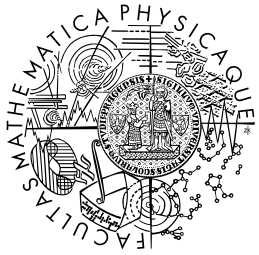

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Study of the effect of spin-orbit interaction in solids

Department of Condensed Matter Physics

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Title: Study of the effect of spin-orbit interaction in solids

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Supervisor: Karel Carva, Department of Condensed Matter Physics

Abstract: One of the effects the spin orbit interaction leads to is the Anomalous Hall effect. In this thesis we describe the origins of the Anomalous Hall effect and its contribution to understanding the solid state physics. We introduce the formalism of linear response theory and other approximations needed to perform calculations of the Anomalous Hall conductivity. We present two different models of the anomalous Hall conductivity. We then compare the models in a simple setting based on Strontium ruthenate.

Keywords: spin-orbit Anomalous Hall effectKubo formalism

I would like to thank my supervisor Karel Carva, who has patiently guided me through the many traps and pitfalls of understanding the modern solid state physics and has offered much invaluable advice.

I would also like to thank my family and friends for bearing with me during my ventures into the marvellous but often exhausting world of physics. Without them I would not be able to ever finish this work.

Contents

Introduction

We live in an era in which our lives are shaped by the results of the modern material science. Even on our everyday commute to work we use technologies which would not exist without the material science such as nanofabrics in our clothes, the liquid crystals in the displays of our cell phones, different kinds of alloys used in the cars we drive and the buses we ride and so forth. Among all the diverse areas of interest that make up the material physics there are two areas of interest which have played a critical role since the onset of the theory - electronic transport and magnetism. The spin-orbit interaction connects both of them.

The spin-orbit interaction is a weak relativistic quantum effect - when we take the low velocity limit of the Dirac Hamiltonian we arrive at a Hamiltonian with many different terms and among them is one term connecting the spin σ and the orbital momentum L of the particle. This term is very small compared to the kinetic terms in the rest of the Hamiltonian, nevertheless it is of great importance in solid state physics as it removes band degeneracy. It therefore gives rise to various effects such as the Rashba-Dresselhaus effect or the anomalous Hall effect. Since covering all the effects in one publication would require at least one rather large book, in this work we will cover only the latter one - the anomalous Hall effect (AHE).

The history of the anomalous Hall effect stretches back to 1881, when Edwin E. Hall found that the Hall effect in ferromagnetic materials was ten times larger than that of the non-magnetic materials. Soon it was empirically found that the Hall resistivity ρ_{xy} is linearly dependent on both the magnetization M_z and the magnetic field H_z: $\rho_{xy} = R_0 H_z + R_s M_z$ (Pugh and Lippert, 1932). However for a long time this effect - now known as the anomalous Hall effect - has eluded all attempts at its theoretical explanation.

The first successful explanation was provided by Karplus and Luttinger in 1954 (Karplus and Luttinger, 1954). According to the Karplus-Luttinger theory, if we apply an external electric field to a ferromagnetic solid, electrons acquire a contribution to their group velocity perpendicular to the electric field now known as the anomalous velocity. The anomalous velocity has its origin in the interband coherence. (See Figure 1) This contribution to the anomalous Hall conductivity is now called the intrinsic contribution and it has been shown that it is in fact connected to the topological properties of the momentum-space. This explanation was however soon rejected by most of the scientific community in favour of skew scattering explanation.

The skew scattering theory has been proposed by Smit in 1955 (Smit, 1955). According to this theory the anomalous Hall effect is caused by the fact, that after each collision with impurity in the crystal lattice the electron scatters asymmetrically due to the spin-orbit interaction.

In 1970 Berger has published an article (Berger, 1970) which considered yet another possible means of origin of the anomalous Hall effect - the side jump. This mechanism was based on the fact that when a Gaussian wave packet is scattered elastically by an impurity in the crystal lattice, the centre of the wave packet shifts depending on the spin associated with it.

