary Hall conductances due to Spin-Orbit coupling and induced magnetization.

As mentioned earlier one should be careful to apply this result as it is based on a variational calculation where only a limited part of the Hilbert space is included. For example there is no reason to believe that this equation will hold in cases where the magnetic or electric field vary on a scale smaller than the with of the wave packed. One should also note that this result as presented here is only valid for quadric dispersions (due to our choice of Hamiltonian), but the Lorentz force and the anomalous velocity are obtained independent of the Hamiltonian. Only the ordinary group velocity changes if another Hamiltonian that commute with the canonical momentum is considered. Having $\dot{\mathbf{r}}\mathrm{m}\dot{\mathbf{k}}$ established, we now turn to actually solving the Boltzmann equation in a specific case.

2.3 The Anomalous Hall Effect

Probably the most notorious consequence of having an anomalous velocity in the driving terms of the semi-classical Boltzmann equation is the possibility of having a Hall current without applying a magnetic field, an effect called the anomalous Hall effect. To derive this from, the Boltzmann equation (2.1.5) and the equations (2.2.49) and (2.2.50) is rather straightforward. To avoid a normal Hall response we assume that the magnetic field is zero, leading the following expression for the $\dot{\mathbf{r}}$ and $\dot{\mathbf{k}}$ [4]

$$\begin{aligned}\dot{\mathbf{k}} &= -e\mathbf{E} \\ \dot{\mathbf{r}} &= \frac{\partial \xi_{\mathbf{k}}}{\partial \mathbf{k}} + e\mathbf{E} \times \boldsymbol{\Omega}_n.\end{aligned} \tag{2.3.1}$$

Note that one needs at least two bands to have a non-vanishing Berry curvature[18], and on should think of the resulting Boltzmann equation as an equation for the electrons in the lowest band. Hence the collision integral can in general contain inter band terms. The resulting Boltzmann equation which determine the dynamics for the lower band is:

$$\frac{\partial}{\partial t}f + \left(\frac{\partial \xi_{\mathbf{k}}}{\partial \mathbf{k}} + e\mathbf{E} \times \boldsymbol{\Omega}_n\right) \cdot \frac{\partial}{\partial \mathbf{r}}f - e\mathbf{E} \cdot \frac{\partial}{\partial \mathbf{k}}f = I_{\mathrm{coll}}. \tag{2.3.2}$$

We approximate the collision integral by the relaxation time approximation[20]. Linearising the Boltzmann equation, assuming that there is no spacial dependencies of temperature and chemical potential, no time dependents of the electric fields, then to linear order in the electric field the Boltzmann equation

[4] We have droped the subscript c again as we do not have to consider operators any more, and to make the notation more sleek.

becomes

$$-e\mathbf{E}\cdot\frac{\partial\xi_{\mathbf{k}}}{\partial\mathbf{k}}\frac{\partial}{\partial\xi_{\mathbf{k}}}f^0=-\frac{f-f^0}{\tau}. \tag{2.3.3}$$

Where f^0 is the Fermi distribution and τ is the relaxation time. The linearisation procedure have rendered the otherwise complicated Boltzmann equation straightforward to solve. The solution is

$$f=f^0+e\mathbf{E}\cdot\frac{\partial\xi_{\mathbf{k}}}{\partial\mathbf{k}}\tau\frac{\partial}{\partial\xi_{\mathbf{k}}}f^0. \tag{2.3.4}$$

To get the actual Hall conductivity one needs to find the current density and then differentiate with respect to the electric field. The current density is in the literature of semi-classical transport theory given as[20][5]:

$$\mathbf{j}=-e\int\frac{\mathrm{d}\mathbf{k}}{(2\pi)^2}\mathbf{v}f, \tag{2.3.5}$$

where $\mathbf{v}$ is the velocity, that one naively would understand in the semi-classical picture as the movement of the center of mass coordinate of the wave packed, hence $\dot{\mathbf{r}}$. However the procedure of finding the current density can be formalized by considering the conservation laws obtained from the Boltzmann equation. This is done along the lines of Kadanoff and Baym[21]. Particle conservation is obtain form the Boltzmann equation by integrating it over momentum $\mathbf{k}$ [6]:

$$\int\frac{\mathrm{d}\mathbf{k}}{(2\pi)^2}\frac{\partial}{\partial t}f+\int\frac{\mathrm{d}\mathbf{k}}{(2\pi)^2}\left(\frac{\partial\xi_{\mathbf{k}}}{\partial\mathbf{k}}+e\mathbf{E}\times\mathbf{\Omega}_n\right)\cdot\frac{\partial}{\partial\mathbf{r}}f-\int\frac{\mathrm{d}\mathbf{k}}{(2\pi)^2}e\mathbf{E}\cdot\frac{\partial}{\partial\mathbf{k}}f=\int\frac{\mathrm{d}\mathbf{k}}{(2\pi)^2}I_{coll}, \tag{2.3.6}$$

we note again that the momentum integral of the collision integral must vanish do to particle conservation[27] if we neglect any inter band scattering, which we do. The last term is a bit more tricky, now in case were f can be argued to go to zero when momentum goes to infinity, one would simply the partial integrating the last term and as the electric field dose not depend on momentum i would be zero. But in the case where this is not true one can often make it vanish to liner order in the electric field, as f^0 only depends on momentum through the dispersion[7]. So the expression simplifys as:

$$\frac{\partial}{\partial t}\int\frac{\mathrm{d}\mathbf{k}}{(2\pi)^2}f+\frac{\partial}{\partial\mathbf{r}}\cdot\int\frac{\mathrm{d}\mathbf{k}}{(2\pi)^2}\left(\frac{\partial\xi_{\mathbf{k}}}{\partial\mathbf{k}}+e\mathbf{E}\times\mathbf{\Omega}_n\right)f=0. \tag{2.3.7}$$

We are left with a continuity equation for the particles, where we can identify the following as respectively the particle density and the particle current density

$$\rho=\int\frac{\mathrm{d}\mathbf{k}}{(2\pi)^2}f, \tag{2.3.8}$$

$$\mathbf{j}_p=\int\frac{\mathrm{d}\mathbf{k}}{(2\pi)^2}\left(\frac{\partial\xi_{\mathbf{k}}}{\partial\mathbf{k}}+e\mathbf{E}\times\mathbf{\Omega}_n\right)f. \tag{2.3.9}$$

The current density $\mathbf{j}$ equals $-e\mathbf{j}_p$ if the particles at hand are electrons. We have now form particle conservation shown that naive choice of velocity in the current density was right.
The found velocity leads to the following explicit expression for the current density to linear order in the electric field:

$$\mathbf{j}=-e\int\frac{\mathrm{d}\mathbf{k}}{(2\pi)^2}\left(\frac{\partial\xi_{\mathbf{k}}}{\partial\mathbf{k}}\left(f^0+e\mathbf{E}\cdot\frac{\partial\xi_{\mathbf{k}}}{\partial\mathbf{k}}\tau\frac{\partial}{\partial\xi_{\mathbf{k}}}f^0\right)+e\mathbf{E}\times\mathbf{\Omega}_nf^0\right). \tag{2.3.10}$$

So we see that the normal Drude response is present but there is also an additional term including the Berry curvature, who can induce transport if the specific $\mathbf{k}$ integration dose not vanish. More over one sees that it will be perpendicular to both the Berry curvature and the electric field, hence it is similar to the Hall response. Let us now specify the electric field to point in the x direction and the Berry curvature

[5] We are here specifying to 2 dimensions, as we would like to apply it to a 2-dimensional model
[6] Note this is only a derivation of the current operator for the problem at hand!
[7] This is the case in the Rashba Hamilton

$\mathbf{\Omega}_n$ to point in the z direction. As we will consider a 2-dimensional model we will have the normal Hall geometry as shown in figure 2.2. Ignoring the Drude response as it is well known and only considering

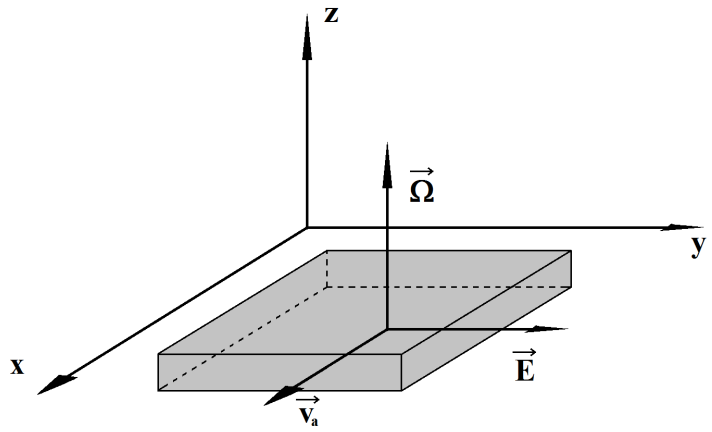

Figure 2.2: A sketch of the geometry behind the anomalous velocity term in a 2-dimensional system. The cross product between $\mathbf{E}$ and $\mathbf{\Omega}_n$ is here called $\mathbf{v}_a$.

the anomalous velocity term we see that the only non-trivial component of the conductivity tensor is σ_{yx}, where the conductivity tensor is the current density differentiated with respect to the electric field.

$$\sigma_{yx} = \frac{\partial \mathbf{j}}{\partial \mathbf{E}_x} \cdot \hat{\mathbf{j}} = -e^2 \int \frac{d\mathbf{k}}{(2\pi)^2} \mathbf{\Omega}_n f^0, \tag{2.3.11}$$

where $\hat{\mathbf{j}}$ is the unit vector in the y-direction. Now to get the actual value of σ_{yx} we need to specify to a model which has a non-trivial momentum integrated Berry curvature, Such and example is given with the Rashba Hamiltonian with Zeeman splitting defined in equation (1.3.1), the Berry curvature in the lowest band is as we calculated in equation (1.3.8) :

$$\mathbf{\Omega}_- = \frac{v_f^2 \Delta}{2\left(v_f^2\left(k_x^2 + k_y^2\right) + \Delta^2\right)^{3/2}} \hat{\mathbf{k}}, \tag{2.3.12}$$

where $\hat{\mathbf{k}}$ is the unit vector in the z direction, Δ is the spin-orbit coupling and v_f is the Fermi velocity. Now we plug this into (2.3.11), and assume half filling so that the lower band is completely filled. Hence the Fermi function is unity for all momenta. We obtain that the conductivity can be written as

$$\sigma_{yx} = -e^2 \int \frac{\mathrm{d}\mathbf{k}}{(2\pi)^2} \frac{v_f^2 \Delta}{2\left(v_f^2\left(k_x^2 + k_y^2\right) + \Delta^2\right)^{3/2}} = -\frac{1}{4\pi} e^2 = -\frac{1}{4\pi} \frac{e^2}{\hbar} = -\frac{1}{2} \frac{e^2}{h}, \tag{2.3.13}$$

Where we have reinstalling $\hbar$ in the third equality. We have found the anomalous Hall coefficient from semi-classical consideration in the Rashba Hamiltonian. The result is consistent with the results obtained from the Kubo formula[15, 26].

Chapter 3

Quantum Anomalous Transport

In this chapter we will go though a full quantum calculation to get a collision less semi-classical Boltzmann equation for each band. The basic idea is to consider Keldysh formalism as done by Rammer and Smith [10], though in the context of a multi-band system which gives raise to anomalous transport phenomena. We then systematically approximate the Keldysh equation through the gradient expansion. However it turns out that in order to get gauge invariant result one has to introduce kinematic variables in both 4-position and 4-momentum. As the Chapter relies on some basic Keldysh formalism which will not be covered one should consult Rammer and Smith[10] for an introduction. Finally it should be mention that one should be able to reach the same result by using the Kadanoff-Bayn contur Green's function introduced by Kadanoff and Baym [21].

3.1 The Keldysh Dyson Equation

In principal we want to treat the behaviour of the multi-band system out of equilibrium exactly (at least formally) by Green's function so we need a non-equilibrium extension of the Dyson equation for non-equilibrium Green's functions. A way to do this according to Rammer and Smith [10] is through the Keldysh formalism[1]. The normal Dyson equation is replaced by the Keldysh Dyson equation, which has the form:

$$\left[\left(\underline{G}_0^{-1} - \underline{\Sigma}\right) \overset{\otimes}{,} \underline{G}\right]_- = 0, \tag{3.1.1}$$

where $[...\overset{\otimes}{,}...]_-$ are the anti commutators with respected to the composition $\otimes$. The composition is defined as the following convolution between to matricides in Keldysh space:

$$\left(\underline{M} \otimes \underline{N}\right)(1,1') = \int \mathrm{d}\mathbf{r} \int \mathrm{d}t_2 \underline{M}(\mathbf{1},\mathbf{2})\underline{N}(\mathbf{2},\mathbf{1}'). \tag{3.1.2}$$

Where $\underline{M}$ and $\underline{N}$ are matrix functions, $\mathbf{1}$ and $\mathbf{1}'$ denote respectively $(t,\mathbf{r})$ and $(t',\mathbf{r}')$ and $\mathbf{2}$ is $(t_2,\mathbf{r}_2)$. The matrix structure of the different terms in equation (3.1.1) is in the rotated Keldysh-space:

$$\underline{G}(\mathbf{1},\mathbf{1}') = \begin{pmatrix} \underline{\underline{G}}^R & \underline{\underline{G}}^K \\ \underline{\underline{0}} & \underline{\underline{G}}^A \end{pmatrix}, \qquad \underline{\Sigma}(\mathbf{1},\mathbf{1}') = \begin{pmatrix} \underline{\underline{\Sigma}}^R & \underline{\underline{\Sigma}}^K \\ \underline{\underline{0}} & \underline{\underline{\Sigma}}^A \end{pmatrix}, \qquad \underline{G}_0^{-1}(\mathbf{1},\mathbf{1}') = \begin{pmatrix} \underline{\underline{G}}_0^{-1} & \underline{\underline{0}} \\ \underline{\underline{0}} & \underline{\underline{G}}_0^{-1} \end{pmatrix}. \tag{3.1.3}$$

The double underlining means the object is a matrix, of dimension $n \times n$ and where n is number of bands, spin , etc. discrete degrees for freedom. Exemplify the form of thesis the matrix functions: $\underline{\underline{G}}^R$, $\underline{\underline{h}}$ which is the distribution function matrix, $\underline{\underline{\Sigma}}^R$, $\underline{\underline{\Sigma}}^A$, $\underline{\underline{G}}_0^{-1}$[2] and $\underline{\underline{G}}^A$ one can writ them out for the

[1] The from of the Keldysh formalism we are using here, we do not take care of initial correlated system as we are not interested in transit effects.

[2] Note that $\underline{\underline{G}}_0^{-1}$ is of the form: $[i\partial_{t_1} - \epsilon(1)]\delta(1-1')$[10].

two-dimensional case, as in Rammer and Smith [10]:

$$\begin{aligned}
\underline{\underline{G}}^R(\mathbf{1},\mathbf{1}') &= \begin{pmatrix} G^R_{11}(\mathbf{1},\mathbf{1}') & G^R_{12}(\mathbf{1},\mathbf{1}') \\ G^R_{21}(\mathbf{1},\mathbf{1}') & G^R_{22}(\mathbf{1},\mathbf{1}') \end{pmatrix}, \qquad \underline{\underline{G}}^A(\mathbf{1},\mathbf{1}') = \begin{pmatrix} G^A_{11}(\mathbf{1},\mathbf{1}') & G^A_{12}(\mathbf{1},\mathbf{1}') \\ G^A_{21}(\mathbf{1},\mathbf{1}') & G^A_{22}(\mathbf{1},\mathbf{1}') \end{pmatrix}, \\
\underline{\underline{G}}_0^{-1}(\mathbf{1},\mathbf{1}') &= \begin{pmatrix} G^{-1}_{0_{(11)}}(\mathbf{1},\mathbf{1}') & G^{-1}_{0_{(12)}}(\mathbf{1},\mathbf{1}') \\ G^{-1}_{0_{(21)}}(\mathbf{1},\mathbf{1}') & G^{-1}_{0_{(22)}}(\mathbf{1},\mathbf{1}') \end{pmatrix}, \qquad \underline{\underline{\Sigma}}^R(\mathbf{1},\mathbf{1}') = \begin{pmatrix} \Sigma^R_{11}(\mathbf{1},\mathbf{1}') & \Sigma^R_{12}(\mathbf{1},\mathbf{1}') \\ \Sigma^R_{21}(\mathbf{1},\mathbf{1}') & \Sigma^R_{22}(\mathbf{1},\mathbf{1}') \end{pmatrix}, \\
\underline{\underline{h}}(\mathbf{1},\mathbf{1}') &= \begin{pmatrix} h_{11}(\mathbf{1},\mathbf{1}') & h_{12}(\mathbf{1},\mathbf{1}') \\ h_{21}(\mathbf{1},\mathbf{1}') & h_{22}(\mathbf{1},\mathbf{1}') \end{pmatrix}, \qquad \underline{\underline{\Sigma}}^A(\mathbf{1},\mathbf{1}') = \begin{pmatrix} \Sigma^A_{11}(\mathbf{1},\mathbf{1}') & \Sigma^A_{12}(\mathbf{1},\mathbf{1}') \\ \Sigma^A_{21}(\mathbf{1},\mathbf{1}') & \Sigma^A_{22}(\mathbf{1},\mathbf{1}') \end{pmatrix}.
\end{aligned} \tag{3.1.4}$$

Having an idea of the structure of this Dyson equation all which is left is to solve the equation for the Green's functions. However as we are mainly interested in transport phenomena and the Keldysh component which is responsible for kinetics [10], we might be able to get an independent equation for the Keldysh component by making some smart tricks. The first step in getting an independent equation for the Keldysh component is to make the following ansatz for G^K

$$\underline{\underline{G}}^K(\mathbf{1},\mathbf{1}') = \left(\underline{\underline{G}}^R \otimes \underline{\underline{h}}\right)(\mathbf{1},\mathbf{1}') - \left(\underline{\underline{h}} \otimes \underline{\underline{G}}^A\right)(\mathbf{1},\mathbf{1}'), \tag{3.1.5}$$

where $\underline{\underline{h}}$ is the matrix distribution function that in its diagonal basis and in equilibrium is $\underline{\underline{h}}_0(\chi) = \tanh(\beta(\underline{\underline{\xi}} - \mu)1/2) = (1 - 2\,\underline{\underline{n_f}})$, where $\underline{\underline{\xi}}$ the dispersion and μ is the chemical potential. We can insert equation (3.1.5) using the Keldysh space structure given in equation (3.1.3), into the Keldysh Dyson equation (3.1.1). Form this one can show that the so called Keldysh component (the (12) component in Keldysh space) of equation (3.1.1) is[3]

$$\begin{aligned}
&\left[\underline{\underline{G}}_0^{-1} - \underline{\underline{Re\Sigma}}^{\otimes}, \underline{\underline{G}}^R \otimes \underline{\underline{h}} - \underline{\underline{h}} \otimes \underline{\underline{G}}^A\right]_- - \left[\underline{\underline{\Sigma}}^K \overset{\otimes}{,} \frac{1}{2}\left(\underline{\underline{G}}^R + \underline{\underline{G}}^A\right)\right]_- \\
&\qquad = \frac{i}{2}\left[\underline{\underline{\Sigma}}^K \overset{\otimes}{,} i\left(\underline{\underline{G}}^R + G^A\right)\right]_+ - \frac{i}{2}\left[\underline{\underline{\Gamma}}^{\otimes}, \underline{\underline{G}}^R \otimes \underline{\underline{h}} - \underline{\underline{h}} \otimes \underline{\underline{G}}^A\right]_+
\end{aligned} \tag{3.1.6}$$

where $\underline{\underline{\Gamma}}$ is the imaginary path of the self-energy. We can similarly find the form of the retarded (the (11) component in Keldysh space) and advandsed (the (22) component in Keldysh space) components of 3.1.1

$$(11) = (\underline{\underline{G}}_0^{-1} - \underline{\underline{\Sigma}}^R) \otimes \underline{\underline{G}}^R - \underline{\underline{G}}^R \otimes (\underline{\underline{G}}_0^{-1} - \underline{\underline{\Sigma}}^R) = 0 \tag{3.1.7}$$

$$(22) = (\underline{\underline{G}}_0^{-1} - \underline{\underline{\Sigma}}^A) \otimes \underline{\underline{G}}^A - \underline{\underline{G}}^A \otimes (\underline{\underline{G}}_0^{-1} - \underline{\underline{\Sigma}}^A) = 0 \tag{3.1.8}$$

Hence basically stating that $\underline{\underline{G}}^R$ commutes with $(\underline{\underline{G}}_0^{-1} - \underline{\underline{\Sigma}}^R)$ and $\underline{\underline{G}}^A$ commutes with $(\underline{\underline{G}}_0^{-1} - \underline{\underline{\Sigma}}^A)$. Expanding the (anti)commutators in equation (3.1.6) along with the use of equations (3.1.7) and (3.1.8) one can show that:

$$\begin{aligned}
&\underline{\underline{G}}^R \otimes \left[\underline{\underline{G}}_0^{-1} - \underline{\underline{Re\Sigma}}^{\otimes}, \underline{\underline{h}}\right]_- - \left[\underline{\underline{G}}_0^{-1} - \underline{\underline{Re\Sigma}}^{\otimes}, \underline{\underline{h}}\right]_- \otimes \underline{\underline{G}}^A \\
&\quad - \frac{1}{2}\underline{\underline{\Sigma}}^K \otimes \underline{\underline{G}}^R - \frac{1}{2}\underline{\underline{\Sigma}}^K \otimes \underline{\underline{G}}^A + \frac{1}{2}\underline{\underline{G}}^R \otimes \underline{\underline{\Sigma}}^K + \frac{1}{2}\underline{\underline{G}}^A \otimes \underline{\underline{\Sigma}}^K \\
&= -\frac{1}{2}\underline{\underline{\Sigma}}^K \otimes \underline{\underline{G}}^R + \frac{1}{2}\Sigma^K \otimes \underline{\underline{G}}^A + \frac{1}{2}\underline{\underline{G}}^R \otimes \underline{\underline{\Sigma}}^K - \frac{1}{2}\underline{\underline{G}}^A \otimes \underline{\underline{\Sigma}}^K \\
&\quad - \frac{i}{2}\underline{\underline{G}}^R \otimes \left[\underline{\underline{\Gamma}}^{\otimes}, \underline{\underline{h}}\right]_+ + \frac{i}{2}\left[\underline{\underline{\Gamma}}^{\otimes}, \underline{\underline{h}}\right]_+ \otimes \underline{\underline{G}}^A.
\end{aligned} \tag{3.1.9}$$

[3]Note the following relation form Rammer and Smith[10] $\underline{\underline{A}} = i(\underline{\underline{G}}^R - \underline{\underline{G}}^A), \underline{\underline{ReG}} = \frac{1}{2}(\underline{\underline{G}}^R + \underline{\underline{G}}^A), \underline{\underline{\Gamma}} = i(\underline{\underline{\Sigma}}^R - \underline{\underline{\Sigma}}^A)$ and $\underline{\underline{Re\Sigma}} = \frac{1}{2,}(\underline{\underline{\Sigma}}^R + \underline{\underline{\Sigma}}^A)$

Now by rearranging the terms it is possible to obtain the following equation

$$\begin{aligned} &- i\,\underline{\underline{G}}^R \otimes \left[\underline{\underline{G}}_0^{-1} - \underline{\underline{Re\Sigma}}^{\otimes}, \underline{\underline{h}}\right]_- + i\left[\underline{\underline{G}}_0^{-1} - \underline{\underline{Re\Sigma}}^{\otimes}, \underline{\underline{h}}\right]_- \otimes \underline{\underline{G}}^A \\ &\quad + i\,\underline{\underline{\Sigma}}^K \otimes \underline{\underline{G}}^R - i\,\underline{\underline{G}}^A \otimes \underline{\underline{\Sigma}}^K + \frac{1}{2}\,\underline{\underline{G}}^R \otimes \left[\underline{\underline{\Gamma}}^{\otimes}, \underline{\underline{h}}\right]_+ - \frac{1}{2}\left[\underline{\underline{\Gamma}}^{\otimes}, \underline{\underline{h}}\right]_+ \otimes \underline{\underline{G}}^A \\ &= 0. \end{aligned} \tag{3.1.10}$$

Introducing the matrix function $\underline{\underline{B}}$

$$\underline{\underline{B}} = -i\left[\underline{\underline{G}}_0^{-1} - \underline{\underline{Re\Sigma}}^{\otimes}, \underline{\underline{h}}\right]_- + \frac{1}{2}\left[\underline{\underline{\Gamma}}^{\otimes}, \underline{\underline{h}}\right]_+ - i\,\underline{\underline{\Sigma}}^K, \tag{3.1.11}$$

one can get the simpler looking form

$$\underline{\underline{G}}^R \otimes \underline{\underline{B}} - \underline{\underline{B}} \otimes \underline{\underline{G}}^A = 0, \tag{3.1.12}$$

Another way of writing equation (3.1.12) which turns out to be nice in conjunction with the gradient expansion is

$$\frac{1}{2}\left[\underline{\underline{B}}^{\otimes}, \underline{\underline{G}}^R - \underline{\underline{G}}^A\right]_+ - \left[\underline{\underline{B}}^{\otimes}, \underline{\underline{ReG}}\right]_- = 0 \tag{3.1.13}$$

Now to make further progress we will note that equation (3.1.12) can be satisfied by requiring $\underline{\underline{B}} = 0$. Which means we have the following equation for $\underline{\underline{h}}$:

$$\underline{\underline{B}} = -i\left[\underline{\underline{G}}_0^{-1} - \underline{\underline{Re\Sigma}}^{\otimes}, \underline{\underline{h}}\right]_- + \frac{1}{2}\left[\underline{\underline{\Gamma}}^{\otimes}, \underline{\underline{h}}\right]_+ - i\,\underline{\underline{\Sigma}}^K = 0. \tag{3.1.14}$$

This is result is exact within our ansatz in equation (3.1.5). Note that we in principle has n^2 coupled equations. However that the equations are coupled is not the only problem as we in general are also not able to perform the convolution integrals. So in order to proceed we need to transform to the Wigner representation where we will have a Moyal product instead of the convolution integral. This transformation will be the topic of the next section.

3.2 Wigner Representation and the Gradient Expansion

The transformation to Wigner representation mainly serves as a way to avoid the convolution integral in favour of a so called Moyal product. The Moyal product is in general not easier to deal with than the convolution integral, however the Moyal product can be viewed as an expansion in the gradients, which under the right conditions may be truncate at finite order. The truncation of the Moyal product is know in the literature as the gradient expansion[10] and is used where a quantum Boltzmann equation for a system is wanted

Now lets us start develop the a Wigner transformation. First note the form of the convolution integral, which we would like to transform is

$$\underline{\underline{C}}\left(\mathbf{x}_1, t_1, \mathbf{x}_{1'}, t_{1'}\right) = \int \mathrm{d}^3\mathbf{x}\mathrm{d}s\, \underline{\underline{A}}\left(\mathbf{x}_1, t_1, \mathbf{x}_2, s\right) \underline{\underline{B}}\left(\mathbf{x}_2, s, \mathbf{x}_{1'}, t_{1'}\right) \tag{3.2.1}$$

$$= \left(\underline{\underline{A}} \otimes \underline{\underline{B}}\right)\left(\mathbf{x}_1, t_1, \mathbf{x}_{1'}, t_{1'}\right). \tag{3.2.2}$$

Lets start by first rewriting the our variables in terms of center-of-mass and relative coordinates[4]:

$$\mathbf{r} = \mathbf{x}_1 - \mathbf{x}_{1'}, \quad \mathbf{R} = \frac{1}{2}\left(\mathbf{x}_1 + \mathbf{x}_{1'}\right), \quad t = t_1 - t_{1'}, \quad T = \frac{1}{2}\left(t_1 + t_{1'}\right). \tag{3.2.3}$$

To make the calculation more convenient we introduce 4-vectors. Note that we use the following convention for the metric $\eta_{\nu\mu} = \mathrm{diag}(-1, 1, 1, 1)$ which will be used throughout the rest of thesis. The 4-vectors

[4]The following is based on Jørgen Rammer's Master thesis (1981) section 2.5

are given as

$$\begin{aligned} x_1^\mu &\equiv (-t_1, \mathbf{x}_1)\,, \\ x^\mu &\equiv (-t, \mathbf{r}) = x_1^\mu - x_{1'}^\mu, \\ X^\mu &\equiv (-T, \mathbf{R}) = \frac{1}{2}(x_1^\mu + x_{1'}^\mu). \end{aligned} \tag{3.2.4}$$

Note that any function of the variables x_1^μ and $x_{1'}^\mu$ can be expressed in terms the center of mass and the relative variables. For a given function $\underline{\underline{A}}(x_1^\mu, x_{1'}^\mu)$ we define a new function $\breve{\underline{\underline{A}}}(X^\mu, x^\mu)$ as

$$\breve{\underline{\underline{A}}}(X^\mu, x^\mu) \equiv \underline{\underline{A}}(X^\mu + \tfrac{1}{2}x^\mu, X^\mu - \tfrac{1}{2}x^\mu) = \underline{\underline{A}}(x_1^\mu, x_{1'}^\mu). \tag{3.2.5}$$

However to be able to perform the Wigner transformation we will also need to note some properties of the Fourier-transform. To do this we need to define the 4-momentum and recall how the scalar product between two 4-vectors is defined:

$$\begin{aligned} p_1^\mu &\equiv (-E_1, \mathbf{p_1}), \\ p_1^\mu \eta_{\mu\nu} x_1^\nu &= p_1^\mu x_{1\,\mu} = -E_1 t_1 + \mathbf{p_1} \cdot \mathbf{x_1}. \end{aligned} \tag{3.2.6}$$

So now we can write the Fourier-transform in the following way, both for $\breve{\underline{\underline{A}}}$ and $\underline{\underline{A}}$

$$\begin{aligned} \underline{\underline{A}}(p_1^\mu, p_{1'}^\mu) &= \int \mathrm{d}^4 x_{1\,\mu} \int \mathrm{d}^4 x_{1'\,\mu} \exp(-i(p_1^\mu x_{1\,\mu} + p_{1'}^\mu x_{1'\,\mu}))\, \underline{\underline{A}}(x_{1\,\mu}, x_{1'\,\mu}), \\ \breve{\underline{\underline{A}}}(P^\mu, p^\mu) &= \int \mathrm{d}^4 x_\mu \int \mathrm{d}^4 X_\mu \exp(-i(p^\mu x_\mu + P^\mu X_\mu))\, \breve{\underline{\underline{A}}}(X_\mu, x_\mu) \\ &= \int \mathrm{d}^4 x_\mu \int \mathrm{d}^4 X_\mu \exp(-i(p^\mu x_\mu + P^\mu X_\mu))\, \underline{\underline{A}}(X_\mu + 1/2 x_\mu, X_\mu - 1/2 x_\mu). \end{aligned} \tag{3.2.7}$$

From this one sees that we can relate the center of mass/the ralative variables with $p_{1'}^\mu$ and p_1^μ as

$$p_1^\mu = \frac{1}{2}P^\mu + p^\mu, \quad p_{1'}^\mu = \frac{1}{2}P^\mu - p^\mu. \tag{3.2.8}$$

Hence we can also relate the functions $\breve{\underline{\underline{A}}}$ and $\underline{\underline{A}}$ in momentum space similar to their relation given in equation (3.2.5)

$$\breve{\underline{\underline{A}}}(P^\mu, p^\mu) = \underline{\underline{A}}\left(\frac{1}{2}P^\mu + p^\mu, \frac{1}{2}P^\mu - p^\mu\right) = \underline{\underline{A}}\,(p_1^\mu, p_{1'}^\mu)\,. \tag{3.2.9}$$

With this relation in place we can now proceed with the Wigner transformation of equation (3.2.1). Staring by looking at the center of mass

$$\begin{aligned} \breve{\underline{\underline{C}}}(X^\mu, x^\mu) &= \int \mathrm{d}^4 x_2^\mu\, \underline{\underline{A}}(X^\mu + \frac{1}{2}x^\mu, x_2^\mu) B(x_2^\mu, X^\mu - \frac{1}{2}x^\mu) \\ &= \int \mathrm{d}^4 x_2^\mu\, \breve{\underline{\underline{A}}}(\frac{1}{2}(X^\mu + \frac{1}{2}x^\mu + x_2^\mu), X^\mu + \frac{1}{2}x^\mu - x_2^\mu)\, \breve{\underline{\underline{B}}}(\frac{1}{2}(X^\mu - \frac{1}{2}x^\mu + x_2^\mu), x_2^\mu - X^\mu + \frac{1}{2}x^\mu), \end{aligned} \tag{3.2.10}$$

where $x_2^\mu = (s, \mathbf{x}_2)$ and we in the second line have used equation (3.2.5).

We proceed by noting that the integration over x_2^μ does not change if we make the following shift of x_2^μ due to the fact that we integrate over all of space-time

$$x_2^\mu \mapsto x_2^\mu - X^\mu - \frac{1}{2}x^\mu. \tag{3.2.11}$$

So equation (3.2.10) can be state as:

$$\breve{\underline{\underline{C}}}(X^\mu, x^\mu) = \int \mathrm{d}^4 x_2^\mu\, \breve{\underline{\underline{A}}}(X^\mu + \frac{1}{2}x_2^\mu, x^\mu - x_2^\mu)\, \breve{\underline{\underline{B}}}(X^\mu - \frac{1}{2}x^\mu + \frac{1}{2}x_2^\mu, x_2^\mu). \tag{3.2.12}$$

To get an equation for the Wigner transformation of $\breve{\underline{\underline{C}}}$, we have to Fourier transform in the relative coordinate x^μ:

$$\breve{\underline{\underline{C}}}(X^\mu, p_\mu) = \int \mathrm{d}^4 x^\mu \exp(-ip_\mu x^\mu) \int \mathrm{d}^4 x_2^\mu \, \breve{\underline{\underline{A}}}(X^\mu + \frac{1}{2}x_2^\mu, x^\mu - x_2^\mu) \, \breve{\underline{\underline{B}}}(X^\mu - \frac{1}{2}x^\mu + \frac{1}{2}x_2^\mu, x_2^\mu). \tag{3.2.13}$$

Now in order to be able to define the Moayl-product we first write $\breve{\underline{\underline{A}}}$ and $\breve{\underline{\underline{B}}}$ as the Fourier transform in the second variable:

$$\begin{aligned}\breve{\underline{\underline{C}}}(X^\mu, p_\mu) = \int \mathrm{d}^4 x^\mu \exp(-ip_\mu x^\mu) \int \mathrm{d}^4 x_2^\mu \int \frac{\mathrm{d}^4 p'_\mu}{(2\pi)^4} \exp(ip'_\mu (x^\mu - x_2^\mu)) \, \breve{\underline{\underline{A}}}(X^\mu + \frac{1}{2}x_2^\mu, p'_\mu) \\ \times \int \frac{\mathrm{d}^4 p''_\mu}{(2\pi)^4} \exp(ip''_\mu x_2^\mu) \, \breve{\underline{\underline{B}}}(X^\mu - \frac{1}{2}x^\mu + 1/2 x_2^\mu, p''_\mu).\end{aligned} \tag{3.2.14}$$

To this point we have not introduced any approximation. To proceed however one has to do a Taylor expansion around X^μ and if one only goes to finite order it will of course be an approximation. We will now do a first order expansion to show how the integral can be evaluated order by order. The expansion point X^μ can be motivated by the classical view that things tend to move around the center of mass. Hence one would think the quantum system would tend to do same up to fast fluctuations. We drop the explicit distinction between the breve and non-breve function and write

$$\begin{aligned}\underline{\underline{C}}(X^\mu, p_\mu) &\approx \int \mathrm{d}^4 x^\mu \int \mathrm{d}^4 x_2^\mu \int \frac{\mathrm{d}^4 p'_\mu}{(2\pi)^4} \int \frac{\mathrm{d}^4 p''_\mu}{(2\pi)^4} \exp(i(-p_\mu x^\mu + p'_\mu (x^\mu - x_2^\mu) + p''_\mu x_2^\mu)) \\ &\quad \times \left[\underline{\underline{A}}(X^\mu, p'_\mu) + \frac{1}{2} x_2^\mu \partial_{X^\mu} \underline{\underline{A}}(X^\mu, p'_\mu) \right] \left[\underline{\underline{B}}(X^\mu, p''_\mu) + \frac{1}{2}(x_2^\mu - x^\mu) \partial_{X^\mu} B(X^\mu, p''_\mu) \right] \\ &= \int \mathrm{d}^4 x^\mu \int \mathrm{d}^4 x_2^\mu \int \frac{\mathrm{d}^4 p'_\mu}{(2\pi)^4} \int \frac{\mathrm{d}^4 p''_\mu}{(2\pi)^4} \exp(i(-p_\mu x^\mu + p'_\mu (x^\mu - x_2^\mu) + p'' - \mu x_2^\mu)) \\ &\quad \times \Bigg[\underline{\underline{A}}(X^\mu, p'_\mu) \, \underline{\underline{B}}(X^\mu, p''_\mu) + \frac{1}{2} x_2^\mu \partial_{X^\mu} \underline{\underline{A}}(X^\mu, p'_\mu) \, \underline{\underline{B}}(X^\mu, p''_\mu) \\ &\quad + \frac{1}{2} \underline{\underline{A}}(X^\mu, p'_\mu)(x_2^\mu - x^\mu) \partial_{X^\mu} \underline{\underline{B}}(X^\mu, p''_\mu) \Bigg].\end{aligned} \tag{3.2.15}$$

In the second equality we have dropped second order terms in the spacial gradient as we only consider a first order expansion. The partial derivative with respect to the 4-vectors of real-space/time and momentum-space/energy are defined as

$$\partial_{X^\mu} \equiv (-\partial_T, \nabla_{\mathbf{R}}), \qquad \partial_{p^\mu} \equiv (-\partial_E, \nabla_{\mathbf{p}}). \tag{3.2.16}$$

This allow us to write $\underline{\underline{C}}$ as

$$\begin{aligned}\underline{\underline{C}}(X^\mu, p_\mu) &\approx \int \mathrm{d}^4 x^\mu \int \mathrm{d}^4 x_2^\mu \int \frac{\mathrm{d}^4 p'_\mu}{(2\pi)^4} \int \frac{\mathrm{d}^4 p''_\mu}{(2\pi)^4} \\ &\quad \times \Big[\underline{\underline{A}}(X^\mu, p'_\mu) \, \underline{\underline{B}}(X^\mu, p''_\mu) \exp(i(-p_\mu x^\mu + p' - \mu(x^\mu - x_2^\mu) + p''_\mu x_2^\mu)) \\ &\quad + \frac{1}{2} \partial_{X^\mu} \underline{\underline{A}}(X^\mu, p'_\mu)(-i) \partial_{p''_\mu} \exp(i(-p_\mu x^\mu + p'_\mu (x^\mu - x_2^\mu) + p''_\mu \cdot x_2^\mu)) \, \underline{\underline{B}}(X^\mu, p''_\mu) \\ &\quad + \frac{1}{2} \underline{\underline{A}}(X^\mu, p'_\mu) i \partial_{p'_\mu} \exp(i(-p_\mu x^\mu + p'_\mu (x^\mu - x_2^\mu) + p''_\mu x_2^\mu)) \partial_{X^\mu} \underline{\underline{B}}(X^\mu, p''_\mu) \Big] \\ &= \int \mathrm{d}^4 x^\mu \int \mathrm{d}^4 x_2^\mu \int \frac{\mathrm{d}^4 p'_\mu}{(2\pi)^4} \int \frac{\mathrm{d}^4 p''_\mu}{(2\pi)^4} \exp(i(-p_\mu x^\mu + p' - \mu \cdot (x^\mu - x_2^\mu) + p''_\mu \cdot x_2^\mu)) \\ &\quad \times \Bigg[\underline{\underline{A}}(X^\mu, p'_\mu) \, \underline{\underline{B}}(X^\mu, p''_\mu) - \frac{i}{2} \partial_{p'_\mu} \underline{\underline{A}}(X^\mu, p'_\mu) \partial_{X^\mu} \underline{\underline{B}}(X^\mu, p''_\mu) \\ &\quad + \frac{i}{2} \partial_{X^\mu} \underline{\underline{A}}(X^\mu, p'_\mu) \partial_{p''_\mu} \underline{\underline{B}}(^\mu, p''_\mu) \Bigg],\end{aligned} \tag{3.2.17}$$

where in the second equality we used integration by parts. The expression above can now be integrated. To demonstrate the technique, integration of the first term is shown here

$$\begin{aligned}\underline{\underline{C}}^0(X^\mu,p_\mu) &= \int \mathrm{d}^4x^\mu \int \mathrm{d}^4x_2^\mu \int \frac{\mathrm{d}^4p'_\mu}{(2\pi)^4}\int \frac{\mathrm{d}^4p''_\mu}{(2\pi)^4}\exp(i(-p_\mu x^\mu + p'_\mu(x^\mu - x_2^\mu) + p''_\mu x_2^\mu)) \\ &\quad \times \underline{\underline{A}}(X^\mu,p'_\mu)\,\underline{\underline{B}}(X^\mu,p''_\mu) \\ &= \int \mathrm{d}^4x^\mu \exp(-ip_\mu x^\mu)\int \mathrm{d}^4x_2^\mu\, \underline{\underline{A}}(X^\mu, x^\mu - x_2^\mu)B(X^\mu,x_2^\mu) \\ &= \underline{\underline{A}}(X^\mu,p_\mu)\,\underline{\underline{B}}(X^\mu,p_\mu).\end{aligned} \tag{3.2.18}$$

where the superscript on $\underline{\underline{C}}$ refer to the order and we in the third line used that the integral is a convolution in the variable x_2^μ. The integration of the two other terms gives

$$\underline{\underline{C}}^1(X^\mu,p_\mu) = -\frac{i}{2}\partial_{p_\mu}\underline{\underline{A}}(X^\mu,p_\mu)\partial_{X^\mu}\underline{\underline{B}}(X^\mu,p_\mu) + \frac{i}{2}\partial_{X^\mu}\underline{\underline{A}}(X^\mu,p_\mu)\partial_{p_\mu}B(X^\mu,p_\mu). \tag{3.2.19}$$

By considering the infinite order Taylor expansion one can show that Wigner transform can be written exactly as

$$\begin{aligned}(\underline{\underline{A}}\otimes\underline{\underline{B}})(X^\mu,p_\mu) &= \underline{\underline{A}}(X^\mu,p_\mu)\exp\left(\frac{i}{2}(\overleftarrow{\partial}_{X^\mu}\overrightarrow{\partial}_{p_\mu} - \overleftarrow{\partial}_{p^\mu}\overrightarrow{\partial}_{X_\mu})\right)\underline{\underline{B}}(X^\mu,p_\mu) \\ &= \underline{\underline{A}}(X^\mu,p_\mu)\bigstar\underline{\underline{B}}(X^\mu,p_\mu).\end{aligned} \tag{3.2.20}$$

Where the arrows above the differentials denote in which direction thy act. The composition $\bigstar$ is called the Moyal product[5] but in the context of transport theory it is also denoted the gradient operator [27, 22]. For the proof of equation (3.2.20) see[22].