For a long time, there was a great controversy as to which of these three

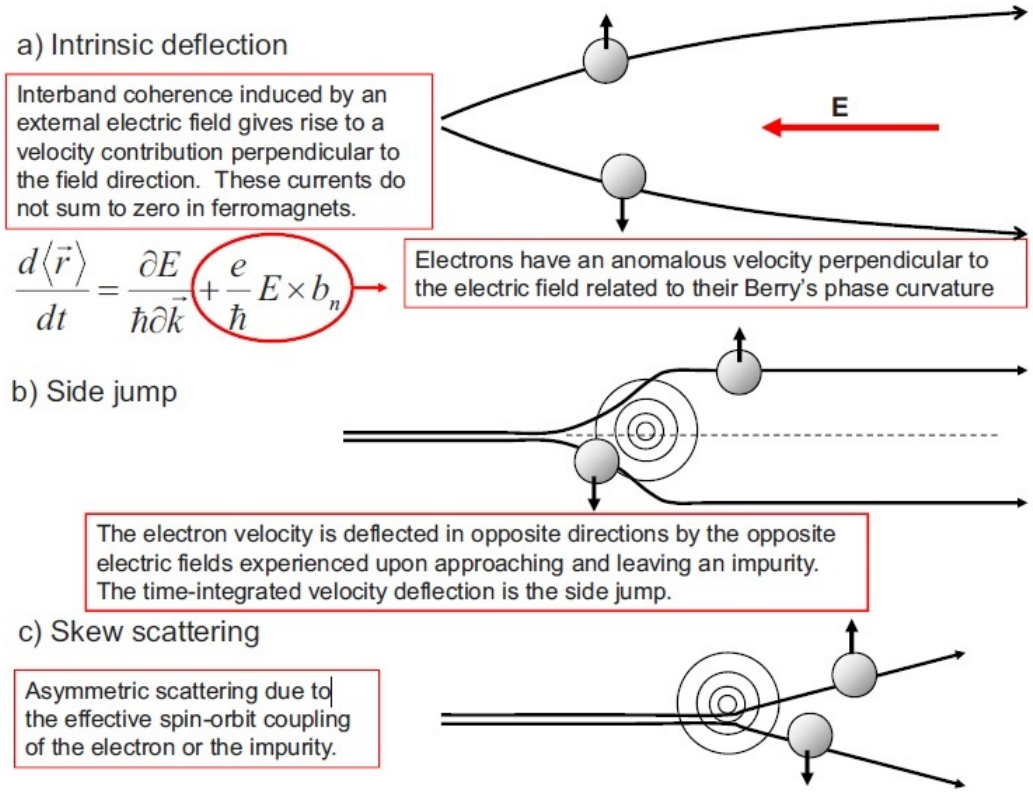

Figure 1: Representation of mechanisms responsible for the anomalous Hall effect. From (Nagaosa et al., 2010)

different theories of the origin of the anomalous Hall effect is the correct one. In the last three decades there has been a great progress in the understanding of AHE and we have since learned that all the three described modes of origin of the AHE are indeed present in solids and in fact compete in creating the anomalous Hall effect. Nevertheless there are still very few good models for computing the anomalous Hall conductivity, so there is still a lot of area for new development.

At the break of the millennium there has been a surge in interest in the anomalous Hall effect, as it became apparent, that it could provide us with much interesting information about the ferromagnetic materials. There is also a prospect of anomalous Hall effect playing a crucial role in spintronics. The anomalous Hall effect is therefore surely worth studying and there is much potential for uncovering results that will lead to a better understanding of solid state physics as well as future new technologies.

In this work we will introduce the framework necessary for the description of the AHE. We will then show how different mechanisms of the AHE come up in this formalism. Then we will turn our attention to two models which describe the AHE, we will describe the models and we will endeavour to compare these two models and show where they differ and what are their areas of applicability.

1. Background

In order to study the anomalous Hall effect we must first lay some groundwork that will allow us to efficiently describe the phenomena that are responsible for it. As was already mentioned in the introduction the AHE is a relativistic quantum effect, so in order to describe the phenomenon in an exact manner we would have to solve a many-body Dirac equation for something like 10^{24} particles. This is not really feasible so, to get some meaningful results, we have to introduce several approximations and work with them.

1.1 Independent electron approximation

The first approximation we will use is the independent electron approximation. This approximation springs out of density functional theory (which is covered e.g. in Lowitzer (2010)) which tells us that the manybody description of the system can in effect be replaced by a description involving only a single electron moving in effective potentials and a term called exchange correlation energy which accounts for the interaction energy of the electrons. In the independent electron approximation we neglect the exchange correlation energy altogether and we work with a single-electron Dirac equation with effective external potentials. This approximation is the most widely used in solid state physics (see e.g. Ashcroft and Mermin (1976)) and it is in fact one of the few means of describing the conductivity.

1.2 The Dirac and Pauli equations

In the relativistic quantum theory the state of an electron is described by a bi-spinor wavefunction Ψ. The evolution of the electron (with charge $e < 0$ and mass m) subjected to an external electric field, given by a scalar potential ϕ and a vector potential A, is characterised by the Dirac equation (Itzykson and Zuber, 2012):

$$\hat{H}\Psi = i\hbar\frac{\partial}{\partial t}\Psi; \qquad \hat{H} = \boldsymbol{\alpha}\cdot(c\mathbf{p} + e\mathbf{A}(\mathbf{r})) + \beta mc^2 - eV(\mathbf{r}) \tag{1.1}$$

where $\mathbf{p}$ is the momentum of the electron and α and β are the Dirac matrices:

$$\boldsymbol{\alpha} = \begin{pmatrix} \boldsymbol{\sigma} & 0 \\ 0 & \boldsymbol{\sigma} \end{pmatrix} \text{ with } \sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \tag{1.2}$$

where σ_i are Pauli matrices and

$$\beta = \begin{pmatrix} I_2 & 0 \\ 0 & -I_2 \end{pmatrix}. \tag{1.3}$$

where I_2 is a 2×2 identity matrix.

It is possible to calculate the AHE via the Dirac equation, however it is too complicated for our purposes and the spin-orbit effects are not so readily apparent in the solution. Therefore we will use the weak relativistic limit of the Dirac equation - the Pauli equation. If we take the weak-relativistic limit of the

conductivity calculated with the Dirac Hamiltonian (Dirac conductivity) and take the terms up to the order of $\frac{1}{c^2}$ it will correspond with the conductivity obtained with the Pauli Hamiltonian (Pauli conductivity).(Crépieux and Bruno, 2001)

The bi-spinor wavefunction can be divided into two spinor wavefunctions - large component ψ and small component χ. In the weak-relativistic limit we can give an approximate relation between the two

$$\begin{aligned}\chi(\boldsymbol{r},t) =& \frac{1}{2mc}\left(\frac{\hbar}{i}\nabla - e\mathbf{A}(\mathbf{r})\right)\cdot\boldsymbol{\sigma}\phi(\boldsymbol{r},t) - \\ &- \frac{1}{4m^2c^3}\left(i\hbar\frac{\partial}{\partial t} - V(\boldsymbol{r}) - mc^2\right)\left(\frac{\hbar}{i}\nabla - e\mathbf{A}(\mathbf{r})\right)\cdot\boldsymbol{\sigma}\phi(\boldsymbol{r},t)\end{aligned} \tag{1.4}$$

thus all the physical meaning is conveyed by the large component. With the assumption of small velocities we can therefore rewrite the Dirac equation so that it acts separately on the large and the small component.

The most simple approximation would lead to the Schroedinger equation. The Schroedinger equation however does not contain any spin-orbit interaction term, so in order to account for the spin-orbit interaction we have to take into account more terms from the Dirac equation. Including all the terms up to the order of $\frac{1}{c^2}$ leads to the Pauli equation (for a detailed derivation of the Pauli equation see e.g. (Strange, 1998)):

$$\begin{aligned}&\left[E + eV(r) - \frac{1}{2m}\left(\mathbf{p}(\mathbf{r}) + \frac{e}{c}\mathbf{A}(\mathbf{r})\right)^2 + \frac{1}{2mc^2}(E + eV(\boldsymbol{r}))^2 + i\frac{\mu_B}{2mc}\mathbf{E}(\mathbf{r})\cdot\mathbf{p} - \right. \\ &\left. - \frac{\mu_B}{2mc}\boldsymbol{\sigma}\cdot(\mathbf{E}(\mathbf{r})\times\mathbf{p}) - \mu_B\boldsymbol{\sigma}\cdot\mathbf{B}(\mathbf{r})\right]\psi = 0,\end{aligned} \tag{1.5}$$

where we have written explicitly the gradient of the scalar potential ϕ and the curl of the vector potential A as electric field E and magnetic field B and we have introduced the Bohr magneton $\mu_B = \frac{e\hbar}{2mc}$ The first three terms in the equation give the ordinary Schroedinger equation, the fourth term is a relativistic correction to the energy due to the change of mass with velocity. The fifth term is called the Darwin term and has no classical analogy.