Now we have reformulated the convolution of $\underline{\underline{A}}$ and $\underline{\underline{B}}$ in the Wigner representation in terms of the Moyal product between the Wigner representationof $\underline{\underline{A}}$ and $\underline{\underline{B}}$. From the definition seams easy to approximate by simply truncating the Moyal product at finite order, which is typically motivated by assuming that potential is slowing varying compared to the typical energy scale of the system.

Let us state the explicit result of the second order gradient expansion of both the commutator and anti commutator with respect to the Moyal product. However we will later consider only the first order as is customary[10]

$$\begin{aligned}\left[\underline{\underline{A}}\overset{\bigstar}{,}\underline{\underline{B}}\right]_- &= \underline{\underline{A}}\exp\left(\frac{i}{2}\left(\overleftarrow{\partial}_{X^\mu}\overrightarrow{\partial}_{p_\mu} - \overleftarrow{\partial}_{p^\mu}\overrightarrow{\partial}_{X_\mu}\right)\right)\underline{\underline{B}} - \underline{\underline{B}}\exp\left(\frac{i}{2}\left(\overleftarrow{\partial}_{X^\mu}\overrightarrow{\partial}_{p_\mu} - \overleftarrow{\partial}_{p^\mu}\overrightarrow{\partial}_{X_\mu}\right)\right)\underline{\underline{A}} \\ &\simeq \left[\underline{\underline{A}},\underline{\underline{B}}\right]_- + \frac{i}{2}\left(\left[\partial_{X_\mu}\underline{\underline{A}},\partial_{p^\mu}\underline{\underline{B}}\right]_+ - \left[\partial_{p_\mu}\underline{\underline{A}},\partial_{X^\mu}\underline{\underline{B}}\right]_+\right) \\ &\quad - \frac{1}{8}\Big(\left[\partial_{p_\mu}\partial_{p_\nu}\underline{\underline{A}},\partial_{X^\mu}\partial_{X^\nu}\underline{\underline{B}}\right]_- + \left[\partial_{X_\mu}\partial_{X_\nu}\underline{\underline{A}},\partial_{p^\mu}\partial_{p^\nu}\underline{\underline{B}}\right]_- \\ &\quad - \left[\partial_{X_\mu}\partial_{p_\nu}\underline{\underline{A}},\partial_{p^\mu}\partial_{X^\nu}\underline{\underline{B}}\right]_- - \left[\partial_{p_\mu}\partial_{X_\nu}\underline{\underline{A}},\partial_{X^\mu}\partial_{p^\nu}\underline{\underline{B}}\right]_-\Big).\end{aligned} \tag{3.2.21}$$

Note especially that the zeroth and the second order always vanish if $\underline{\underline{A}}$ and $\underline{\underline{B}}$ are scaler quantities[6], and that the zeroth order can be made to vanish if $\underline{\underline{A}}$ and $\underline{\underline{B}}$ have the same eigenvectors. The anti-commutator

[5] As a side remark it can be mention that the Moyal product is closely relate to the phase-space or Weyl-Wigner-Moyal representation of quantum mechanics which is a non-operator based formulation of quantum mechanics.

[6] It is customary to write the first order term in the scalar case as $[A,B]_{\mathbf{R}} \equiv (\partial_{X^\mu}A)\left(\partial_{p_\mu}B\right) - \left(\partial_{p^\mu}A\right)\left(\partial_{X_\mu}B\right)$ which is referred to as the generalized Poisson brackets

have the following expansion:

$$\left[\underline{\underline{A}}^{\bigstar}, \underline{\underline{B}}\right]_+ = \underline{\underline{A}} \exp\left(\frac{i}{2}\left(\overleftarrow{\partial}_{X^\mu}\overrightarrow{\partial}_{p_\mu} - \overleftarrow{\partial}_{p^\mu}\overrightarrow{\partial}_{X_\mu}\right)\right)\underline{\underline{B}} + \underline{\underline{B}} \exp\left(\frac{i}{2}\left(\overleftarrow{\partial}_{X^\mu}\overrightarrow{\partial}_{p_\mu} - \overleftarrow{\partial}_{p^\mu}\overrightarrow{\partial}_{X_\mu}\right)\right)\underline{\underline{A}} \quad (3.2.22)$$

$$\simeq \left[\underline{\underline{A}}, \underline{\underline{B}}\right]_+ + \frac{i}{2}\left(\left[\partial_{X_\mu}\underline{\underline{A}}, \partial_{p^\mu}\underline{\underline{B}}\right]_- - \left[\partial_{p_\mu}\underline{\underline{A}}, \partial_{X^\mu}\underline{\underline{B}}\right]_-\right)$$
$$- \frac{1}{8}\left(\left[\partial_{p_\mu}\partial_{p_\nu}\underline{\underline{A}}, \partial_{X^\mu}\partial_{X^\nu}\underline{\underline{B}}\right]_+ + \left[\partial_{X_\mu}\partial_{X_\nu}\underline{\underline{A}}, \partial_{p^\mu}\partial_{p^\nu}\underline{\underline{B}}\right]_+\right.$$
$$\left. - \left[\partial_{X_\mu}\partial_{p_\nu}\underline{\underline{A}}, \partial_{p^\mu}\partial_{X^\nu}\underline{\underline{B}}\right]_+ - \left[\partial_{p_\mu}\partial_{X_\nu}\underline{\underline{A}}, \partial_{X^\mu}\partial_{p^\nu}\underline{\underline{B}}\right]_+\right).$$

These two equations, along with the fact that we can transform the convolution to Moyal products, allow us write equation (3.1.14) using the Wigner representation as

$$\underline{\underline{B}} = -i\left[\underline{\underline{G}}_0^{-1} - \underline{\underline{Re\Sigma}}^{\bigstar}, \underline{\underline{h}}\right]_- + \frac{1}{2}\left[\underline{\underline{\Gamma}}^{\bigstar}, \underline{\underline{h}}\right]_+ - i\,\underline{\underline{\Sigma}}^K = 0. \quad (3.2.23)$$

Note that $\underline{\underline{G}}_0^{-1}$ is now a function of the form $\underline{\underline{1}}\omega - \underline{\underline{H}}(X^\mu, p^\mu)$. However there is still the problem that we have n^2 coupled differential equation. In the next section we will show how to decouple the equations order by order in the gradient expansion and develop an intra-band kinetic equation for each band.

3.3 Decoupling of the Matrix Kinetic Equation

In this section we will go through the process of decoupling the equations contained in (3.2.23) however only in the case where we can safely ignore the collision terms, hence where $\underline{\underline{\Gamma}}$ and $\underline{\underline{\Sigma}}^K$ can be set to zero. The real path of the self energy is not as complicated to include as it's imaginary or Keldysh counterparts. So we will show how to decouple the equations

$$\underline{\underline{B}} = -i\left[\underline{\underline{G}}_0^{-1} - \underline{\underline{Re\Sigma}}^{\bigstar}, \underline{\underline{h}}\right]_- = 0. \quad (3.3.1)$$

Note that in the rest for the section we will use the inverse Green's function $\underline{\underline{G}}^{-1}$ to make the notation more smooth which is defined as $\underline{\underline{G}}^{-1} = \underline{\underline{G}}_0^{-1} - \underline{\underline{Re\Sigma}}$.

The naive guess on how to decouple the equations would be to use the unitary transformation $\underline{\underline{\mathcal{U}}}_{(0)}(X^\mu, p^\mu)$[7] that diagonalizes the matrix $\underline{\underline{G}}^{-1}(X^\mu, p^\mu)$:

$$\underline{\underline{\mathcal{U}}}_{(0)}\underline{\underline{\mathcal{U}}}^\dagger_{(0)} = \underline{\underline{\mathcal{U}}}^\dagger_{(0)}\underline{\underline{\mathcal{U}}}_{(0)} = 1, \quad (3.3.2)$$

$$\underline{\underline{\mathcal{U}}}_{(0)}\underline{\underline{G}}^{-1}\underline{\underline{\mathcal{U}}}^\dagger_{(0)} \equiv \underline{\underline{\tilde{G}}}^{-1}_{(0)} \quad (3.3.3)$$

where the subscript in a parenthesis on the $\underline{\underline{\mathcal{U}}}$ is the order in the gradient which will be come clear in following, the tilde denotes that the matrix is diagonal and the index (0) is on the inverse Green's function means that diagonalization is done by the matrix product with $\underline{\underline{\mathcal{U}}}_{(0)}$ [8] . However the only way to include $\underline{\underline{\mathcal{U}}}_{(0)}$ in equation (3.3.1) is to insert it as complete sets as follows

$$\underline{\underline{B}} = -i\left[\underline{\underline{\mathcal{U}}}^\dagger_{(0)}\underline{\underline{\mathcal{U}}}_{(0)}\underline{\underline{G}}^{-1}\underline{\underline{\mathcal{U}}}^\dagger_{(0)}\underline{\underline{\mathcal{U}}}_{(0)}^{\bigstar}, \underline{\underline{h}}\right]_- = 0. \quad (3.3.4)$$

This obviously does not make any change to the left hand side of the equation, so we have to find an other way to diagonalize it. Now assuming there exist a more general unitary transformation $\underline{\underline{\mathcal{U}}}(X^\mu, p^\mu)$[9]

[7] This transformation will not denpend on the energy if no self-energy is included as the energy dependence of $\underline{\underline{G}}_0^{-1}(X^\mu, p^\mu)$ is proportional to the identity.

[8] Comparer with section 1.4: $\underline{\underline{\mathcal{U}}}_{(0)}$ should be identified with $\underline{\underline{U}}^\dagger$ and $\underline{\underline{\mathcal{U}}}^\dagger_{(0)}$ should be identified with $\underline{\underline{U}}$

[9] This will also only depend on energy in the presence of a slef-energy.

which has the following properties

$$\underline{\underline{\mathcal{U}}}\bigstar\underline{\underline{\mathcal{U}}}^{\dagger} = \underline{\underline{\mathcal{U}}}^{\dagger}\bigstar\underline{\underline{\mathcal{U}}} = 1 \tag{3.3.5}$$

$$\underline{\underline{\mathcal{U}}}\bigstar\underline{\underline{G}}^{-1}\bigstar\underline{\underline{\mathcal{U}}}^{\dagger} = \underline{\underline{\tilde{G}}}^{-1} \tag{3.3.6}$$

where the tilde denote that the function is diagonal. Now applying this to equation (3.3.1) and by using that the Moyal product is associative we can get the following

$$\begin{aligned}\underline{\underline{\mathcal{U}}}\bigstar\underline{\underline{B}}\bigstar\underline{\underline{\mathcal{U}}}^{\dagger} &= -i\underline{\underline{\mathcal{U}}}\bigstar\left[\underline{\underline{G}}^{-1}\bigstar\underline{\underline{\mathcal{U}}}^{\dagger}\bigstar\underline{\underline{\mathcal{U}}}\overset{\bigstar}{,}\underline{\underline{h}}\right]_{-}\bigstar\underline{\underline{\mathcal{U}}}^{\dagger} \\ &= -i\left[\underline{\underline{\mathcal{U}}}\bigstar\underline{\underline{G}}^{-1}\bigstar\underline{\underline{\mathcal{U}}}^{\dagger}\overset{\bigstar}{,}\underline{\underline{\mathcal{U}}}\bigstar\underline{\underline{h}}\bigstar\underline{\underline{\mathcal{U}}}^{\dagger}\right]_{-} \\ &= -i\left[\underline{\underline{\tilde{G}}}^{-1}\overset{\bigstar}{,}\underline{\underline{\breve{h}}}\right]_{-} = 0,\end{aligned} \tag{3.3.7}$$

where $\underline{\underline{\breve{h}}} = \underline{\underline{\mathcal{U}}}\bigstar\underline{\underline{h}}\bigstar\underline{\underline{\mathcal{U}}}^{\dagger}$ is just a matrix. The same can be defined for $\underline{\underline{B}}$. Now let us writ out this equation explicitly for the two by two case, to see that this in fact decouples the diagonal equations:

$$\begin{aligned}\underline{\underline{\breve{B}}} &= -i\left[\begin{pmatrix}\tilde{G}_1^{-1} & 0\\ 0 & \tilde{G}_2^{-1}\end{pmatrix}\overset{\bigstar}{,}\begin{pmatrix}\breve{h}_{11} & \breve{h}_{12}\\ \breve{h}_{21} & \breve{h}_{22}\end{pmatrix}\right]_{-} \\ &= -i\begin{pmatrix}\tilde{G}_1^{-1}\bigstar\breve{h}_{11} - \breve{h}_{11}\bigstar\tilde{G}_1^{-1} & \tilde{G}_1^{-1}\bigstar\breve{h}_{12} - \breve{h}_{12}\bigstar\tilde{G}_2^{-1}\\ \tilde{G}_2^{-1}\bigstar\breve{h}_{21} - \breve{h}_{21}\bigstar\tilde{G}_1^{-1} & \tilde{G}_2^{-1}\bigstar\breve{h}_{22} - \breve{h}_{22}\bigstar\tilde{G}_2^{-1}\end{pmatrix} = 0.\end{aligned} \tag{3.3.8}$$

We see that the intra-band equations decouples, hence the equations on the diagonal, by the transformation $\underline{\underline{\mathcal{U}}}$. So as we interested in are the intra-band transport we can introduce the band-projectors $\mathcal{P}_i$. Applying the band projectors to $\underline{\underline{\breve{B}}}$ and summing them gives:

$$\sum_{i=1}^{n}\mathcal{P}_i\,\underline{\underline{\breve{B}}}\mathcal{P}_i = -i\begin{pmatrix}\tilde{G}_1^{-1}\bigstar\breve{h}_{11} - \breve{h}_{11}\bigstar\tilde{G}_1^{-1} & 0\\ 0 & \tilde{G}_2^{-1}\bigstar\breve{h}_{22} - \breve{h}_{22}\bigstar\tilde{G}_2^{-1}\end{pmatrix} = 0. \tag{3.3.9}$$

However we are left with one rather significant problem: We do not known the transformation $\underline{\underline{\mathcal{U}}}$ In the general $\underline{\underline{\mathcal{U}}}$ depends on both X_μ and p_μ ans it is not possible to obtain it exactly. However in the case where the gradient expansion is valid one can obtain it perturbatively. This case will be the subject of the following subsection.

3.3.1 Perturbative Treatment of the Unitary Transformation and the Diagonalization of the Inverse Green's Function

Even though it is in general not possible to find $\underline{\underline{\mathcal{U}}}$ exactly, we can find it perturbatively in the cases where the gradient expansion is valid. The reason is that the Moyal product in this case can the viewed as an expansion in some small parameter λ. The idea of doing this kind of expansion stems form Wickles and Blezig [9]. Others have used similar methods [8]. To get started on the perturbativ diagonalization let us expand both the unitary transformation $\underline{\underline{\mathcal{U}}}$ and the diagonalized inverse free Green's fuction $\underline{\underline{\tilde{G}}}^{-1}$ in the small parameter λ as follows

$$\underline{\underline{\mathcal{U}}} = \underline{\underline{\mathcal{U}}}_{(0)} + \underline{\underline{\bar{\mathcal{U}}}}_{(1)}\underline{\underline{\mathcal{U}}}_{(0)} + \underline{\underline{\bar{\mathcal{U}}}}_{(2)}\underline{\underline{\mathcal{U}}}_{(0)} + ... \tag{3.3.10}$$

$$\underline{\underline{\tilde{G}}}^{-1} = \underline{\underline{\tilde{G}}}^{-1}_{(0)} + \underline{\underline{\tilde{G}}}^{-1}_{(1)} + \underline{\underline{\tilde{G}}}^{-1}_{(2)} + ..., \tag{3.3.11}$$

where the extra index in parentheses on the function gives the order in λ, $\underline{\underline{\bar{\mathcal{U}}}}_{(1)}\underline{\underline{\mathcal{U}}}_{(0)} = \underline{\underline{\mathcal{U}}}_{(1)}$ and $\underline{\underline{\tilde{G}}}^{-1}_{(0)}$ is given through equation (3.3.3). Now let us explore the definition in equation (3.3.6) to first order in the

gradient. Before we start on this we need to define the matrix Berry connections $\underline{\underline{\mathcal{A}}}$

$$\underline{\underline{\mathcal{A}}}_{x^\mu} = i\underline{\underline{\mathcal{U}}}_{(0)}\partial_{X^\mu}\underline{\underline{\mathcal{U}}}^\dagger_{(0)} = -i\left(\partial_{X^\mu}\underline{\underline{\mathcal{U}}}_{(0)}\right)\underline{\underline{\mathcal{U}}}^\dagger_{(0)} = \underline{\underline{\mathcal{A}}}^\dagger_{x^\mu} \tag{3.3.12}$$

$$\underline{\underline{\mathcal{A}}}_{p^\mu} = i\underline{\underline{\mathcal{U}}}_{(0)}\partial_{p^\mu}\underline{\underline{\mathcal{U}}}^\dagger_{(0)} = -i\left(\partial_{p^\mu}\underline{\underline{\mathcal{U}}}_{(0)}\right)\underline{\underline{\mathcal{U}}}^\dagger_{(0)} = \underline{\underline{\mathcal{A}}}^\dagger_{p^\mu}. \tag{3.3.13}$$