The last two terms involve the spin of the electron. The last one is the Zeeman energy of the electron. It corresponds to a coupling of an external magnetic field to the spin of the electron.

The last-but-one term can be rewritten as:

$$\frac{\mu_B}{2mc}\boldsymbol{\sigma}\cdot(\mathbf{E}(\mathbf{r})\times\mathbf{p}) = \frac{\mu_B}{2}\boldsymbol{\sigma}\cdot\left(\frac{1}{c}\mathbf{E}(\mathbf{r})\times\mathbf{v}\right) = \frac{\mu_B}{2}\boldsymbol{\sigma}\cdot\boldsymbol{B}_0, \tag{1.6}$$

where $\boldsymbol{B}_0$ is a magnetic field that emerges in the local frame of the electron due to the movement of the electron through the electric field.

In a spherically symmetrical potential $V(r)$ we can give another expression for the last-but-one term:

$$\boldsymbol{\sigma}\cdot(\mathbf{E}(\mathbf{r})\times\mathbf{p}) = \boldsymbol{\sigma}\cdot(\nabla V(r)\times\mathbf{p}) = \frac{1}{r}\frac{dV(r)}{dr}\boldsymbol{\sigma}\cdot(\mathbf{r}\times\mathbf{p}) = \frac{1}{r}\frac{dV(r)}{dr}\boldsymbol{\sigma}\cdot L = \lambda\boldsymbol{\sigma}\cdot L \tag{1.7}$$

where we have introduced the spin-orbit coupling constant λ. This term is the spin-orbit coupling term. It connects the spin of the electron with its angular

momentum and thus with its transport properties. We therefore see that this term encompasses the magnetic properties of solids as well as their transport properties.

1.3 Kubo formula

The effective potentials appearing in the Pauli equation make it impossible to solve the equation exactly. We therefore have to introduce another approximation. The kinetic energy term in the Pauli equation is much larger than the electric potential and spin orbit coupling terms. We can therefore consider the spin-orbit coupling and the electric potential to be a small perturbation of an unperturbed Hamiltonian. When the perturbation is small enough we may assume that the response of the system is directly proportional to the perturbation and neglect all higher orders of the perturbation series. We call this case a linear response of the system.

The linear response theory entails the Kubo formalism which makes the formulation and subsequent solution of the conductivity problem much more simple. We will develop the Kubo formalism in this section.

Suppose we have a system in a stationary state described by a state operator ρ and an unperturbed time-independent Hamiltonian H_0. In order to calculate the conductivity we would like to know what will be the expectation value for the current density $\langle j \rangle$ if we add a small time-dependent perturbation $W(t)$ that accounts for an electric field $E(t)$.

In the Schrödinger picture the expectation value of the current density $\hat{j}$ for a system described by a time dependent state operator $\rho(t)$ is defined as: $\langle j \rangle_t = Tr\left\{\rho(t)A\right\}$ (Ballentine, 1998). The equation of motion for the state operator in the Schrödinger picture is

$$\frac{d\rho(t)}{dt} = -\frac{i}{\hbar}\left[H(t), \rho(t)\right], \tag{1.8}$$

where $H(t) = H_0 + W(t)$ is the complete Hamiltonian of the system. To get the time dependence of the state operator it is advantageous to transform into a Dirac picture, where the state operator has the form

$$\rho_D(t) = e^{\frac{i}{\hbar}H_0 t}\rho(t)e^{-\frac{i}{\hbar}H_0 t} \tag{1.9}$$

The equation of motion for the state operator in the Dirac picture has the form

$$\frac{d\rho_D(t)}{dt} = \frac{i}{\hbar}e^{\frac{i}{\hbar}H_0 t}\left[H_0, \rho(t)\right]e^{-\frac{i}{\hbar}H_0 t} + e^{\frac{i}{\hbar}H_0 t}\frac{\partial\rho(t)}{\partial t}e^{-\frac{i}{\hbar}H_0 t} \tag{1.10}$$

$$= \frac{i}{\hbar}e^{\frac{i}{\hbar}H_0 t}\left[H_0, \rho(t)\right]e^{-\frac{i}{\hbar}H_0 t} - \frac{i}{\hbar}\left[H_0 + W(t), \rho(t)\right] \tag{1.11}$$

$$= -\frac{i}{\hbar}e^{\frac{i}{\hbar}H_0 t}\left[W(t), \rho(t)\right]e^{-\frac{i}{\hbar}H_0 t} \tag{1.12}$$

$$= -\frac{i}{\hbar}\left[W_D(t), \rho_D(t)\right], \tag{1.13}$$

with $W_D(t) = e^{\frac{i}{\hbar}H_0 t}W(t)e^{-\frac{i}{\hbar}H_0 t}$. The equation of motion (1.13) along with the initial condition $\rho_D(0) = \rho_0$ is clearly satisfied by $\rho_D(t)$ in the form:

$$\rho_D(t) = \rho_0 - \frac{i}{\hbar}\int_{-\infty}^{t} dt'\left[W_D(t'), \rho_D(t')\right] \tag{1.14}$$

By iteration we obtain the solution in form of an infinite series

$$\rho_D(t) = \rho_0 + \sum_{n=1}^{\infty} \left(\frac{-i}{\hbar}\right)^n \int_{-\infty}^{t} dt_1 \int_{-\infty}^{t_1} dt_2 \cdots \int_{-\infty}^{t_{n-1}} dt_n \cdot \\ \cdot [W_D(t_1), [W_D(t_2), [\cdots, [W_D(t_n), \rho_0] \cdots]]] \tag{1.15}$$

This expression is exact and the only condition for it to be true is that the sum on the right side converges. Now we will exploit the fact, that the perturbation $W(t)$ is small and we will keep only the leading term in the series.

$$\rho_D(t) = \rho_0 - \frac{i}{\hbar} \int_{-\infty}^{t} dt' \, [W_D(t'), \rho_0] \tag{1.16}$$

We can now transform the approximated state operator back into the Schrödinger picture obtaining

$$\rho(t) = \rho_0 - \frac{i}{\hbar} \int_{-\infty}^{t} dt' e^{-\frac{i}{\hbar}H_0 t} \, [W_D(t'), \rho_0] \, e^{\frac{i}{\hbar}H_0 t}. \tag{1.17}$$

With the use of the equation 1.17 we can now write the expectation value of the current density as

$$\left\langle \hat{j} \right\rangle_t = Tr\left\{\rho_0 \hat{j}\right\} - \frac{i}{\hbar} Tr\left\{\int_{-\infty}^{t} dt' e^{-\frac{i}{\hbar}H_0 t} \, [W_D(t'), \rho_0] \, e^{\frac{i}{\hbar}H_0 t} \hat{j}\right\} \tag{1.18}$$

$$= -\frac{i}{\hbar} Tr\left\{\int_{-\infty}^{t} dt' \, [W_D(t'), \rho_0] \, \hat{j}_D(t)\right\} \tag{1.19}$$

$$= -\frac{i}{\hbar} \int_{-\infty}^{t} dt' \, \langle [j_D(t), W_D(t')] \rangle \tag{1.20}$$

where the first term in equation 1.18 vanishes as there is no current in the unperturbed system. We have used invariance of trace under cyclic permutations and we have set $j_D(t) = e^{\frac{i}{\hbar}H_0 t} \hat{j} e^{-\frac{i}{\hbar}H_0 t}$.

We can now insert the explicit form of the perturbation into the equation 1.20. We will consider an electric field with the form $\boldsymbol{E}(t) = \boldsymbol{E}_0 e^{-i(\omega+\delta i)t}$ with $\delta \to 0^+$ (the term $i\delta$ ensures that for $t \to -\infty$ the electric field vanishes and the system is unperturbed). The perturbation associated with the electric field has the form

$$W(t) = -\mathbf{E}(\mathbf{t}) \cdot \mathbf{P}, \tag{1.21}$$

where $\boldsymbol{P} = \sum_{i=1}^{N} q_i \hat{r}_i$ is the electric dipole moment, with q_i the electric charge and $\hat{r}_i$ the position of the particle. Using this form of the perturbation in the equation 1.20 we get the explicit relation between the current density expectation value and the electric field

$$\left\langle \hat{j}_\mu \right\rangle_t = \frac{i}{\hbar} \sum_{\nu} \int_{-\infty}^{t} dt' \, \langle [j_{\mu,D}(t), P_{\nu,D}(t')] \rangle \, E_{0,\nu} e^{-i(\omega+\delta i)t'} \tag{1.22}$$