The second equality comes from differentiating equation (3.3.2) with respect to X^μ and p^μ respectively. In the third equality we recognize the Hermitian conjugate of the Berry connection so we see that it is in fact Hermitian, which will important later. To avoid complications with defining the Berry curvatures and to make the process as clear as possible we will restric ourselves to the case of Abelian Berry connections. Hence we will not consider degenerate bands nor will we treat the problem of a band crossing[10]. With the expansions of equations (3.3.12), (3.3.13) in place we are ready to handle equation (3.3.6) to first order in the gradient, as we already know how to treat the zero order through equation (3.3.3). Let us start by rewriting the left side of equation (3.3.6):

$$\begin{aligned}
\underline{\underline{\mathcal{U}}}\bigstar\left(\underline{\underline{G}}^{-1}\bigstar\underline{\underline{\mathcal{U}}}^\dagger\right) &= \underline{\underline{\mathcal{U}}}\bigstar\left(\underline{\underline{G}}^{-1}\left(1+\frac{i}{2}\left(+\overleftarrow{\partial}_{X^\mu}\overrightarrow{\partial}_{p^\mu}-\overleftarrow{\partial}_{p^\mu}\overrightarrow{\partial}_{X^\mu}\right)\right)\underline{\underline{\mathcal{U}}}^\dagger\right) \\
&= \underline{\underline{\mathcal{U}}}\left(1+\frac{i}{2}\left(+\overleftarrow{\partial}_{X^\mu}\overrightarrow{\partial}_{p^\mu}-\overleftarrow{\partial}_{p^\mu}\overrightarrow{\partial}_{X^\mu}\right)\right) \\
&\quad\times\left(\underline{\underline{G}}^{-1}\underline{\underline{\mathcal{U}}}^\dagger+\frac{i}{2}\left(+\partial_{X^\mu}\underline{\underline{G}}^{-1}\partial_{p^\mu}\underline{\underline{\mathcal{U}}}^\dagger_{(0)}-\partial_{p^\mu}\underline{\underline{G}}^{-1}\partial_{X^\mu}\underline{\underline{\mathcal{U}}}^\dagger_{(0)}\right)\right)+\mathcal{O}(\lambda^2) \\
&= \tilde{\underline{\underline{G}}}^{-1}_{(0)}+\bar{\underline{\underline{\mathcal{U}}}}_{(1)}\tilde{\underline{\underline{G}}}^{-1}_{(0)}+\tilde{\underline{\underline{G}}}^{-1}_{(0)}\bar{\underline{\underline{\mathcal{U}}}}^\dagger_{(1)} \\
&\quad+\frac{i}{2}\left(-\underline{\underline{\mathcal{U}}}_{(0)}\partial_{p^\mu}\underline{\underline{G}}^{-1}\partial_{X^\mu}\underline{\underline{\mathcal{U}}}^\dagger_{(0)}+\underline{\underline{\mathcal{U}}}_{(0)}\partial_{X^\mu}\underline{\underline{G}}^{-1}\partial_{p^\mu}\underline{\underline{\mathcal{U}}}^\dagger_{(0)}\right) \\
&\quad+\frac{i}{2}\left(-\partial_{p^\mu}\underline{\underline{\mathcal{U}}}_{(0)}\partial_{X^\mu}\left(\underline{\underline{G}}^{-1}\underline{\underline{\mathcal{U}}}^\dagger_{(0)}\right)+\partial_{X^\mu}\underline{\underline{\mathcal{U}}}_{(0)}\partial_{p^\mu}\left(\underline{\underline{G}}^{-1}\underline{\underline{\mathcal{U}}}^\dagger_{(0)}\right)\right)+\mathcal{O}(\lambda^2),
\end{aligned} \tag{3.3.14}$$

where we have expanded to first order in the gradient. Then using equation (3.3.3) we get

$$\begin{aligned}
&\tilde{\underline{\underline{G}}}^{-1}_{(0)}+\bar{\underline{\underline{\mathcal{U}}}}_{(1)}\tilde{\underline{\underline{G}}}^{-1}_{(0)}+\tilde{\underline{\underline{G}}}^{-1}_{(0)}\bar{\underline{\underline{\mathcal{U}}}}^\dagger_{(1)}+\frac{i}{2}\left(-\underline{\underline{\mathcal{U}}}_{(0)}\partial_{p^\mu}\left(\underline{\underline{\mathcal{U}}}^\dagger_{(0)}\tilde{\underline{\underline{G}}}^{-1}_{(0)}\underline{\underline{\mathcal{U}}}_{(0)}\right)\partial_{X^\mu}\underline{\underline{\mathcal{U}}}^\dagger_{(0)}\right. \\
&\quad\left.+\underline{\underline{\mathcal{U}}}_{(0)}\partial_{X^\mu}\left(\underline{\underline{\mathcal{U}}}^\dagger_{(0)}\tilde{\underline{\underline{G}}}^{-1}_{(0)}\underline{\underline{\mathcal{U}}}_{(0)}\right)\partial_{p^\mu}\underline{\underline{\mathcal{U}}}^\dagger_{(0)}\right) \\
&\quad+\frac{i}{2}\left(-\partial_{p^\mu}\underline{\underline{\mathcal{U}}}_{(0)}\partial_{X^\mu}\left(\underline{\underline{\mathcal{U}}}^\dagger_{(0)}\tilde{\underline{\underline{G}}}^{-1}_{(0)}\right)+\partial_{X^\mu}\underline{\underline{\mathcal{U}}}_{(0)}\partial_{p^\mu}\left(\underline{\underline{\mathcal{U}}}^\dagger_{(0)}\tilde{\underline{\underline{G}}}^{-1}_{(0)}\right)\right)+\mathcal{O}(\lambda^2),
\end{aligned} \tag{3.3.15}$$

expanding the equation leads to

$$\begin{aligned}
&\tilde{\underline{\underline{G}}}^{-1}_{(0)}+\bar{\underline{\underline{\mathcal{U}}}}_{(1)}\tilde{\underline{\underline{G}}}^{-1}_{(0)}+\tilde{\underline{\underline{G}}}^{-1}_{(0)}\bar{\underline{\underline{\mathcal{U}}}}^\dagger_{(1)} \\
&\quad+\frac{i}{2}\left(-\underline{\underline{\mathcal{U}}}_{(0)}\partial_{p^\mu}\underline{\underline{\mathcal{U}}}^\dagger_{(0)}\tilde{\underline{\underline{G}}}^{-1}_{(0)}\underline{\underline{\mathcal{U}}}_{(0)}\partial_{X^\mu}\underline{\underline{\mathcal{U}}}^\dagger_{(0)}-\partial_{p^\mu}\tilde{\underline{\underline{G}}}^{-1}_{(0)}\underline{\underline{\mathcal{U}}}_{(0)}\partial_{X^\mu}\underline{\underline{\mathcal{U}}}^\dagger_{(0)}\right. \\
&\quad-\tilde{\underline{\underline{G}}}^{-1}_{(0)}\partial_{p^\mu}\underline{\underline{\mathcal{U}}}_{(0)}\partial_{X^\mu}\underline{\underline{\mathcal{U}}}^\dagger_{(0)}+\underline{\underline{\mathcal{U}}}_{(0)}\partial_{X^\mu}\underline{\underline{\mathcal{U}}}^\dagger_{(0)}\tilde{\underline{\underline{G}}}^{-1}_{(0)}\underline{\underline{\mathcal{U}}}_{(0)}\partial_{p^\mu}\underline{\underline{\mathcal{U}}}^\dagger_{(0)} \\
&\quad\left.+\partial_{X^\mu}\tilde{\underline{\underline{G}}}^{-1}_{(0)}\underline{\underline{\mathcal{U}}}_{(0)}\partial_{p^\mu}\underline{\underline{\mathcal{U}}}^\dagger_{(0)}+\tilde{\underline{\underline{G}}}^{-1}_{(0)}\partial_{X^\mu}\underline{\underline{\mathcal{U}}}_{(0)}\partial_{p^\mu}\underline{\underline{\mathcal{U}}}^\dagger_{(0)}\right) \\
&\quad+\frac{i}{2}\left(-\partial_{p^\mu}\underline{\underline{\mathcal{U}}}_{(0)}\partial_{X^\mu}\underline{\underline{\mathcal{U}}}^\dagger_{(0)}\tilde{\underline{\underline{G}}}^{-1}_{(0)}+\partial_{p^\mu}\underline{\underline{\mathcal{U}}}_{(0)}\underline{\underline{\mathcal{U}}}^\dagger_{(0)}\partial_{X^\mu}\tilde{\underline{\underline{G}}}^{-1}_{(0)}\right. \\
&\quad\left.+\partial_{X^\mu}\underline{\underline{\mathcal{U}}}_{(0)}\partial_{p^\mu}\underline{\underline{\mathcal{U}}}^\dagger_{(0)}\tilde{\underline{\underline{G}}}^{-1}_{(0)}-\partial_{X^\mu}\underline{\underline{\mathcal{U}}}_{(0)}\underline{\underline{\mathcal{U}}}^\dagger_{(0)}\partial_{p^\mu}\tilde{\underline{\underline{G}}}^{-1}_{(0)}\right)+\mathcal{O}(\lambda^2).
\end{aligned} \tag{3.3.16}$$

[10]The complications in treating non-Abelian Berry connections are manageable and Wickles and Blezig [9] do it

The using the equations (3.3.12) and (3.3.13) to rewrite the equation yield

$$\begin{aligned}\tilde{\underline{\underline{G}}}^{-1}_{(0)} &+ \bar{\underline{\underline{\mathcal{U}}}}_{(1)}\tilde{\underline{\underline{G}}}^{-1}_{(0)} + \tilde{\underline{\underline{G}}}^{-1}_{(0)}\bar{\underline{\underline{\mathcal{U}}}}^{\dagger}_{(1)} + \frac{i}{2}\Big(+\underline{\underline{\mathcal{A}}}_{p^\mu}\tilde{\underline{\underline{G}}}^{-1}_{(0)}\underline{\underline{\mathcal{A}}}_{X^\mu} + i\partial_{p^\mu}\tilde{\underline{\underline{G}}}^{-1}_{(0)}\underline{\underline{\mathcal{A}}}_{X^\mu} \\ &- \tilde{\underline{\underline{G}}}^{-1}_{(0)}\underline{\underline{\mathcal{A}}}_{p^\mu}\underline{\underline{\mathcal{A}}}_{X^\mu} - \underline{\underline{\mathcal{A}}}_{X^\mu}\tilde{\underline{\underline{G}}}^{-1}_{(0)}\underline{\underline{\mathcal{A}}}_{p^\mu} - i\partial_{X^\mu}\tilde{\underline{\underline{G}}}^{-1}_{(0)}\underline{\underline{\mathcal{A}}}_{p^\mu} + \tilde{\underline{\underline{G}}}^{-1}_{(0)}\underline{\underline{\mathcal{A}}}_{X^\mu}\underline{\underline{\mathcal{A}}}_{p^\mu}\Big) \\ &+ \frac{i}{2}\Big(-\underline{\underline{\mathcal{A}}}_{p^\mu}\underline{\underline{\mathcal{A}}}_{X^\mu}\tilde{\underline{\underline{G}}}^{-1}_{(0)} - i\,\underline{\underline{\mathcal{A}}}_{p^\mu}\partial_{X^\mu}\tilde{\underline{\underline{G}}}^{-1}_{(0)} + \underline{\underline{\mathcal{A}}}_{X^\mu}\underline{\underline{\mathcal{A}}}_{p^\mu}\tilde{\underline{\underline{G}}}^{-1}_{(0)} + i\,\underline{\underline{\mathcal{A}}}_{X^\mu}\partial_{p^\mu}\tilde{\underline{\underline{G}}}^{-1}_{(0)}\Big) \\ &+ \mathcal{O}(\lambda^2).\end{aligned} \tag{3.3.17}$$

Finally rewriting it using (anti)-commutators

$$\begin{aligned}\tilde{\underline{\underline{G}}}^{-1}_{(0)} &+ \bar{\underline{\underline{\mathcal{U}}}}_{(1)}\tilde{\underline{\underline{G}}}^{-1}_{(0)} + \tilde{\underline{\underline{G}}}^{-1}_{(0)}\bar{\underline{\underline{\mathcal{U}}}}^{\dagger}_{(1)} - \frac{1}{2}\Big\{\underline{\underline{\mathcal{A}}}_{X^\mu}, \partial_{p^\mu}\tilde{\underline{\underline{G}}}^{-1}_{(0)}\Big\} \\ &+ \frac{1}{2}\Big\{\underline{\underline{\mathcal{A}}}_{p^\mu}, \partial_{X^\mu}\tilde{\underline{\underline{G}}}^{-1}_{(0)}\Big\} - \frac{i}{2}\Big\{\underline{\underline{\mathcal{A}}}_{p^\mu}\underline{\underline{\mathcal{A}}}_{X^\mu}, \tilde{\underline{\underline{G}}}^{-1}_{(0)}\Big\} + \frac{i}{2}\Big\{\underline{\underline{\mathcal{A}}}_{X^\mu}\underline{\underline{\mathcal{A}}}_{p^\mu}, \tilde{\underline{\underline{G}}}^{-1}_{(0)}\Big\} \\ &- \frac{i}{2}\Big(\underline{\underline{\mathcal{A}}}_{X^\mu}\tilde{\underline{\underline{G}}}^{-1}_{(0)}\underline{\underline{\mathcal{A}}}_{p^\mu} - \underline{\underline{\mathcal{A}}}_{p^\mu}\tilde{\underline{\underline{G}}}^{-1}_{(0)}\underline{\underline{\mathcal{A}}}_{X^\mu}\Big) + \mathcal{O}(\lambda^2).\end{aligned} \tag{3.3.18}$$

Note that if $\tilde{\underline{\underline{G}}}^{-1}$ only depends on either X^μ or p^μ, the diagonalization of the inverse Green's function becomes exact at first order in the gradient. Now using the expression in equation (3.3.11) to first order in the gradients one arrives at the following equation for $\tilde{\underline{\underline{G}}}^{-1}_{1}$:

$$\begin{aligned}\tilde{\underline{\underline{G}}}^{-1}_{(1)} &= \bar{\underline{\underline{\mathcal{U}}}}_{(1)}\tilde{\underline{\underline{G}}}^{-1}_{(0)} + \tilde{\underline{\underline{G}}}^{-1}_{(0)}\bar{\underline{\underline{\mathcal{U}}}}^{\dagger}_{(1)} - \frac{1}{2}\Big\{\underline{\underline{\mathcal{A}}}_{X^\mu}, \partial_{p^\mu}\tilde{\underline{\underline{G}}}^{-1}_{(0)}\Big\} \\ &+ \frac{1}{2}\Big\{\underline{\underline{\mathcal{A}}}_{p^\mu}, \partial_{X^\mu}\tilde{\underline{\underline{G}}}^{-1}_{(0)}\Big\} - \frac{i}{2}\Big\{\underline{\underline{\mathcal{A}}}_{p^\mu}\underline{\underline{\mathcal{A}}}_{X^\mu}, \tilde{\underline{\underline{G}}}^{-1}_{(0)}\Big\} + \frac{i}{2}\Big\{\underline{\underline{\mathcal{A}}}_{X^\mu}\underline{\underline{\mathcal{A}}}_{p^\mu}, \tilde{\underline{\underline{G}}}^{-1}_{(0)}\Big\} \\ &- \frac{i}{2}\Big(\underline{\underline{\mathcal{A}}}_{X^\mu}\tilde{\underline{\underline{G}}}^{-1}_{(0)}\underline{\underline{\mathcal{A}}}_{p^\mu} - \underline{\underline{\mathcal{A}}}_{p^\mu}\tilde{\underline{\underline{G}}}^{-1}_{(0)}\underline{\underline{\mathcal{A}}}_{X^\mu}\Big)\end{aligned} \tag{3.3.19}$$

However we also need an equation for $\bar{\underline{\underline{\mathcal{U}}}}_{(1)}$ in order to find $\tilde{\underline{\underline{G}}}^{-1}_{(1)}$. Such an equation can be obtained simply by replacing $\tilde{\underline{\underline{G}}}^{-1}_{(0)}$ with the identity $\underline{\underline{1}}$ in equation (3.3.18) along with using equation (3.3.5). This gives

$$\bar{\underline{\underline{\mathcal{U}}}}_{(1)} + \bar{\underline{\underline{\mathcal{U}}}}^{\dagger}_{(1)} - \frac{i}{2}\Big[\underline{\underline{\mathcal{A}}}_{p^\mu}, \underline{\underline{\mathcal{A}}}_{X^\mu}\Big] = 0. \tag{3.3.20}$$

This equation fixes the Hermitian part of $\bar{\underline{\underline{\mathcal{U}}}}_{(1)}$. It is intriguing to make the following ansatz

$$\bar{\underline{\underline{\mathcal{U}}}}_{(1)} = +\frac{i}{4}\Big[\underline{\underline{\mathcal{A}}}_{p^\mu}, \underline{\underline{\mathcal{A}}}_{X^\mu}\Big] + \underline{\underline{\mathcal{Y}}}_{(1)}. \tag{3.3.21}$$

Where $\underline{\underline{\mathcal{Y}}}_{(1)}$ is taken to be anti-Hermitian, that is $\underline{\underline{\mathcal{Y}}}_{(1)} = -\underline{\underline{\mathcal{Y}}}^{\dagger}_{(1)}$, in order to satisfy equation (3.3.20). Now plugging the ansatz form equation (3.3.21) into equation (3.3.19), gives

$$\begin{aligned}\tilde{\underline{\underline{G}}}^{-1}_{(0)} &= \Big[\underline{\underline{\mathcal{Y}}}_{(1)}, \tilde{\underline{\underline{G}}}^{-1}_{(0)}\Big]_{-} - \frac{1}{2}\Big\{\underline{\underline{\mathcal{A}}}_{X^\mu}, \partial_{p^\mu}\tilde{\underline{\underline{G}}}^{-1}_{(0)}\Big\} \\ &+ \frac{1}{2}\Big\{\underline{\underline{\mathcal{A}}}_{p^\mu}, \partial_{X^\mu}\tilde{\underline{\underline{G}}}^{-1}_{(0)}\Big\} - \frac{i}{4}\Big\{\underline{\underline{\mathcal{A}}}_{p^\mu}\underline{\underline{\mathcal{A}}}_{X^\mu}, \tilde{\underline{\underline{G}}}^{-1}_{(0)}\Big\} + \frac{i}{4}\Big\{\underline{\underline{\mathcal{A}}}_{X^\mu}\underline{\underline{\mathcal{A}}}_{p^\mu}, \tilde{\underline{\underline{G}}}^{-1}_{(0)}\Big\} \\ &- \frac{i}{2}\Big(\underline{\underline{\mathcal{A}}}_{X^\mu}\tilde{\underline{\underline{G}}}^{-1}_{(0)}\underline{\underline{\mathcal{A}}}_{p^\mu} - \underline{\underline{\mathcal{A}}}_{p^\mu}\tilde{\underline{\underline{G}}}^{-1}_{(0)}\underline{\underline{\mathcal{A}}}_{X^\mu}\Big).\end{aligned} \tag{3.3.22}$$

The imagery part of the diagonal of $\underline{\underline{\mathcal{Y}}}_{(1)}$ is in contrast to its real part not restricted by the requirement that $\underline{\underline{\mathcal{Y}}}_{(1)}$ is anti-Hermitian to be zero. However it can be put to zero with our loss of generality as it can be absorbed by the U(1) gauge freedom in each band. The detailed discussion of the gauge freedom will be postponed. With this observation at hand we can choose $\Big[\underline{\underline{\mathcal{Y}}}_{(1)}, \tilde{\underline{\underline{G}}}^{-1}_{(0)}\Big]_{-}$ to be completely off diagonal.

Hence we can use it to absorb the off-diagonal components of the remaining terms in equation (3.3.22). Now calling these off-diagonal components $\underline{\underline{\mathcal{R}}}_{(0)}$ we, for the two band case, get the following equation if the of diagonal part of equation (3.3.22) should vanish

$$\begin{pmatrix} 0 & \left(\tilde{G}^{-1}_{(0)\,1} - \tilde{G}^{-1}_{(0)\,2}\right)\mathcal{Y}_{12(1)} \\ \left(\tilde{G}^{-1}_{(0)\,2} - \tilde{G}^{-1}_{(0)\,1}\right)\mathcal{Y}_{21(1)} & 0 \end{pmatrix} = \begin{pmatrix} 0 & \mathcal{R}_{12} \\ \mathcal{R}_{21} & 0 \end{pmatrix}. \tag{3.3.23}$$

Hence the solution for $\underline{\underline{\mathcal{Y}}}_{(1)}$ is

$$\begin{pmatrix} \mathcal{Y}_{12(1)} & 0 \\ 0 & \mathcal{Y}_{21(1)} \end{pmatrix} = \begin{pmatrix} \frac{\mathcal{R}_{12}}{\tilde{G}^{-1}_{(0)\,1} - \tilde{G}^{-1}_{(0)\,2}} & 0 \\ 0 & \frac{\mathcal{R}_{21}}{\tilde{G}^{-1}_{(0)\,2} - \tilde{G}^{-1}_{(0)\,1}} \end{pmatrix}. \tag{3.3.24}$$

Here we see that the off-diagonal components are inversely proportional to the energy spacing of the bands in the system. Hence it is reasonable to use the gradient expansion if $\mathcal{R}_{(0)}$ is small compared to the energy gap. This is actually the statement that has been used to justify of the Boltzmann equation in Smith and Jensen[20]. Note this result can be extended to more than two bands but it gives no new insight in our discussion[9].