In this form the expression for the current density is still not suitable for calculating the conductivity as there is integral over all electric fields in time $t' < t$. We will have to get rid of the dependence of the electric field on time t'. In order to

do this we will first rewrite the expectation value of the commutator in equation (1.22) so that only the polarisation will be time dependent.

$$\begin{aligned}\langle [j_{\mu,D}(t), P_{\nu,D}(t')]\rangle = Tr\Big\{\rho_0\Big(e^{\frac{i}{\hbar}H_0 t} j_\mu e^{\frac{i}{\hbar}H_0(t'-t)} P_\nu e^{-\frac{i}{\hbar}H_0 t'} - \\ - e^{\frac{i}{\hbar}H_0 t'} P_\nu e^{-\frac{i}{\hbar}H_0(t'-t)} j_\mu e^{-\frac{i}{\hbar}H_0 t}\Big)\Big\} \qquad (1.23)\end{aligned}$$

$$= \langle [j_\mu, P_{\nu,D}(t'-t)]\rangle \qquad (1.24)$$

We can now rewrite the equation 1.22 as:

$$\left\langle \hat{j}_\mu \right\rangle_t = \frac{i}{\hbar}\sum_\nu \int_{-\infty}^{t} dt' \,\langle [j_\mu, P_{\nu,D}(t'-t)]\rangle \, E_{0,\nu} e^{-i(\omega+\delta i)t'} \qquad (1.25)$$

$$= \frac{i}{\hbar}\sum_\nu \int_{-\infty}^{\infty} dt' \Theta(t'-t) \,\langle [j_\mu, P_{\nu,D}(t'-t)]\rangle \, e^{-i(\omega+\delta i)(t'-t)} E_{0,\nu} e^{-i(\omega+\delta i)t} \qquad (1.26)$$

$$= \frac{i}{\hbar}\sum_\nu \int_{-\infty}^{\infty} dt'' \Theta(-t'') \,\langle [j_\mu, P_{\nu,D}(t'')]\rangle \, e^{-i(\omega+\delta i)(t'')} E_\nu(t) \qquad (1.27)$$

where we have introduced the Heaviside function $\Theta(t)$. With the relation between the current density and the electric field in this form we may now finally write down the formula for conductivity tensor:

$$\sigma_{\mu\nu} = \frac{i}{\hbar}\int_{-\infty}^{\infty} dt \Theta(-t) \,\langle [j_\mu, P_{\nu,D}(t)]\rangle \, e^{-i(\omega+\delta i)(t)} \qquad (1.28)$$

However this form of relationship is still not suitable for the calculations as there appears the dipole moment. In order to get rid of the dipole moment we will use the Kubo identity (Kubo, 1957) which is valid for any operator $\hat{A}$

$$\left[\hat{A}(t), \rho\right] = -i\hbar\rho \int_0^{(k_B T)^{-1}} d\lambda \dot{\hat{A}}(t - i\hbar\lambda). \qquad (1.29)$$

We will use Kubo formula along with a relation $\dot{\hat{P}} = V\hat{j}$ where V is the volume of the system we investigate. The conductivity tensor can then be rewritten as

$$\sigma_{\mu\nu} = \frac{i}{\hbar}\sum_\nu \int_{-\infty}^{\infty} dt \Theta(-t) Tr\left\{[j_\mu, P_{\nu,D}(t)]\,\rho_0\right\} e^{-i(\omega+\delta i)(t)} \qquad (1.30)$$

$$= \frac{i}{\hbar}\int_{-\infty}^{\infty} dt \Theta(-t) Tr\left\{[P_{\nu,D}(t), \rho_0]\, j_\mu\right\} e^{-i(\omega+\delta i)(t)} \qquad (1.31)$$

$$= \int_0^\beta d\lambda \int_{-\infty}^{\infty} dt \Theta(-t) Tr\left\{\rho_0 \dot{\hat{P}}_{\nu,D}(t - i\hbar\lambda) j_\mu\right\} e^{-i(\omega+\delta i)(t)} \qquad (1.32)$$

$$= V\int_0^\beta d\lambda \int_{-\infty}^{\infty} dt \Theta(-t) Tr\left\{\rho_0 j_{\nu,D}(t - i\hbar\lambda) j_\mu\right\} e^{-i(\omega+\delta i)(t)} \qquad (1.33)$$

$$= V\int_0^\beta d\lambda \int_{-\infty}^{\infty} dt \Theta(t) Tr\left\{\rho_0 j_\nu j_{\mu,D}(t + i\hbar\lambda)\right\} e^{i(\omega+\delta i)(t)} \qquad (1.34)$$

This is the Kubo formula

1.4 Bastin and Kubo-Středa formula

The Kubo formula is still too inconvenient to work with as it contains the integrals over current densities. It is often hard to express the current densities explicitly and even should we succeed the integrals in the Kubo formula are not generally manageable. We will therefore derive the Kubo-Středa formula, which will be much more convenient for the actual calculations. The Kontani model in the next chapter will be based on the Kubo-Středa formula.