Having shown that we can systematic get rid of the off-diagonal components of $\underline{\underline{\tilde{G}}}^{-1}_{(0)}$, let us just project the off-diagonal out of $\underline{\underline{\tilde{G}}}^{-1}$ to first order in the gradient. This will be done with the previously used band projectors $\underline{\underline{\mathcal{P}}}_i$. Before doing this let us define the band projected Berry connection as

$$\underline{\underline{\tilde{\mathcal{A}}}}_{p^\mu} = \sum_{i=1}^{n} \underline{\underline{\mathcal{P}}}_i \underline{\underline{\mathcal{A}}}_{p^\mu} \underline{\underline{\mathcal{P}}}_i, \tag{3.3.25}$$

where we notice that $\underline{\underline{\tilde{\mathcal{A}}}}_{p^\mu}$ is a diagonal matrix. Note that diagonal matrices commute. So the projected inverse free Green's function can to first order in the gradient be written as

$$\begin{aligned} \underline{\underline{\tilde{G}}}^{-1} = \underline{\underline{\tilde{G}}}^{-1}_{(0)} &+ \underline{\underline{\tilde{\mathcal{A}}}}_{p^\mu}\left[\partial_{X^\mu}\underline{\underline{\tilde{G}}}^{-1}_{(0)}\right] - \underline{\underline{\tilde{\mathcal{A}}}}_{X^\mu}\partial_{p^\mu}\underline{\underline{\tilde{G}}}^{-1}_{(0)} \\ &+ \sum_{i=1}^{n}\underline{\underline{\mathcal{P}}}_i\left[-\frac{i}{4}\left\{\underline{\underline{\mathcal{A}}}_{p^\mu}\underline{\underline{\mathcal{A}}}_{X^\mu}, \underline{\underline{\tilde{G}}}^{-1}_{(0)}\right\} + \frac{i}{4}\left\{\underline{\underline{\mathcal{A}}}_{X^\mu}\underline{\underline{\mathcal{A}}}_{p^\mu}, \underline{\underline{\tilde{G}}}^{-1}_{(0)}\right\}\right. \\ &\left. - \frac{i}{2}\left(\underline{\underline{\mathcal{A}}}_{X^\mu}\underline{\underline{\tilde{G}}}^{-1}_{(0)}\underline{\underline{\mathcal{A}}}_{p^\mu} - \underline{\underline{\mathcal{A}}}_{p^\mu}\underline{\underline{\tilde{G}}}^{-1}_{(0)}\underline{\underline{\mathcal{A}}}_{X^\mu}\right)\right]\underline{\underline{\mathcal{P}}}_i + \mathcal{O}(\lambda^2). \end{aligned} \tag{3.3.26}$$

The projection sum(the fourth term) can quite straightforwardly be shown to be zero because $\underline{\underline{\tilde{G}}}^{-1}_{(0)}$ is diagonal an the Berry connection is Hermitian. Our finally result for the form of $\underline{\underline{\tilde{G}}}^{-1}$ is

$$\underline{\underline{\tilde{G}}}^{-1} = \underline{\underline{\tilde{G}}}^{-1}_{(0)} + \underline{\underline{\tilde{\mathcal{A}}}}_{p^\mu}\partial_{X^\mu}\underline{\underline{\tilde{G}}}^{-1}_{(0)} - \underline{\underline{\tilde{\mathcal{A}}}}_{X^\mu}\partial_{p^\mu}\underline{\underline{\tilde{G}}}^{-1}_{(0)} + \mathcal{O}(\lambda^2). \tag{3.3.27}$$

With this equation at hand we will now turn to the problem that $\underline{\underline{\mathcal{U}}}_{(0)}$ is not uniquely defined. In fact there is a local gauge phase that depends on both X^μ and p^μ in each band. The gauge phase originates because the eigenvectors of a matrix are only defined up to a complex phase. This means that both the unitary transformation $\underline{\underline{\mathcal{U}}}_{(0)}$ and $\underline{\underline{\mathcal{U}}}'_{(0)}$ will diagonalize $\underline{\underline{\tilde{G}}}^{-1}$if they are related by the transformation $\underline{\underline{\tilde{\Phi}}}\underline{\underline{\mathcal{U}}}_{(0)} = \underline{\underline{\mathcal{U}}}'_{(0)}$, where $\underline{\underline{\tilde{\Phi}}}$ is Given in the two band case as

$$\underline{\underline{\tilde{\Phi}}}(X^\mu, p^\mu) = \begin{pmatrix} e^{i\chi_1(X^\mu,p^\mu)} & 0 \\ 0 & e^{i\chi_2(X^\mu,p^\mu)} \end{pmatrix}. \tag{3.3.28}$$

Here $\chi_i(X^\mu, p^\mu)$ is an arbitrary real function. However such a transformation does not leave our Berry connection invariant. In fact it is straightforward to calculate that it transforms as[11]

$$\underline{\underline{\mathcal{A}}}'_{p^\mu} = i\underline{\underline{\mathcal{U}}}'_{(0)}\partial_{p^\mu}\underline{\underline{\mathcal{U}}}'^{\dagger}_{(0)} = \underline{\underline{\tilde{\Phi}}}\,\underline{\underline{\mathcal{A}}}_{p^\mu}\underline{\underline{\tilde{\Phi}}}^{\dagger} + i\underline{\underline{\tilde{\Phi}}}\partial_{p^\mu}\underline{\underline{\tilde{\Phi}}}^{\dagger}. \tag{3.3.29}$$

Hence band projecting the transformed Berry curvature gives

$$\underline{\underline{\tilde{\mathcal{A}}}}'_{p^\mu} = \underline{\underline{\tilde{\mathcal{A}}}}_{p^\mu} + i\underline{\underline{\tilde{\Phi}}}\partial_{p^\mu}\underline{\underline{\tilde{\Phi}}}^{\dagger}. \tag{3.3.30}$$

This kind of transformation look all most like the gauge transformations known form electrodynamics. Note that the ith component of $i\underline{\underline{\tilde{\Phi}}}\partial_{p^\mu}\underline{\underline{\tilde{\Phi}}}^{\dagger}$ is just

$$\partial_{p^\mu}\chi_i. \tag{3.3.31}$$

The relation (3.3.30) implies that equation (3.3.27) transforms to

$$\underline{\underline{\tilde{G}}}^{-1} = \underline{\underline{\tilde{G}}}^{-1}_{(0)} + \underline{\underline{\tilde{\mathcal{A}}}}'_{p^\mu}\partial_{X^\mu}\underline{\underline{\tilde{G}}}^{-1}_{(0)} - \underline{\underline{\tilde{\mathcal{A}}}}'_{X^\mu}\partial_{p^\mu}\underline{\underline{\tilde{G}}}^{-1}_{(0)} + \mathcal{O}(\lambda^2). \tag{3.3.32}$$

This is obviously not a the same as before, hence not gauge invariant quantity. So we need, like in the case of electromagnetism, to find some kinetic variables which yield gauge invariant equations. Instead of introducing kinetic variables we can obtain the same result by going to second order i the Moyal product while keeping only terms which are of first order in the gradient[8]. However this is extremely cumbersome. We now find the kinetic variables by first writing equation (3.3.27) with all it arguments explicitly:

$$\underline{\underline{\tilde{G}}}^{-1} = \underline{\underline{\tilde{G}}}^{-1}_{(0)}(X^\mu, p^\mu) + \underline{\underline{\tilde{\mathcal{A}}}}_{p^\mu}(X^\mu, p^\mu)\partial_{X^\mu}\underline{\underline{\tilde{G}}}^{-1}_{(0)}(X^\mu, p^\mu) - \underline{\underline{\tilde{\mathcal{A}}}}_{X^\mu}(X^\mu, p^\mu)\partial_{p^\mu}\underline{\underline{\tilde{G}}}^{-1}_{(0)}(X^\mu, p^\mu) + \mathcal{O}(\lambda^2). \tag{3.3.33}$$

Now this can be viewed as a first order Taylor expansion around p^μ and X^μ of $\underline{\underline{\tilde{G}}}^{-1}_{(0)}$ if it had the following variables:

$$\underline{\underline{\tilde{G}}}^{-1}_{(0)}(X^\mu + \underline{\underline{\tilde{\mathcal{A}}}}_{p^\mu}, p^\mu - \underline{\underline{\tilde{\mathcal{A}}}}_{X^\mu}) + \mathcal{O}(\lambda^2). \tag{3.3.34}$$

Note this only holds as both $\underline{\underline{\tilde{G}}}^{-1}_{(0)}$, $\underline{\underline{\tilde{\mathcal{A}}}}_{p^\mu}$ and $\underline{\underline{\tilde{\mathcal{A}}}}_{X^\mu}$ are diagonal and hence effectively act as scalars under multiplication. However this also implies that one could introduce kinetic variables in each band as:

$$\underline{\underline{\tilde{\Upsilon}}}_{\mu} = X^\mu + \underline{\underline{\tilde{\mathcal{A}}}}_{p^\mu} \tag{3.3.35}$$

$$\underline{\underline{\tilde{\Pi}}}_{\mu} = p^\mu - \underline{\underline{\tilde{\mathcal{A}}}}_{X^\mu}, \tag{3.3.36}$$

which should be understood in the way that in the i-ed band the variable will be $X^\mu - (\underline{\underline{\tilde{\mathcal{A}}}}_{p^\mu})_{ii}$. So equation (3.3.27) can now be put to first order in the gradient in the following elegant form

$$\underline{\underline{\tilde{G}}}^{-1} = \underline{\underline{\tilde{G}}}^{-1}_{(0)}(\Upsilon^\mu, \Pi^\mu) + \mathcal{O}(\lambda^2). \tag{3.3.37}$$

As the Berry connections only occur in first order terms, one dose not need to distinguish between $\underline{\underline{\tilde{\mathcal{A}}}}_{p^\mu}(X^\mu, p^\mu)$ and $\underline{\underline{\tilde{\mathcal{A}}}}_{p^\mu}(\Upsilon^\mu, \Pi^\mu)$ as the differences are of first order in the gradient. With this result at hand we can rewrite equation (3.3.7) to first order as

$$-i\left[\underline{\underline{\tilde{G}}}^{-1}_{(0)}(\Upsilon^\mu, \Pi^\mu) \bigstar, \breve{\underline{\underline{h}}}(\Upsilon^\mu, \Pi^\mu)\right] = 0. \tag{3.3.38}$$

Note that we have also changed variables in the distribution function and hence it is principle not the same function as before which is expressed through the breve over the distribution function h. The only problem left is that the Moyal product is taken with respect to the variables X^μ and p^μ and we would

[11] Of cause the same equality holds similarly for $\underline{\underline{\mathcal{A}}}_{X^\mu}$

like it to be with respect to the kinetic variables. So all there is left to do is to find the Moyal product in the kinetic variables. This is in principle the same approach Rammer and Smith[10] used to derive a quantum Boltzmann equation that contained electromagnetism, but with some expect complication due to the facet that the Berry connection depends on both real-space and momentum. This processes will also show that the kinetic variables in fact restore gauge invariants. Let us find the derivatives with respect to X^μ and p^μ expressed through the band kinetic variables to first order in the gradient

$$\vec{\partial}_{X^\mu} = \frac{\partial \Upsilon^\nu}{\partial X^\mu}\vec{\partial}_{\Upsilon^\nu} + \frac{\partial \Pi^\nu}{\partial X^\mu}\vec{\partial}_{\Pi^\nu} = \vec{\partial}_{\Upsilon^\mu} + \frac{\partial \underline{\underline{\tilde{\mathcal{A}}}}_{\Pi^\nu}}{\partial \Upsilon^\mu}\vec{\partial}_{\Upsilon^\nu} - \frac{\partial \underline{\underline{\tilde{\mathcal{A}}}}_{\Upsilon^\nu}}{\partial \Upsilon^\mu}\vec{\partial}_{\Pi^\nu} + \mathcal{O}(\lambda^2), \tag{3.3.39}$$

$$\overleftarrow{\partial}_{X^\mu} = \overleftarrow{\partial}_{\Upsilon^\nu}\frac{\partial \Upsilon^\nu}{\partial X^\mu} + \overleftarrow{\partial}_{\Pi^\nu}\frac{\partial \Pi^\nu}{\partial X^\mu} = \overleftarrow{\partial}_{\Upsilon^\mu} + \overleftarrow{\partial}_{\Upsilon^\nu}\frac{\partial \underline{\underline{\tilde{\mathcal{A}}}}_{\Pi^\nu}}{\partial \Upsilon^\mu} - \overleftarrow{\partial}_{\Pi^\nu}\frac{\partial \underline{\underline{\tilde{\mathcal{A}}}}_{\Upsilon^\nu}}{\partial \Upsilon^\mu} + \mathcal{O}(\lambda^2), \tag{3.3.40}$$

$$\vec{\partial}_{p^\mu} = \frac{\partial \Pi^\nu}{\partial p^\mu}\vec{\partial}_{\Pi^\nu} + \frac{\partial \Upsilon^\nu}{\partial p^\mu}\vec{\partial}_{\Upsilon^\nu} = \vec{\partial}_{\Pi^\mu} - \frac{\partial \underline{\underline{\tilde{\mathcal{A}}}}_{\Upsilon^\nu}}{\partial \Pi^\mu}\vec{\partial}_{\Pi^\nu} + \frac{\partial \underline{\underline{\tilde{\mathcal{A}}}}_{\Pi^\nu}}{\partial \Pi^\mu}\vec{\partial}_{\Upsilon^\nu} + \mathcal{O}(\lambda^2), \tag{3.3.41}$$

$$\overleftarrow{\partial}_{p^\mu} = \overleftarrow{\partial}_{\Pi^\nu}\frac{\partial \Pi^\nu}{\partial p^\mu} + \overleftarrow{\partial}_{\Upsilon^\nu}\frac{\partial \Upsilon^\nu}{\partial p^\mu} = \overleftarrow{\partial}_{\Pi^\mu} - \overleftarrow{\partial}_{\Pi^\nu}\frac{\partial \underline{\underline{\tilde{\mathcal{A}}}}_{\Upsilon^\nu}}{\partial \Pi^\mu} + \overleftarrow{\partial}_{\Upsilon^\nu}\frac{\partial \underline{\underline{\tilde{\mathcal{A}}}}_{\Pi^\nu}}{\partial \Pi^\mu} + \mathcal{O}(\lambda^2). \tag{3.3.42}$$

This we can use to expand $\overleftarrow{\partial}_{X^\mu}\vec{\partial}_{p_\mu} - \overleftarrow{\partial}_{p^\mu}\vec{\partial}_{X_\mu}$ separately

$$\begin{aligned}
\overleftarrow{\partial}_{X^\mu}\vec{\partial}_{p_\mu} &= \left(\overleftarrow{\partial}_{\Upsilon^\mu} + \overleftarrow{\partial}_{\Upsilon^\nu}\partial_{\Upsilon_\mu}\underline{\underline{\tilde{\mathcal{A}}}}_{\Pi^\nu} - \overleftarrow{\partial}_{\Pi^\nu}\partial_{\Upsilon_\mu}\underline{\underline{\tilde{\mathcal{A}}}}_{\Upsilon^\nu}\right) \\
&\quad\times\left(\vec{\partial}_{\Pi_\mu} - \partial_{\Pi_\mu}\underline{\underline{\tilde{\mathcal{A}}}}_{\Upsilon_\delta}\vec{\partial}_{\Pi^\delta} + \partial_{\Pi_\mu}\underline{\underline{\tilde{\mathcal{A}}}}_{\Pi_\delta}\vec{\partial}_{\Upsilon^\delta}\right) + \mathcal{O}(\lambda^2) \\
&= \overleftarrow{\partial}_{\Upsilon^\mu}\vec{\partial}_{\Pi_\mu} - \overleftarrow{\partial}_{\Upsilon^\mu}\partial_{\Pi_\mu}\underline{\underline{\tilde{\mathcal{A}}}}_{\Upsilon_\delta}\vec{\partial}_{\Pi^\delta} + \overleftarrow{\partial}_{\Upsilon^\mu}\partial_{\Pi_\mu}\underline{\underline{\tilde{\mathcal{A}}}}_{\Pi_\delta}\vec{\partial}_{\Upsilon^\delta} \\
&\quad+ \overleftarrow{\partial}_{\Upsilon^\nu}\partial_{\Upsilon_\mu}\underline{\underline{\tilde{\mathcal{A}}}}_{\Pi^\nu}\vec{\partial}_{\Pi_\mu} - \overleftarrow{\partial}_{\Upsilon^\nu}\partial_{\Upsilon_\mu}\underline{\underline{\tilde{\mathcal{A}}}}_{\Pi^\nu}\partial_{\Pi_\mu}\underline{\underline{\tilde{\mathcal{A}}}}_{\Upsilon_\delta}\vec{\partial}_{\Pi^\delta} + \overleftarrow{\partial}_{\Upsilon^\nu}\partial_{\Upsilon_\mu}\underline{\underline{\tilde{\mathcal{A}}}}_{\Pi^\nu}\partial_{\Pi_\mu}\underline{\underline{\tilde{\mathcal{A}}}}_{\Pi_\delta}\vec{\partial}_{\Upsilon^\delta} \\
&\quad- \overleftarrow{\partial}_{\Pi^\nu}\partial_{\Upsilon_\mu}\underline{\underline{\tilde{\mathcal{A}}}}_{\Upsilon^\nu}\vec{\partial}_{\Pi_\mu} + \overleftarrow{\partial}_{\Pi^\nu}\partial_{\Upsilon_\mu}\underline{\underline{\tilde{\mathcal{A}}}}_{\Upsilon^\nu}\partial_{\Pi_\mu}\underline{\underline{\tilde{\mathcal{A}}}}_{\Upsilon_\delta}\vec{\partial}_{\Pi^\delta} - \overleftarrow{\partial}_{\Pi^\nu}\partial_{\Upsilon_\mu}\underline{\underline{\tilde{\mathcal{A}}}}_{\Upsilon^\nu}\partial_{\Pi_\mu}\underline{\underline{\tilde{\mathcal{A}}}}_{\Pi_\delta}\vec{\partial}_{\Upsilon^\delta} + \mathcal{O}(\lambda^2)
\end{aligned} \tag{3.3.43}$$

and

$$\begin{aligned}
-\overleftarrow{\partial}_{p^\mu}\vec{\partial}_{X_\mu} &= \left(-\overleftarrow{\partial}_{\Pi_\mu} + \overleftarrow{\partial}_{\Pi^\delta}\partial_{\Pi_\mu}\underline{\underline{\tilde{\mathcal{A}}}}_{\Upsilon_\delta} - \overleftarrow{\partial}_{\Upsilon^\delta}\partial_{\Pi_\mu}\underline{\underline{\tilde{\mathcal{A}}}}_{\Pi_\delta}\right) \\
&\quad\times\left(\vec{\partial}_{\Upsilon^\mu} + \partial_{\Upsilon_\mu}\underline{\underline{\tilde{\mathcal{A}}}}_{\Pi^\nu}\vec{\partial}_{\Upsilon^\nu} - \partial_{\Upsilon_\mu}\underline{\underline{\tilde{\mathcal{A}}}}_{\Upsilon^\nu}\vec{\partial}_{\Pi^\nu}\right) + \mathcal{O}(\lambda^2) \\
&= -\overleftarrow{\partial}_{\Pi_\mu}\vec{\partial}_{\Upsilon^\mu} - \overleftarrow{\partial}_{\Pi_\mu}\partial_{\Upsilon_\mu}\underline{\underline{\tilde{\mathcal{A}}}}_{\Pi^\nu}\vec{\partial}_{\Upsilon^\nu} + \overleftarrow{\partial}_{\Pi_\mu}\partial_{\Upsilon_\mu}\underline{\underline{\tilde{\mathcal{A}}}}_{\Upsilon^\nu}\vec{\partial}_{\Pi^\nu} \\
&\quad+ \overleftarrow{\partial}_{\Pi^\delta}\partial_{\Pi_\mu}\underline{\underline{\tilde{\mathcal{A}}}}_{\Upsilon_\delta}\vec{\partial}_{\Upsilon^\mu} + \overleftarrow{\partial}_{\Pi^\delta}\partial_{\Pi_\mu}\underline{\underline{\tilde{\mathcal{A}}}}_{\Upsilon_\delta}\partial_{\Upsilon_\mu}\underline{\underline{\tilde{\mathcal{A}}}}_{\Pi^\nu}\vec{\partial}_{\Upsilon^\nu} - \overleftarrow{\partial}_{\Pi^\delta}\partial_{\Pi_\mu}\underline{\underline{\tilde{\mathcal{A}}}}_{\Upsilon_\delta}\partial_{\Upsilon_\mu}\underline{\underline{\tilde{\mathcal{A}}}}_{\Upsilon^\nu}\vec{\partial}_{\Pi^\nu} \\
&\quad- \overleftarrow{\partial}_{\Upsilon^\delta}\partial_{\Pi_\mu}\underline{\underline{\tilde{\mathcal{A}}}}_{\Pi_\delta}\vec{\partial}_{\Upsilon^\mu} - \overleftarrow{\partial}_{\Upsilon^\delta}\partial_{\Pi_\mu}\underline{\underline{\tilde{\mathcal{A}}}}_{\Pi_\delta}\partial_{\Upsilon_\mu}\underline{\underline{\tilde{\mathcal{A}}}}_{\Pi^\nu}\vec{\partial}_{\Upsilon^\nu} + \overleftarrow{\partial}_{\Upsilon^\delta}\partial_{\Pi_\mu}\underline{\underline{\tilde{\mathcal{A}}}}_{\Pi_\delta}\partial_{\Upsilon_\mu}\underline{\underline{\tilde{\mathcal{A}}}}_{\Upsilon^\nu}\vec{\partial}_{\Pi^\nu} + \mathcal{O}(\lambda^2).
\end{aligned} \tag{3.3.44}$$

Combining this two terms, gives to first order in the gradients

$$\begin{aligned}
\overleftarrow{\partial}_{X^\mu}\vec{\partial}_{p_\mu} - \overleftarrow{\partial}_{p^\mu}\vec{\partial}_{X_\mu} &= \overleftarrow{\partial}_{\Upsilon^\mu}\vec{\partial}_{\Pi_\mu} - \overleftarrow{\partial}_{\Pi^\mu}\vec{\partial}_{\Upsilon_\mu} + \overleftarrow{\partial}_{\Upsilon_\nu}\left(\partial_{\Pi^\nu}\underline{\underline{\tilde{\mathcal{A}}}}_{\Pi^\mu} - \partial_{\Pi^\mu}\underline{\underline{\tilde{\mathcal{A}}}}_{\Pi^\nu}\right)\vec{\partial}_{\Upsilon_\mu} \\
&\quad+ \overleftarrow{\partial}_{\Pi_\nu}\left(\partial_{\Upsilon^\nu}\underline{\underline{\tilde{\mathcal{A}}}}_{\Upsilon^\mu} - \partial_{\Upsilon^\mu}\underline{\underline{\tilde{\mathcal{A}}}}_{\Upsilon^\nu}\right)\vec{\partial}_{\Pi_\mu} - \overleftarrow{\partial}_{\Pi_\mu}\left(\partial_{\Upsilon^\mu}\underline{\underline{\tilde{\mathcal{A}}}}_{\Pi^\nu} - \partial_{\Pi^\nu}\underline{\underline{\tilde{\mathcal{A}}}}_{\Upsilon^\mu}\right)\vec{\partial}_{\Upsilon_\nu} \\
&\quad- \overleftarrow{\partial}_{\Upsilon_\mu}\left(\partial_{\Pi^\mu}\underline{\underline{\tilde{\mathcal{A}}}}_{\Upsilon^\nu} - \partial_{\Upsilon^\nu}\underline{\underline{\tilde{\mathcal{A}}}}_{\Pi^\mu}\right)\vec{\partial}_{\Pi_\nu} + \mathcal{O}(\lambda^2).
\end{aligned} \tag{3.3.45}$$

Let us now expand all of this expression by dropping the 4-vector notation. The terms containing the Berry connection will be treated term by term. Note that the 4-vector is given as $\Upsilon_\mu = (\tau, \boldsymbol{\rho})$,

$\Pi^\mu = (-\omega, \boldsymbol{\pi})$. letus start with the term

$$\begin{aligned}\overleftarrow{\partial}_{\Upsilon_\nu}\left(\partial_{\Pi^\nu}\underline{\underline{\tilde{\mathcal{A}}}}_{\Pi^\mu} - \partial_{\Pi^\mu}\underline{\underline{\tilde{\mathcal{A}}}}_{\Pi^\nu}\right)\overrightarrow{\partial}_{\Upsilon_\mu} &= -\overleftarrow{\partial}_\tau\left(\partial_\omega\underline{\underline{\tilde{\mathcal{A}}}}_{\boldsymbol{\pi}} - \partial_{\boldsymbol{\pi}}\underline{\underline{\tilde{\mathcal{A}}}}_{\omega}\right)\cdot\overrightarrow{\partial}_{\boldsymbol{\rho}} \\ &\quad - \overleftarrow{\partial}_{\boldsymbol{\rho}}\cdot\left(\partial_{\boldsymbol{\pi}}\underline{\underline{\tilde{\mathcal{A}}}}_{\omega} - \partial_\omega\underline{\underline{\tilde{\mathcal{A}}}}_{\boldsymbol{\pi}}\right)\overrightarrow{\partial}_\tau + \overleftarrow{\partial}_{\rho_i}\left(\partial_{\pi_i}\underline{\underline{\tilde{\mathcal{A}}}}_{\pi_j} - \partial_{\pi_j}\underline{\underline{\tilde{\mathcal{A}}}}_{\pi_i}\right)\overrightarrow{\partial}_{\rho_j} \\ &= +\overleftarrow{\partial}_\tau\boldsymbol{\mathcal{E}}^{\boldsymbol{\pi}_\omega}\cdot\overrightarrow{\partial}_{\boldsymbol{\rho}} - \overleftarrow{\partial}_{\boldsymbol{\rho}}\cdot\boldsymbol{\mathcal{E}}^{\boldsymbol{\pi}_\omega}\overrightarrow{\partial}_\tau - \overleftarrow{\partial}_{\boldsymbol{\rho}}\times\boldsymbol{\Omega}^{\boldsymbol{\pi}}\cdot\overrightarrow{\partial}_{\boldsymbol{\rho}},\end{aligned} \tag{3.3.46}$$

where the last equality defines $\boldsymbol{\mathcal{E}}^{\boldsymbol{\pi}_\omega}$ and $\boldsymbol{\Omega}^{\boldsymbol{\pi}}$. we turn to the next term:

$$\begin{aligned}\overleftarrow{\partial}_{\Pi_\nu}\left(\partial_{\Upsilon^\nu}\underline{\underline{\tilde{\mathcal{A}}}}_{\Upsilon^\mu} - \partial_{\Upsilon^\mu}\underline{\underline{\tilde{\mathcal{A}}}}_{\Upsilon^\nu}\right)\overrightarrow{\partial}_{\Pi_\mu} &= -\overleftarrow{\partial}_\omega\left(\partial_\tau\underline{\underline{\tilde{\mathcal{A}}}}_{\boldsymbol{\rho}} - \partial_{\boldsymbol{\rho}}\underline{\underline{\tilde{\mathcal{A}}}}_{\tau}\right)\cdot\overrightarrow{\partial}_{\boldsymbol{\pi}} \\ &\quad - \overleftarrow{\partial}_{\boldsymbol{\pi}}\left(\partial_{\boldsymbol{\rho}}\underline{\underline{\tilde{\mathcal{A}}}}_{\tau} - \partial_\tau\underline{\underline{\tilde{\mathcal{A}}}}_{\boldsymbol{\rho}}\right)\overrightarrow{\partial}_\omega + \overleftarrow{\partial}_{\pi_i}\left(\partial_{\rho_i}\underline{\underline{\tilde{\mathcal{A}}}}_{\rho_j} - \partial_{\rho_j}\underline{\underline{\tilde{\mathcal{A}}}}_{\rho_i}\right)\overrightarrow{\partial}_{\pi_j} \\ &= +\overleftarrow{\partial}_\omega\boldsymbol{\mathcal{E}}^{\boldsymbol{\rho}_\tau}\cdot\overrightarrow{\partial}_{\boldsymbol{\pi}} - \overleftarrow{\partial}_{\boldsymbol{\pi}}\cdot\boldsymbol{\mathcal{E}}^{\boldsymbol{\rho}_\tau}\overrightarrow{\partial}_\omega - \overleftarrow{\partial}_{\boldsymbol{\pi}}\times\boldsymbol{\Omega}^{\boldsymbol{\rho}}\cdot\overrightarrow{\partial}_{\boldsymbol{\pi}},\end{aligned} \tag{3.3.47}$$

where the last equality defines $\boldsymbol{\mathcal{E}}^{\boldsymbol{\rho}_\tau}$ and $\boldsymbol{\Omega}^{\boldsymbol{\rho}}$. The next term yields

$$\begin{aligned}-\overleftarrow{\partial}_{\Pi_\mu}\left(\partial_{\Upsilon^\mu}\underline{\underline{\tilde{\mathcal{A}}}}_{\Pi^\nu} - \partial_{\Pi^\nu}\underline{\underline{\tilde{\mathcal{A}}}}_{\Upsilon^\mu}\right)\overrightarrow{\partial}_{\Upsilon_\nu} &= +\overleftarrow{\partial}_{\boldsymbol{\pi}}\cdot\left(\partial_{\boldsymbol{\rho}}\underline{\underline{\tilde{\mathcal{A}}}}_{\omega} - \partial_\omega\underline{\underline{\tilde{\mathcal{A}}}}_{\boldsymbol{\rho}}\right)\overrightarrow{\partial}_\tau \\ &\quad + \overleftarrow{\partial}_\omega\left(\partial_\tau\underline{\underline{\tilde{\mathcal{A}}}}_{\boldsymbol{\pi}} - \partial_{\boldsymbol{\pi}}\underline{\underline{\tilde{\mathcal{A}}}}_{\tau}\right)\cdot\overrightarrow{\partial}_{\boldsymbol{\rho}} - \overleftarrow{\partial}_{\pi_i}\left(\partial_{\rho_i}\underline{\underline{\tilde{\mathcal{A}}}}_{\pi_j} - \partial_{\pi_j}\underline{\underline{\tilde{\mathcal{A}}}}_{\rho_i}\right)\overrightarrow{\partial}_{\rho_j} \\ &\quad - \overleftarrow{\partial}_\omega\left(\partial_\tau\underline{\underline{\tilde{\mathcal{A}}}}_{\omega} - \partial_\omega\underline{\underline{\tilde{\mathcal{A}}}}_{\tau}\right)\overrightarrow{\partial}_\tau \\ &= +\overleftarrow{\partial}_{\boldsymbol{\pi}}\cdot\boldsymbol{\mathcal{E}}^{\boldsymbol{\rho}_\omega}\overrightarrow{\partial}_\tau - \overleftarrow{\partial}_\omega\boldsymbol{\mathcal{E}}^{\boldsymbol{\pi}_\tau}\cdot\overrightarrow{\partial}_{\boldsymbol{\rho}} - \overleftarrow{\partial}_{\pi_i}\Theta_{ij}^{\boldsymbol{\rho}\boldsymbol{\pi}}\overrightarrow{\partial}_{\rho_j} - \overleftarrow{\partial}_\omega\Xi\overrightarrow{\partial}_\tau,\end{aligned} \tag{3.3.48}$$

where the last equality defines $\boldsymbol{\mathcal{E}}^{\boldsymbol{\rho}_\omega}$,$\boldsymbol{\mathcal{E}}^{\phi_\tau}$,$\Theta_{ij}^{\boldsymbol{\rho}\boldsymbol{\pi}}$ and Ξ. We turn to the last term

$$\begin{aligned}-\overleftarrow{\partial}_{\Upsilon_\mu}\left(\partial_{\Pi^\mu}\underline{\underline{\tilde{\mathcal{A}}}}_{\Upsilon^\nu} - \partial_{\Upsilon^\nu}\underline{\underline{\tilde{\mathcal{A}}}}_{\Pi^\mu}\right)\overrightarrow{\partial}_{\Pi_\nu} &= +\overleftarrow{\partial}_{\boldsymbol{\rho}}\cdot\left(\partial_{\boldsymbol{\pi}}\underline{\underline{\tilde{\mathcal{A}}}}_{\tau} - \partial_\tau\underline{\underline{\tilde{\mathcal{A}}}}_{\boldsymbol{\pi}}\right)\overrightarrow{\partial}_\omega \\ &\quad + \overleftarrow{\partial}_\tau\left(\partial_\omega\underline{\underline{\tilde{\mathcal{A}}}}_{\boldsymbol{\rho}} - \partial_{\boldsymbol{\rho}}\underline{\underline{\tilde{\mathcal{A}}}}_{\omega}\right)\cdot\overrightarrow{\partial}_{\boldsymbol{\pi}} - \overleftarrow{\partial}_{\rho_i}\left(\partial_{\pi_i}\underline{\underline{\tilde{\mathcal{A}}}}_{\rho_j} - \partial_{\rho_j}\underline{\underline{\tilde{\mathcal{A}}}}_{\pi_i}\right)\overrightarrow{\partial}_{\pi_j} \\ &\quad + \overleftarrow{\partial}_\tau\left(\partial_\omega\underline{\underline{\tilde{\mathcal{A}}}}_{\tau} - \partial_\tau\underline{\underline{\tilde{\mathcal{A}}}}_{\omega}\right)\overrightarrow{\partial}_\omega \\ &= +\overleftarrow{\partial}_{\boldsymbol{\rho}}\cdot\boldsymbol{\mathcal{E}}^{\boldsymbol{\pi}_\tau}\overrightarrow{\partial}_\omega - \overleftarrow{\partial}_\tau\boldsymbol{\mathcal{E}}^{\boldsymbol{\rho}_\omega}\cdot\overrightarrow{\partial}_{\boldsymbol{\pi}} + \overleftarrow{\partial}_{\rho_i}\left(\Theta_{ij}^{\boldsymbol{\rho}\boldsymbol{\pi}}\right)^T\overrightarrow{\partial}_{\pi_j} + \overleftarrow{\partial}_\tau\Xi\overrightarrow{\partial}_\omega.\end{aligned} \tag{3.3.49}$$

With all this we can write equation (3.3.45) as:

$$\begin{aligned}\overleftarrow{\partial}_{X^\mu}\overrightarrow{\partial}_{p_\mu} - \overleftarrow{\partial}_{p^\mu}\overrightarrow{\partial}_{X_\mu} &= \overleftarrow{\partial}_{\boldsymbol{\rho}}\cdot\overrightarrow{\partial}_{\boldsymbol{\pi}} - \overleftarrow{\partial}_{\boldsymbol{\pi}}\cdot\overrightarrow{\partial}_{\boldsymbol{\rho}} - \overleftarrow{\partial}_\tau\overrightarrow{\partial}_\omega + \overleftarrow{\partial}_\omega\overrightarrow{\partial}_\tau + \overleftarrow{\partial}_\tau\boldsymbol{\mathcal{E}}^{\boldsymbol{\pi}_\omega}\cdot\overrightarrow{\partial}_{\boldsymbol{\rho}} \\ &\quad - \overleftarrow{\partial}_{\boldsymbol{\rho}}\cdot\boldsymbol{\mathcal{E}}^{\boldsymbol{\pi}_\omega}\overrightarrow{\partial}_\tau - \overleftarrow{\partial}_{\boldsymbol{\rho}}\times\boldsymbol{\Omega}^{\boldsymbol{\pi}}\cdot\overrightarrow{\partial}_{\boldsymbol{\rho}} + \overleftarrow{\partial}_\omega\boldsymbol{\mathcal{E}}^{\boldsymbol{\rho}_\tau}\cdot\overrightarrow{\partial}_{\boldsymbol{\pi}} - \overleftarrow{\partial}_{\boldsymbol{\pi}}\cdot\boldsymbol{\mathcal{E}}^{\boldsymbol{\rho}_\tau}\overrightarrow{\partial}_\omega \\ &\quad - \overleftarrow{\partial}_{\boldsymbol{\pi}}\times\boldsymbol{\Omega}^{\boldsymbol{\rho}}\cdot\overrightarrow{\partial}_{\boldsymbol{\pi}} + \overleftarrow{\partial}_{\boldsymbol{\pi}}\cdot\boldsymbol{\mathcal{E}}^{\boldsymbol{\rho}_\omega}\overrightarrow{\partial}_\tau - \overleftarrow{\partial}_\omega\boldsymbol{\mathcal{E}}^{\boldsymbol{\pi}_\tau}\cdot\overrightarrow{\partial}_{\boldsymbol{\rho}} - \overleftarrow{\partial}_{\pi_i}\Theta_{ij}^{\boldsymbol{\rho}\boldsymbol{\pi}}\overrightarrow{\partial}_{\rho_j} - \overleftarrow{\partial}_\omega\Xi\overrightarrow{\partial}_\tau \\ &\quad + \overleftarrow{\partial}_{\boldsymbol{\rho}}\cdot\boldsymbol{\mathcal{E}}^{\boldsymbol{\pi}_\tau}\overrightarrow{\partial}_\omega - \overleftarrow{\partial}_\tau\boldsymbol{\mathcal{E}}^{\boldsymbol{\rho}_\omega}\cdot\overrightarrow{\partial}_{\boldsymbol{\pi}} + \overleftarrow{\partial}_{\rho_i}\left(\Theta_{ij}^{\boldsymbol{\rho}\boldsymbol{\pi}}\right)^T\overrightarrow{\partial}_{\pi_j} + \overleftarrow{\partial}_\tau\Xi\overrightarrow{\partial}_\omega. + \mathcal{O}(\lambda^2)\end{aligned} \tag{3.3.50}$$

This is in principled the fist order correction to the Moyal product, and we see that it is explicitly gauge invariant, so the kinetic variables restored the guage invariants.

The Berry Field Strength and The Quantum Boltzmann equation

With equation (3.3.50) at hand we can now straightforwardly write down a collision-less quantum Boltzmann equation for a multi-band system by applying our result from equation (3.3.50) to equation (3.3.38). Similarly straightforwardly we can apply equation (3.3.50) to the band projection of equation (3.3.38). This yields independent equation for all the bands.

Before doing this we would like to first note the that equation (3.3.50) can be written in terms of a

field strength $\mathcal{F}$, which will be called the Berry field strength as:

$$\overleftarrow{\partial}_{X^\mu}\overrightarrow{\partial}_{p_\mu} - \overleftarrow{\partial}_{p^\mu}\overrightarrow{\partial}_{X_\mu} = \overleftarrow{\partial}_{\Upsilon^\mu}\overrightarrow{\partial}_{\Pi_\mu} - \overleftarrow{\partial}_{\Pi^\mu}\overrightarrow{\partial}_{\Upsilon_\mu} + \begin{pmatrix}\overleftarrow{\partial}_\Pi \overleftarrow{\partial}_\Upsilon\end{pmatrix}\mathcal{F}\begin{pmatrix}\overrightarrow{\partial}_\Pi \\ \overrightarrow{\partial}_\Upsilon\end{pmatrix} + \mathcal{O}(\lambda^2) \tag{3.3.51}$$

where:

$$\begin{pmatrix}\overleftarrow{\partial}_\Pi, \overleftarrow{\partial}_\Upsilon\end{pmatrix} = (-\omega, \boldsymbol{\pi}, -\tau, \boldsymbol{\rho}), \quad \begin{pmatrix}\overrightarrow{\partial}_\Pi \\ \overrightarrow{\partial}_\Upsilon\end{pmatrix} = \begin{pmatrix}-\omega \\ \boldsymbol{\pi} \\ -\tau \\ \boldsymbol{\rho}\end{pmatrix} \tag{3.3.52}$$

Hence the Berry field strength is defined in the following way:

$$\mathcal{F} = \begin{pmatrix} 0 & -\boldsymbol{\mathcal{E}}_{\boldsymbol{\rho}_\tau} & -\Xi & \boldsymbol{\mathcal{E}}_{\boldsymbol{\pi}_\tau} \\ \boldsymbol{\mathcal{E}}_{\boldsymbol{\rho}_\tau} & \epsilon_{ijk}\Omega_{\boldsymbol{\rho}\,k} & -\boldsymbol{\mathcal{E}}_{\boldsymbol{\rho}_\omega} & -\Theta_{ij}^{\boldsymbol{\rho},\boldsymbol{\pi}} \\ \Xi & \boldsymbol{\mathcal{E}}_{\boldsymbol{\rho}_\omega} & 0 & -\boldsymbol{\mathcal{E}}_{\boldsymbol{\pi}_\omega} \\ -\boldsymbol{\mathcal{E}}_{\boldsymbol{\pi}_\tau} & \left(\Theta_{ij}^{\boldsymbol{\rho},\boldsymbol{\pi}}\right)^T & \boldsymbol{\mathcal{E}}_{\boldsymbol{\pi}_\omega} & \epsilon_{ijk}\Omega_{\boldsymbol{\pi}\,k} \end{pmatrix}, \tag{3.3.53}$$

or in the more compact way

$$\mathcal{F} = \partial_i \underline{\underline{\tilde{\mathcal{A}}}}_j - \partial_j \underline{\underline{\tilde{\mathcal{A}}}}_i \tag{3.3.54}$$

where, i an j runs over $\omega, \boldsymbol{\pi}, \tau, \boldsymbol{\rho}$. Having this field strength we can to first order in the gradient write the Moyal product as

$$\bigstar = \exp\left(\frac{i}{2}\left(\overleftarrow{\partial}_{\Upsilon^\mu}\overrightarrow{\partial}_{\Pi_\mu} - \overleftarrow{\partial}_{\Pi^\mu}\overrightarrow{\partial}_{\Upsilon_\mu} + \begin{pmatrix}\overleftarrow{\partial}_{\Pi_\nu} \overleftarrow{\partial}_{\Upsilon_\nu}\end{pmatrix}\mathcal{F}\begin{pmatrix}\overleftarrow{\partial}_{\Pi_\nu} \\ \overleftarrow{\partial}_{\Upsilon_\nu}\end{pmatrix}\right)\right) + \mathcal{O}(\lambda^2). \tag{3.3.55}$$

We now apply this exprission of the Moyal product to the band projection of equation (3.3.38). We get a quantum Boltzman equation for each of the bands:

$$\begin{aligned} -i\mathcal{P}_i\left[\underline{\underline{\tilde{G}}}_{(0)}^{-1} \bigstar \underline{\underline{\breve{h}}}\right]\mathcal{P}_i = \Big[&\Big(-(1-\Xi_i)\partial_\tau \tilde{G}^{-1}_{(0)\,i} - \partial_{\boldsymbol{\pi}}\tilde{G}^{-1}_{(0)\,i}\cdot\boldsymbol{\mathcal{E}}_i^{\boldsymbol{\rho}_\tau} + \partial_{\boldsymbol{\rho}}\tilde{G}^{-1}_{(0)\,i}\cdot\boldsymbol{\mathcal{E}}_i^{\boldsymbol{\pi}_\tau}\Big)\partial_\omega \\ &+ \Big(\partial_\omega \tilde{G}^{-1}_{(0)\,i}\boldsymbol{\mathcal{E}}_i^{\boldsymbol{\rho}_\tau} - \partial_{\boldsymbol{\pi}}\tilde{G}^{-1}_{(0)\,i}\times\boldsymbol{\Omega}_i^{\boldsymbol{\rho}} - \partial_\tau \tilde{G}^{-1}_{(0)\,i}\boldsymbol{\mathcal{E}}_i^{\boldsymbol{\rho}_\omega} + \partial_{\boldsymbol{\rho}}\tilde{G}^{-1}_{(0)\,i}(1-\Theta_i^{\boldsymbol{\rho}\boldsymbol{\pi}})\Big)\cdot\partial_{\boldsymbol{\pi}} \\ &+ \Big((1-\Xi_i)\partial_\omega \tilde{G}^{-1}_{(0)\,i} + \partial_{\boldsymbol{\pi}}\tilde{G}^{-1}_{(0)\,i}\cdot\boldsymbol{\mathcal{E}}_i^{\boldsymbol{\rho}_\omega} - \partial_{\boldsymbol{\rho}}\tilde{G}^{-1}_{(0)\,i}\cdot\boldsymbol{\mathcal{E}}_i^{\boldsymbol{\pi}_\omega}\Big)\partial_\tau \\ &+ \Big(-\partial_\omega \tilde{G}^{-1}_{(0)\,i}\boldsymbol{\mathcal{E}}_i^{\boldsymbol{\pi}_\tau} - \partial_{\boldsymbol{\pi}}\tilde{G}^{-1}_{(0)\,i}(\underline{1} - (\underline{\Theta}^{\boldsymbol{\rho}\boldsymbol{\pi}})_i^T) \\ &+ \partial_\tau \tilde{G}^{-1}_{(0)\,i}\boldsymbol{\mathcal{E}}_i^{\boldsymbol{\pi}_\omega} - \partial_{\boldsymbol{\rho}}\tilde{G}^{-1}_{(0)\,i}\times\boldsymbol{\Omega}_i^{\boldsymbol{\pi}}\Big)\cdot\partial_{\boldsymbol{\rho}}\Big]\breve{h}_i = 0, \end{aligned} \tag{3.3.56}$$

where the index i refers to the band and a single underlining means a matrix in real-space and momentum-space.

Physical Understanding of the Berry Curvature

Having derived a quantum Boltzmann equation we now want to understand the different terms. This will be done by comparison with a one band quantum Boltzmann equation with a general electromagnetic field present. The derivation of such an equation is in principle contained above, so it will not be discussed here. However it can be found in Rammer and Smith [10] or in Maciejko [22]. It yields the following one band quantum Boltzmann equation:

$$\begin{aligned} -i\left[G_0^{-1}\bigstar\tilde{h}\right] = \big[&\partial_\omega G_0^{-1}\partial_T - \left(\partial_T G_0^{-1} + \partial_{\boldsymbol{\pi}}G_0^{-1}\cdot e\mathbf{E}\right)\partial_\omega - \partial_{\boldsymbol{\pi}}G_0^{-1}\cdot\partial_{\mathbf{R}} \\ &+ \left(\partial_\omega G_0^{-1} e\mathbf{E} - e\partial_{\boldsymbol{\pi}}G_0^{-1}\times\mathbf{B} + \partial_{\mathbf{R}}G_0^{-1}\right)\cdot\partial_{\boldsymbol{\pi}}\big]\,h, \end{aligned} \tag{3.3.57}$$

where $\mathbf{E}$ is the electric field and $\mathbf{B}$ is the magnetic field. So now by comparing equation (3.3.56) and (3.3.57) one straightforwardly sees that $\boldsymbol{\mathcal{E}}_i^{\boldsymbol{\rho}_\tau}$ orcures in the same way as the electric field does and that $\boldsymbol{\Omega}_i^{\boldsymbol{\rho}}$ orcures in the same way as the magnetic field does. Hence they can be viewed as a renormalization to respectively the electric and magnetic fields. The term $\boldsymbol{\Omega}_i^{\boldsymbol{\pi}}$ can be seen as a momentum-"magnetic" field and is in the literature typical refereed to as the anomalous velocity. This term the anomalous Hall response in section 2.3. The term $\boldsymbol{\mathcal{E}}_i^{\boldsymbol{\pi}_\omega}$ can similarly be viewed as momentum-"electric" field, it should be mentioned that this term is only non-vanishing if the real part of the self energy $\underline{\underline{Re\Sigma}}$ depends on the energy E. The reaming terms can be viewed as the changes of the metric by the transformation from the canonical to the kinetic variables in the following way

$$\mathrm{d}\Upsilon_\mu = \left(\delta_\mu{}^\nu + \partial_{X^\nu}\mathcal{A}_{p_\mu}\right)\mathrm{d}X_\nu \tag{3.3.58}$$

$$\mathrm{d}\Pi^\mu = \left(\delta_\nu{}^\mu - \partial_{p_\nu}\mathcal{A}_{X^\mu}\right)\mathrm{d}p^\nu. \tag{3.3.59}$$

We take the inner product between them to first order in the small parameter λ

$$\mathrm{d}\Upsilon_\mu \mathrm{d}\Pi^\mu = \mathrm{d}X_\nu\left(\delta_\delta{}^\nu + \left(\partial_{X^\nu}\mathcal{A}_{p_\delta} - \partial_{p_\delta}\mathcal{A}_{X^\nu}\right)\right)\mathrm{d}p^\delta + \mathcal{O}(\lambda^2) \tag{3.3.60}$$

The last two terms containing the Berry connection is precisely the term expanded in equation (3.3.48).

The next section will be concerned with energy integrating the quantum Boltzmann equation to get a semi-classical Boltzmann equation.

3.4 Energy integration of the Quantum Boltzmann Equation

In this section we will energy integrate(integration over ω) our quantum Boltzmann equation in order to get an equation which is comparable with the semi-classical Boltzmann equation we found in the second chapter. But there is some subtlety in integration of the quantum Boltzmann equation which was derived by letting the matrix function $\underline{\underline{B}}$ be equal to zero, because it is the Keldysh Dyson equation that gives the actual physics. The equation that actually governs the physics is equation (3.1.13) which in the Wigner repesentation is

$$\frac{1}{2}\left[\underline{\underline{B}}(X^\mu,p^\mu)\overset{\star}{,}\underline{\underline{G}}^R(X^\mu,p^\mu) - \underline{\underline{G}}^A(X^\mu,p^\mu)\right]_+ - \left[\underline{\underline{B}}(X^\mu,p^\mu)\overset{\star}{,}\underline{\underline{ReG}}(X^\mu,p^\mu)\right]_- = 0 \tag{3.4.1}$$

Off course this equation has the full matrix structure and as we want a equation for the band projected equations for h. So we need to motivate that we can in fact meaningfully restrict this equation to band projected equations. To do this we transform the equation with the generalized unitary transformation $\underline{\underline{\mathcal{U}}}$ to first order in the gradient. Equation (3.4.1) becomes

$$\frac{1}{2}\left[\breve{\underline{\underline{B}}}(\Upsilon^\mu,\Pi^\mu)\overset{\star}{,}\breve{\underline{\underline{G}}}^R(\Upsilon^\mu,\Pi^\mu) - \breve{\underline{\underline{G}}}^A(\Upsilon^\mu,\Pi^\mu)\right]_+ - \left[\breve{\underline{\underline{B}}}(\Upsilon^\mu,\Pi^\mu)\overset{\star}{,}\breve{\underline{\underline{ReG}}}(\Upsilon^\mu,\Pi^\mu)\right]_- = 0. \tag{3.4.2}$$

Now we need the matrix structure of the spectral function $\breve{\underline{\underline{A}}}$[12] along with the real part of the Green's function $\breve{\underline{\underline{ReG}}}$. As our inverse bare Green's function plus real part of the self-energy is diagonal in the basis we have transformed to, their inverse, the Green's function, would also be diagonal. Now as the spectral function is proportional to imaginary part of the Green's function[19], we should be able to write $\breve{\underline{\underline{A}}}$ and $\breve{\underline{\underline{ReG}}}$ as $\tilde{\underline{\underline{A}}}$ and $\tilde{\underline{\underline{ReG}}}$. With this constrain on the matrix form of $\tilde{\underline{\underline{A}}}$ and $\tilde{\underline{\underline{ReG}}}$ we again see that we decouple the bands. Moreover we note as $\tilde{\underline{\underline{B}}}$ is first order in the gradient(λ) already the term involving $\tilde{\underline{\underline{ReG}}}$ will vanish when projected into the bands to first order in the gradient. So we end up with the following band projected equation

$$i\sum_i \mathcal{P}_i\,\breve{\underline{\underline{B}}}(\Upsilon^\mu,\Pi^\mu)\,\tilde{\underline{\underline{A}}}(\Upsilon^\mu,\Pi^\mu)\mathcal{P}_i = 0. \tag{3.4.3}$$

[12]Remember That $\breve{\underline{\underline{A}}} = i\left(\breve{\underline{\underline{G}}}^R - \breve{\underline{\underline{G}}}^A\right)$

More explicitly using the result from equation (3.3.56) the ith equation gives

$$
\begin{aligned}
A_i \Big[\Big(& -(1-\Xi_i)\partial_\tau \tilde{G}^{-1}_{(0)\,i} - \partial_{\boldsymbol{\pi}} \tilde{G}^{-1}_{(0)\,i} \cdot \boldsymbol{\mathcal{E}}^{\boldsymbol{\rho}_\tau}_i + \partial_{\boldsymbol{\rho}} \tilde{G}^{-1}_{(0)\,i} \cdot \boldsymbol{\mathcal{E}}^{\boldsymbol{\pi}_\tau}_i \Big) \partial_\omega \\
& + \Big(\underbrace{\partial_\omega \tilde{G}^{-1}_{(0)\,i} \boldsymbol{\mathcal{E}}^{\boldsymbol{\rho}_\tau}_i}_{\mathcal{D}_{\omega I}} - \underbrace{\partial_{\boldsymbol{\pi}} \tilde{G}^{-1}_{(0)\,i} \times \boldsymbol{\Omega}^{\boldsymbol{\rho}}_i}_{\mathcal{D}_{\boldsymbol{\pi} I}} - \underbrace{\partial_\tau \tilde{G}^{-1}_{(0)\,i} \boldsymbol{\mathcal{E}}^{\boldsymbol{\rho}_\omega}_i}_{\mathcal{D}_{\tau I}} + \underbrace{\partial_{\boldsymbol{\rho}} \tilde{G}^{-1}_{(0)\,i} (1 - \Theta^{\boldsymbol{\rho}\boldsymbol{\pi}}_i)}_{\mathcal{D}_{\boldsymbol{\rho} I}} \Big) \cdot \partial_{\boldsymbol{\pi}} \\
& + \Big(\underbrace{(1-\Xi_i)\partial_\omega \tilde{G}^{-1}_{(0)\,i}}_{\mathcal{D}_{\omega II}} + \underbrace{\partial_{\boldsymbol{\pi}} \tilde{G}^{-1}_{(0)\,i} \cdot \boldsymbol{\mathcal{E}}^{\boldsymbol{\rho}_\omega}_i}_{\mathcal{D}_{\boldsymbol{\pi} II}} - \underbrace{\partial_{\boldsymbol{\rho}} \tilde{G}^{-1}_{(0)\,i} \cdot \boldsymbol{\mathcal{E}}^{\boldsymbol{\pi}_\omega}_i}_{\mathcal{D}_{\boldsymbol{\rho} II}} \Big) \partial_\tau \\
& + \Big(\underbrace{-\partial_\omega \tilde{G}^{-1}_{(0)\,i} \boldsymbol{\mathcal{E}}^{\boldsymbol{\pi}_\tau}_i}_{\mathcal{D}_{\omega III}} - \underbrace{\partial_{\boldsymbol{\pi}} \tilde{G}^{-1}_{(0)\,i} (\underline{1} - (\underline{\Theta}^{\boldsymbol{\rho}\boldsymbol{\pi}})^T_i)}_{\mathcal{D}_{\boldsymbol{\pi} III}} + \underbrace{\partial_\tau \tilde{G}^{-1}_{(0)\,i} \boldsymbol{\mathcal{E}}^{\boldsymbol{\pi}_\omega}_i}_{\mathcal{D}_{\tau I}} - \underbrace{\partial_{\boldsymbol{\rho}} \tilde{G}^{-1}_{(0)\,i} \times \boldsymbol{\Omega}^{\boldsymbol{\pi}}_i}_{\mathcal{D}_{\boldsymbol{\rho} III}} \Big) \cdot \partial_{\boldsymbol{\rho}} \Big] \breve{h}_i = 0,
\end{aligned}
\tag{3.4.4}
$$

where A_i is the spectral function of the ith band. The $\mathcal{D}$ are placed to mark the different terms for later use. Remember that $\tilde{G}^{-1}_{(0)\,i} = \omega - \mathcal{P}_i \left(\underline{\underline{\breve{H}}} + \underline{\underline{R\breve{e}\Sigma}} \right) \mathcal{P}_i$ which we want to write as $\tilde{G}^{-1}_{(0)\,i} = \omega - \xi_i(\boldsymbol{\pi}, \tau, \boldsymbol{\rho}) - Re\Sigma_i(\Upsilon^\mu, \Pi^\mu)$ to make look similar to the normal one-band case [10]. Now our quantum Boltzmann equation also takes the spectral function into account explicitly. Hence we are ready to energy integrate as soon as we establish the form of the spectral function. However in order to also be in the semi-classical regime the spectral function should be sharply peaked so there is a unique relation between the renormalized dispersion $\xi_i + Re\Sigma_i$[13] and the energy ω i.e. the spectral function can be approximated by a delta function. Let us first consider the typical form for a spectral function in case of a scattering potential, namely the Lorentzian, it should be stressed that this is in fact the from for the spectral function out of equilibrium for the one band case as shown by Kadanoff and Baym [21]:

$$
A_i = \frac{\Gamma_i}{(\omega - \xi_i - Re\Sigma_i)^2 + (\frac{\Gamma_i}{2})^2}. \tag{3.4.5}
$$

Here Γ_i is the imagery part of the self-energy in the ith band. Now we see that the semi-classical criterion is satisfied either by having an altogether vanishing self-energy or just having a real self-energy. To have a vanishing imaginary part it is also necessary to have a collision-less Boltzmann equation which we have restricted ourselves to. If the real part of the self-energy is kept it gives rise to a renormalized Boltzmann equation which will be seen later. In the case of a vanishing imaginary part of the self-energy the form of the spectral function simplifies to

$$
A(\Upsilon^\mu, \Pi^\mu) \approx 2\pi\delta(\Omega - \xi_i(\tau, \boldsymbol{\rho}, \boldsymbol{\pi}) - Re\Sigma_i(\Upsilon^\mu, \Pi^\mu)). \tag{3.4.6}
$$

Having the from of the spectral function in place we are nearly ready perform do the energy integration of equation (3.4.4). However with the delta function form of the spectral function it is normal to make the ansatz [14] that the distribution function is independent of energy. Hence the three terms that dependences on an energy derivative of the distribution function are zero. To make it clear we call the ω independent distribution function $h_{\pi i}$

Finally before the integration lets remember how to shift variables in a delta function:

$$
A = 2\pi\delta\left(\omega - \xi_i - Re\Sigma_i\right) = \frac{2\pi}{1 - \frac{\partial Re\Sigma_i}{\partial\omega}\Big|_{\omega=\xi^*_i}} \delta\left(\omega - \xi^*_i\right) = Z_i 2\pi\delta\left(\omega - \xi^*_i\right). \tag{3.4.7}
$$

Here Z_i is defined by the last equality and ξ^*_i is self-consistently defined as $\xi^*_i = \xi_i + Re\Sigma|_{\omega=\xi^*_i}$. Now all is in place to perform the energy integration of equation (3.4.4). Let us start by doing all the terms

[13] Be awere that ξ can depend on both position, time and momentum.

[14] This ansatz on h seems to be good in the sens that it leads to solvable equations. Most works on the topics assume this with out hardly any discussion, Kadanoff and Baym 1961 page 142 mentions that in the case of a delta function spectral function one can clearly do this!? How ever under this ansatz the resulting Boltzmann equation remains possible to solve as seen more or less throughout all of Højgaard and Smith 1989, and the Berry curvature doses not seem to introduce new complication in that sense.

where the inverse Green's function is differentiated with respect to energy:

$$\begin{aligned}\mathcal{D}_{\omega I} &= +\int_{-\infty}^{\infty}\frac{d\omega}{2\pi i}2\pi i\delta(\omega-\xi_i-Re\Sigma_i)\partial_\omega\left(\omega-\xi_i-Re\Sigma_i\right)\boldsymbol{\mathcal{E}}_i^{\boldsymbol{\rho}_\tau}\cdot\partial_{\boldsymbol{\pi}}h_{\pi i} \\ &= Z_i\left(1-\partial_\omega Re\Sigma\right)|_{\omega=\xi_i^*}\boldsymbol{\mathcal{E}}_i^{\boldsymbol{\rho}_\tau}\big|_{\omega=\xi_i^*}\cdot\partial_{\boldsymbol{\pi}}h_{\pi i} \\ &= Z_iZ_i^{-1}\boldsymbol{\mathcal{E}}_i^{\boldsymbol{\rho}_\tau}\big|_{\omega=\xi_i^*}\cdot\partial_{\boldsymbol{\pi}}h_{\pi i},\end{aligned} \tag{3.4.8}$$

$$\begin{aligned}\mathcal{D}_{\omega II} &= +\int_{-\infty}^{\infty}\frac{d\omega}{2\pi i}2\pi i\delta(\omega-\xi_i-Re\Sigma_i)(1-\Xi_i)\,\partial_\omega\left(\omega-\xi_i-Re\Sigma_i\right)\partial_\tau h_{\pi i} \\ &= Z_i\left(1-\partial_\omega Re\Sigma\right)|_{\omega=\xi_i^*}\left(1-\Xi_i|_{\omega=\xi_i^*}\right)\partial_\tau h_{\pi i} \\ &= Z_iZ_i^{-1}\left(1-\Xi_i|_{\omega=\xi_i^*}\right)\partial_\tau h_{\pi i}\end{aligned} \tag{3.4.9}$$

$$\begin{aligned}\mathcal{D}_{\omega III} &= -\int_{-\infty}^{\infty}\frac{d\omega}{2\pi i}2\pi i\delta(\omega-\xi_i-Re\Sigma_i)\partial_\omega\left(\omega-\xi_i-Re\Sigma_i\right)\boldsymbol{\mathcal{E}}_i^{\boldsymbol{\pi}_\tau}\cdot\partial_{\boldsymbol{\rho}}h_{\pi i} \\ &= -Z_i\left(1-\partial_\omega Re\Sigma\right)|_{\omega=\xi_i^*}\boldsymbol{\mathcal{E}}_i^{\boldsymbol{\pi}_\tau}|_{\omega=\xi_i^*}\cdot\partial_{\boldsymbol{\rho}}h_{\pi i} \\ &= -Z_iZ_i^{-1}\boldsymbol{\mathcal{E}}_i^{\boldsymbol{\pi}_\tau}|_{\omega=\xi_i^*}\cdot\partial_{\boldsymbol{\rho}}h_{\pi i}\end{aligned} \tag{3.4.10}$$

So we se that these terms only renormalise due to the changes in the dispersion and only if our $\underline{\underline{\mathcal{U}}}_0$ depends on ω. Now let us integrate the terms where the inverse Green's function is differentiated with respect to momentum:

$$\begin{aligned}\mathcal{D}_{\boldsymbol{\pi}I} &= -\int_{-\infty}^{\infty}\frac{d\omega}{2\pi i}2\pi i\delta(\omega-\xi_i-Re\Sigma_i)\partial_{\boldsymbol{\pi}}\left(\omega-\xi_i-Re\Sigma_i\right)\times\boldsymbol{\Omega}_i^{\boldsymbol{\rho}}\cdot\partial_{\boldsymbol{\pi}}h_{\pi i} \\ &= Z_i\left(\partial_{\boldsymbol{\pi}}\xi_i+\partial_{\boldsymbol{\pi}}Re\Sigma_i\right)|_{\omega=\xi_i^*}\times\boldsymbol{\Omega}_i^{\boldsymbol{\rho}}|_{\omega=\xi_i^*}\cdot\partial_{\boldsymbol{\pi}}h_{\pi i}\end{aligned} \tag{3.4.11}$$

$$\begin{aligned}\mathcal{D}_{\boldsymbol{\pi}II} &= +\int_{-\infty}^{\infty}\frac{d\omega}{2\pi i}2\pi i\delta(\omega-\xi_i-Re\Sigma_i)\partial_{\boldsymbol{\pi}}\left(\omega-\xi_i-Re\Sigma_i\right)\cdot\boldsymbol{\mathcal{E}}_i^{\boldsymbol{\rho}_\omega}\partial_\tau h_{\pi i} \\ &= -Z_i\left(\partial_{\boldsymbol{\pi}}\xi_i+\partial_{\boldsymbol{\pi}}Re\Sigma_i\right)|_{\omega=\xi_i^*}\cdot\boldsymbol{\mathcal{E}}_i^{\boldsymbol{\rho}_\omega}\big|_{\omega=\xi_i^*}\partial_\tau h_{\pi i}\end{aligned} \tag{3.4.12}$$

$$\begin{aligned}\mathcal{D}_{\boldsymbol{\pi}III} &= -\int_{-\infty}^{\infty}\frac{d\omega}{2\pi i}2\pi i\delta(\omega-\xi_i-Re\Sigma_i)\partial_{\boldsymbol{\pi}}\left(\omega-\xi_i-Re\Sigma_i\right)\left(\underline{1}-(\underline{\Theta}^{\boldsymbol{\rho}\boldsymbol{\pi}})_i^T\right)\cdot\partial_{\boldsymbol{\rho}}h_{\pi i} \\ &= Z_i\left(\partial_{\boldsymbol{\pi}}\xi_i+\partial_{\boldsymbol{\pi}}Re\Sigma_i\right)|_{\omega=\xi_i^*}\left(\underline{1}-(\underline{\Theta}^{\boldsymbol{\rho}\boldsymbol{\pi}})_i^T\Big|_{\omega=\xi_i^*}\right)\cdot\partial_{\boldsymbol{\rho}}h_{\pi i}\end{aligned} \tag{3.4.13}$$

This can be simplified by noting the following relation:

$$\partial_{\boldsymbol{\pi}}\left((\xi_i+Re\Sigma)|_{\omega=\xi_i^*}\right)=\partial_\omega Re\Sigma|_{\omega=\xi_i^*}\,\partial_{\boldsymbol{\pi}}\left((\xi_i+Re\Sigma)|_{\omega=\xi_i^*}\right)+\left(\partial_{\boldsymbol{\pi}}(\xi_i+Re\Sigma)\right)|_{\omega=\xi_i^*}, \tag{3.4.14}$$

which can be rearranged as

$$\left(\partial_{\boldsymbol{\pi}}(\xi_i+Re\Sigma)\right)|_{\omega=\xi_i^*}=\partial_{\boldsymbol{\pi}}\left((\xi_i+Re\Sigma)|_{\omega=\xi_i^*}\right)\left(1-\partial_\omega Re\Sigma|_{\omega=\xi_i^*}\right). \tag{3.4.15}$$

As we would like to think of $\partial_{\boldsymbol{\pi}}\xi_i$ as the velocity $\mathbf{v}$. We now define the renormalizes velocity $\mathbf{v}^*$ in the following way

$$\mathbf{v}^*=\partial_{\boldsymbol{\pi}}\left((\xi_i+Re\Sigma)|_{\omega=\xi_i^*}\right). \tag{3.4.16}$$

Hence the three equations (3.4.11),(3.4.12) and (3.4.13) can respectively be written as

$$\mathbf{v}^* \times \boldsymbol{\Omega}_i^{\boldsymbol{\rho}}\big|_{\omega=\xi_i^*} \cdot \partial_{\boldsymbol{\pi}} h_{\pi i} \tag{3.4.17}$$

$$-\mathbf{v}^* \cdot \boldsymbol{\mathcal{E}}_i^{\boldsymbol{\rho}_\omega}\big|_{\omega=\xi_i^*} \partial_\tau h_{\pi i} \tag{3.4.18}$$

$$\mathbf{v}^* \left(\underline{1} - (\underline{\Theta}^{\boldsymbol{\rho\pi}})_i^T \Big|_{\omega=\xi_i^*} \right) \cdot \partial_{\boldsymbol{\rho}} h_{\pi i} \tag{3.4.19}$$

We proceed by integrating the terms where the inverse Green's function is differentiated with respect to time:

$$\begin{aligned} \mathcal{D}_{\tau I} &= -\int_{-\infty}^{\infty} \frac{d\omega}{2\pi i} 2\pi i \delta(\omega - \xi_i - Re\Sigma_i) \partial_\tau \left(\omega - \xi_i - Re\Sigma_i\right) \boldsymbol{\mathcal{E}}_i^{\boldsymbol{\rho}_\omega} \cdot \partial_{\boldsymbol{\pi}} h_{\pi i} \\ &= Z_i \left(\partial_\tau \xi_i + \partial_\tau Re\Sigma_i)|_{\omega=\xi_i^*} \boldsymbol{\mathcal{E}}_i^{\boldsymbol{\rho}_\omega}\right|_{\omega=\xi_i^*} \cdot \partial_{\boldsymbol{\pi}} h_{\pi i} \end{aligned} \tag{3.4.20}$$

$$\begin{aligned} \mathcal{D}_{\tau II} &= +\int_{-\infty}^{\infty} \frac{d\omega}{2\pi i} 2\pi i \delta(\omega - \xi_i - Re\Sigma_i) \partial_\tau \left(\omega - \xi_i - Re\Sigma_i\right) \boldsymbol{\mathcal{E}}_i^{\boldsymbol{\pi}_\omega} \cdot \partial_{\boldsymbol{\rho}} h_{\pi i} \\ &= -Z_i \left(\partial_\tau \xi_i + \partial_\tau Re\Sigma_i)|_{\omega=\xi_i^*} \boldsymbol{\mathcal{E}}_i^{\boldsymbol{\pi}_\omega}|_{\omega=\xi_i^*} \cdot \partial_{\boldsymbol{\rho}} h_{\pi i} \end{aligned} \tag{3.4.21}$$

As in the momentum case this can be simplified by noting a similar relation:

$$\partial_\tau \left((\xi_i + Re\Sigma)|_{\omega=\xi_i^*} \right) = \partial_\omega Re\Sigma|_{\omega=\xi_i^*} \partial_\tau \left((\xi_i + Re\Sigma)|_{\omega=\xi_i^*} \right) + \left(\partial_\tau (\xi_i + Re\Sigma)\right)|_{\omega=\xi_i^*} . \tag{3.4.22}$$

This can be rearranged as

$$\left(\partial_\tau (\xi_i + Re\Sigma)\right)|_{\omega=\xi_i^*} = \partial_\tau \left((\xi_i + Re\Sigma)|_{\omega=\xi_i^*} \right) \left(1 - \partial_\omega Re\Sigma|_{\omega=\xi_i^*} \right). \tag{3.4.23}$$

As we would like to think of $\partial_\tau \xi_i$ as a power $\mathfrak{P}$. We define the renormalizes power $\mathfrak{P}^*$ in the following way :

$$\mathfrak{P}^* = \partial_\tau \left((\xi_i + Re\Sigma)|_{\omega=\xi_i^*} \right). \tag{3.4.24}$$

Hence we can rewrite equations (3.4.20) and (3.4.21) respectively as

$$\mathfrak{P}^* \, \boldsymbol{\mathcal{E}}_i^{\boldsymbol{\rho}_\omega}\big|_{\omega=\xi_i^*} \cdot \partial_{\boldsymbol{\pi}} h_{\pi i} \tag{3.4.25}$$

$$-\mathfrak{P}^* \, \boldsymbol{\mathcal{E}}_i^{\boldsymbol{\pi}_\omega}|_{\omega=\xi_i^*} \cdot \partial_{\boldsymbol{\rho}} h_{\pi i} \tag{3.4.26}$$

Finally we take care of the integration of the terms where the inverse Green's function is differentiated with respect to position:

$$\begin{aligned} \mathcal{D}_{\boldsymbol{\rho} I} &= +\int_{-\infty}^{\infty} \frac{d\omega}{2\pi i} 2\pi i \delta(\omega - \xi_i - Re\Sigma_i) \partial_{\boldsymbol{\rho}} \left(\omega - \xi_i - Re\Sigma_i\right) \left(\underline{1} - \underline{\Theta}_i^{\boldsymbol{\rho\pi}}\right) \cdot \partial_{\boldsymbol{\pi}} h_{\pi i} \\ &= -Z_i \left(\partial_{\boldsymbol{\rho}} \xi_i + \partial_{\boldsymbol{\rho}} Re\Sigma_i)|_{\omega=\xi_i^*} \left(\underline{1} - \underline{\Theta}_i^{\boldsymbol{\rho\pi}}\right)|_{\omega=\xi_i^*} \cdot \partial_{\boldsymbol{\pi}} h_{\pi i} \end{aligned} \tag{3.4.27}$$

$$\begin{aligned} \mathcal{D}_{\boldsymbol{\rho} I} &= -\int_{-\infty}^{\infty} \frac{d\omega}{2\pi i} 2\pi i \delta(\omega - \xi_i - Re\Sigma_i) \partial_{\boldsymbol{\rho}} \left(\omega - \xi_i - Re\Sigma_i\right) \cdot \boldsymbol{\mathcal{E}}_i^{\boldsymbol{\pi}_\omega} \partial_\tau h_{\pi i} \\ &= Z_i \left(\partial_{\boldsymbol{\rho}} \xi_i + \partial_{\boldsymbol{\rho}} Re\Sigma_i)|_{\omega=\xi_i^*} \cdot \boldsymbol{\mathcal{E}}_i^{\boldsymbol{\pi}_\omega}|_{\omega=\xi_i^*} \partial_\tau h_{\pi i} \end{aligned} \tag{3.4.28}$$

$$\begin{aligned} \mathcal{D}_{\boldsymbol{\rho} I} &= -\int_{-\infty}^{\infty} \frac{d\omega}{2\pi i} 2\pi i \delta(\omega - \xi_i - Re\Sigma_i) \partial_{\boldsymbol{\rho}} \left(\omega - \xi_i - Re\Sigma_i\right) \times \boldsymbol{\Omega}_i^{\boldsymbol{\pi}} \cdot \partial_{\boldsymbol{\rho}} h_{\pi i} \\ &= Z_i \left(\partial_{\boldsymbol{\rho}} \xi_i + \partial_{\boldsymbol{\rho}} Re\Sigma_i)|_{\omega=\xi_i^*} \times \boldsymbol{\Omega}_i^{\boldsymbol{\pi}}|_{\omega=\xi_i^*} \cdot \partial_{\boldsymbol{\rho}} h_{\pi i} \end{aligned} \tag{3.4.29}$$

Once again we can simplify this in the same way in the previous two cases

$$\partial_{\boldsymbol{\rho}}\left((\xi_i + Re\Sigma)|_{\omega=\xi_i^*}\right) = \partial_\omega Re\Sigma|_{\omega=\xi_i^*}\,\partial_{\boldsymbol{\rho}}\left((\xi_i + Re\Sigma)|_{\omega=\xi_i^*}\right) + (\partial_{\boldsymbol{\rho}}(\xi_i + Re\Sigma))|_{\omega=\xi_i^*}, \tag{3.4.30}$$

which can be rearrange like so

$$(\partial_{\boldsymbol{\rho}}(\xi_i + Re\Sigma))|_{\omega=\xi_i^*} = \partial_{\boldsymbol{\rho}}\left((\xi_i + Re\Sigma)|_{\omega=\xi_i^*}\right)\left(1 - \partial_\omega Re\Sigma|_{\omega=\xi_i^*}\right). \tag{3.4.31}$$

We would like to think of $\partial_{\boldsymbol{\rho}}\xi_i$ as a force $\mathbf{F}$. So we now defining the renormalizes force $\mathbf{F}^*$ in the following way

$$\mathbf{F}^* = \partial_{\boldsymbol{\rho}}\left((\xi_i + Re\Sigma)|_{\omega=\xi_i^*}\right). \tag{3.4.32}$$

Hence the three equations (3.4.27),(3.4.28) and (3.4.29) can respectively be written as

$$-\mathbf{F}^*\,(\underline{1} - \underline{\Theta}_i^{\boldsymbol{\rho\pi}})|_{\omega=\xi_i^*} \cdot \partial_{\boldsymbol{\pi}} h_{\pi i} \tag{3.4.33}$$

$$\mathbf{F}^* \cdot \boldsymbol{\mathcal{E}}_i^{\boldsymbol{\pi}_\omega}|_{\omega=\xi_i^*}\,\partial_\tau h_{\pi i} \tag{3.4.34}$$

$$\mathbf{F}^* \times \boldsymbol{\Omega}_i^{\boldsymbol{\pi}}|_{\omega=\xi_i^*} \cdot \partial_{\boldsymbol{\rho}} h_{\pi i} \tag{3.4.35}$$

Having done the energy integration we can now write down a fully renormalized collision-less semi-classical Boltzmann equation. However to get it into a more recognizable form let us write it as an equation of the function $f = \frac{1}{2}(1 - h_{\pi i})$

$$\begin{aligned}
&\Big[\Big(\mathbf{F}^* \cdot \boldsymbol{\mathcal{E}}_i^{\boldsymbol{\pi}_\omega}|_{\omega=\xi_i^*} - \mathbf{v}^* \cdot \boldsymbol{\mathcal{E}}_i^{\boldsymbol{\rho}_\omega}\big|_{\omega=\xi_i^*} + \left(1 - \Xi_i|_{\omega=\xi_i^*}\right)\Big)\,\partial_\tau \\
&+ \left(\mathfrak{P}^*\,\boldsymbol{\mathcal{E}}_i^{\boldsymbol{\rho}_\omega}\big|_{\omega=\xi_i^*} - \mathbf{F}^*\,(\underline{1} - \underline{\Theta}_i^{\boldsymbol{\rho\pi}})|_{\omega=\xi_i^*} + \boldsymbol{\mathcal{E}}_i^{\boldsymbol{\rho}_\tau}\big|_{\omega=\xi_i^*} + \mathbf{v}^* \times \boldsymbol{\Omega}_i^{\boldsymbol{\rho}}|_{\omega=\xi_i^*}\right) \cdot \partial_{\boldsymbol{\pi}} \\
&+ \left(\mathbf{v}^*\left(\underline{1} - (\underline{\Theta}^{\boldsymbol{\rho\pi}})_i^T\Big|_{\omega=\xi_i^*}\right) - \boldsymbol{\mathcal{E}}_i^{\boldsymbol{\pi}_\tau}|_{\omega=\xi_i^*} - \mathfrak{P}^*\,\boldsymbol{\mathcal{E}}_i^{\boldsymbol{\pi}_\omega}|_{\omega=\xi_i^*} + \mathbf{F}^* \times \boldsymbol{\Omega}_i^{\boldsymbol{\pi}}|_{\omega=\xi_i^*}\right) \cdot \partial_{\boldsymbol{\rho}}\Big]\, f = 0
\end{aligned} \tag{3.4.36}$$

We see that we have obtained a much richer equation due to the multi-band structure of our original problem, even without considering electromagnetic effects. General electromagnetic fields can be introduced rather straightforwardly, see Wickles and Belzig[9]. However it is a tedious procedure, and we can without more work include static electric fields, so we will not bother to inculde the full electromagnetic gauge freedom. It should be stated that the result in (3.4.36) have not been found before, and it is the most general form a semi-classical Boltzmann equaiton can have without including electromagnetic fields, by only considering first order terms. Having found the rather general equation (3.4.36) we should try to specify to the case we discuessed in the first chapter, namely the anomalous Hall effect. This will be done in the following section.

3.4.1 The Anomalous Hall Effect, Revisited

In order to get the anomalous Hall effect let us consider a two band Hamiltonian of the following form

$$\underline{\underline{H}}(\mathbf{r}, \mathbf{p}) = \underline{\underline{\xi}}(\mathbf{p}) - e\varphi(\mathbf{r})\,\underline{1}, \tag{3.4.37}$$

where $\underline{\underline{\xi}}$ is some general hermitian matrix function of momentum which gives am energy gap. $\underline{\underline{\xi}}$ also includes the chemical potential, and φ is the electric potential of a static electric field such that $\partial_{\mathbf{r}}\varphi = -\mathbf{E}$. This along with neglecting all self-energy effect leads to the following semi-classical Boltzmann equation as can be seen from equation (3.4.36)

$$(\partial_t - \mathbf{F}_i \cdot \partial_{\boldsymbol{\pi}} + (\mathbf{v} + \mathbf{F}_i \times \boldsymbol{\Omega}_i^{\boldsymbol{\pi}}) \cdot \partial_{\boldsymbol{\rho}})\, f = (\partial_t - e\mathbf{E} \cdot \partial_{\boldsymbol{\pi}} + (\mathbf{v} + e\mathbf{E} \times \boldsymbol{\Omega}_i^{\boldsymbol{\pi}}) \cdot \partial_{\boldsymbol{\rho}})\, f = 0. \tag{3.4.38}$$

Note that there are no differences between $\mathbf{p}$ and $\boldsymbol{\pi}$ in this case. Now in order to get the transport properties from this equation we need to solve it. But in order to do that we will need to specify a chemical potential. We will put it in the gap as in section 2.3. In this case there is however a simple solution, namely that $f = f_0$, where f_0 is the Fermi-Dirac distribution, which will in the lover band will

be a constant as we place the chemical potential in the gap.

Having a solution we just have to find the continuity equations by performing the momentum integrations as in equation (2.3.6)[15]. Hence we get that the particle density and the particle current density are given as

$$\rho = \int \frac{\mathrm{d}\boldsymbol{\pi}}{(2\pi)^2} f, \tag{3.4.39}$$

$$\mathbf{j}_p = \int \frac{\mathrm{d}\boldsymbol{\pi}}{(2\pi)^2} \left(\mathbf{v} + e\mathbf{E} \times \boldsymbol{\Omega}_i^{\boldsymbol{\pi}}\right) f. \tag{3.4.40}$$

Now plugging our solution for f in we get the following expression for the current density

$$\mathbf{j} = -e \int \frac{\mathrm{d}\boldsymbol{\pi}}{(2\pi)^2} \left(\mathbf{v} + e\mathbf{E} \times \boldsymbol{\Omega}_i^{\boldsymbol{\pi}}\right) f^0. \tag{3.4.41}$$

Now let us find the conductivity tensor in the case of the Hall geometry in figure 2.2. The result is given in equation (2.3.11) which we restate here for convenience, note that $\boldsymbol{\rho} = (x, y, z)$,

$$\sigma_{yx} = \frac{\partial \mathbf{j}}{\partial \mathbf{E}_x} \cdot \hat{j} = -e^2 \int \frac{d\boldsymbol{\pi}}{(2\pi)^2} \boldsymbol{\Omega}_i^{\boldsymbol{\pi}} f^0, \tag{3.4.42}$$

If we specified the model to the Rashba Hamiltonian with Zeeman splitting we will of course get the same result as in equation (2.3.13). So we have shown that the more generally derived semi-classical Boltzmann equation is able to reproduce this well established result. However we now have better understanding of its validity, in the sens that we have a clear expansion parameter giving in equation (3.3.24). More over we have the possibility to account for self-energy effects.

[15] This case is in fact simpler as it is collision-less.

Chapter 4

Summary and Outlook

4.1 Summary

We have, in this thesis first given a derivation of a semi-classical Boltzmann equation, using the time dependent variational method. This gave us an understanding of which kind of new terms to expect form a more general approach. It also enabled us to investigate the underlying symmetries of the semi-classical equation, as one step was to calculate a Lagrangian for the semi-classical variables. Surprisingly, the symmetry found was a local gauge symmetry in both space and momentum. Having a Boltzmann equation with an anomalous velocity term made it possible to derive the anomalous Hall effect, which is one of the hallmark phenomena for Berry curvature in transport theory.

With some physical insight to what properties to expect form a multi-band system we proceed with the Keldysh based derivation. One of the important steps in that derivation was to do the Wigner transformation so we could treat momentum and space on equal footing, leading to the insight that the local gauge symmetry in both space and momentum is in fact present in quantum mechanics, one just has to choose the right representation. Using the gauge symmetry we where able to perturbatively decouple the kinetic equation and show that in the band-projected chase, this could be viewed as a minimal coupling to the space and momentum Berry connection. Transforming to the kinetic space and momentum we where able to arrive at a renormalized collision-less quantum Boltzmann equation for a multi-band Hamiltonian. With a quantum Boltzmann equation at hand we continued by integrating out the energies arriving at a semi-classical Boltzmann equation, which have not been done before. From the semi-classical Boltzmann equation we could again derive the anomalous Hall effect, hence showing consistency.

4.2 Outlook

As we have not considered the full effect of electromagnetism, this would be the natural next step. This has in fact to some extent been discussed by Wickles and Belzing[9] and should not pose major new difficulties. The real challenges of further progress will be the systematic inclusion of collision terms with none trivial matrix structure. Trivial meaning they are proportional to the identity and therefore only able to induce intra band scattering, in fact such terms could have been introduced in our calculation nearly without any further complications. We did not do it since such simple collisions-terms seems to be unphysical. The Keldysh treatment should be done in order to establish a more systematic understanding of side-jumps and skew-scattering as reviewed by Sinitsyn in 2008[16] possibly yielding new phenomena. A Keldysh derivation will also allow for renormalization to be discussed in conjunction with collision.

One could in principal also try to refine the variational method by choosing a more elaborate wave function. However, it is unlikely tolead to any new insight because of the limitation of the method. So this should not be pursued, except for purely academic reasons.

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