As an intermediate step in the derivation of the Kubo-Středa formula we will first derive the Bastin formula. In derivation of the Bastin formula we start with the Kubo formula and then we employ the free electron approximation. (Note that in derivation of the Kubo formula we did not use the free electron approximation, so the Kubo formula could be used in a broader class of problems in the linear response framework.) In order to account for the scattering of electrons on impurities we will now use the configurational average of the operators in the trace which we will denote as $\langle \cdots \rangle_c$ [1] :

$$\sigma_{\mu\nu} = V \int_0^\beta d\lambda \int_0^\infty dt Tr \left\langle \rho_0 j_\nu j_{\mu,D}(t + i\hbar\lambda) \right\rangle_c e^{\frac{i}{\hbar}(\hbar\omega + \delta i)(t)}. \tag{1.35}$$

We will now take a step aside and transform the trace in the integral into a more manageable form. This will permit us to explicitly integrate the expression. The first step is to change the Dirac picture current density into the Schrödinger picture

$$\langle n|J_{D,\mu}(t + i\hbar\lambda)|m\rangle = e^{\frac{i}{\hbar}(t+i\hbar\lambda)(\varepsilon_n - \varepsilon_m)} \langle n|J_\mu|m\rangle , \tag{1.36}$$

with $|n\rangle$and $|m\rangle$the eigenstates of the unperturbed Hamiltonian H_0 with the energy ε_n and ε_m. The free-electron approximation lets us assume that the unperturbed Hamiltonian H_0 can be expanded as a simple series of creation and annihilation operators: $H_0 = \sum_n \epsilon_n a_n^+ a_n$. We can also expand the current density operators this way (Büttiker, 1992)

$$j_\mu = \sum_{m,n} \langle m|j_\mu|n\rangle \, a_m^+ a_n. \tag{1.37}$$

This allows us to write the trace in equation (1.35) as

$$Tr\left[\rho_0 j_\nu j_{D,\mu}(t + i\hbar\lambda)\right] = \sum_{mnkl} \langle m|j_\nu|n\rangle \langle k|j_\mu|l\rangle \, e^{\frac{i}{\hbar}(t+i\hbar\lambda)(\varepsilon_k - \varepsilon_l)} Tr\left[\rho_0 a_m^+ a_n a_k^+ a_l\right] \tag{1.38}$$

$$= \sum_{mnkl} \langle m|j_\nu|n\rangle \langle k|j_\mu|l\rangle \, e^{\frac{i}{\hbar}(t+i\hbar\lambda)(\varepsilon_k - \varepsilon_l)} \delta_{ml}\delta_{nk} f(\varepsilon_n)\left[1 - f(\varepsilon_m)\right] \tag{1.39}$$

$$= \sum_{mn} \langle m|j_\nu|n\rangle \langle n|j_\mu|m\rangle \, e^{\frac{i}{\hbar}(t+i\hbar\lambda)(\varepsilon_n - \varepsilon_m)} f(\varepsilon_n)\left[1 - f(\varepsilon_m)\right]. \tag{1.40}$$

[1] We will not evaluate on the question of form of the configurational average since this work focusses mainly on the scattering-independent type of the AHE.

Where we have used the relation between the trace of equilibrium state operator ρ_0 and the Fermi-Dirac distribution $f(\varepsilon) = \frac{1}{1+e^{\beta(\varepsilon-\mu)}}$:

$$\left[\rho_0 a_m^+ a_n a_k^+ a_l\right] = \delta_{ml}\delta_{nk} f(\varepsilon_n)\left[1 - f(\varepsilon_m)\right]. \tag{1.41}$$

Using the equation (1.40) we can rewrite the integral in equation (1.35) as

$$\begin{aligned}\sigma_{\mu\nu} =& V \int_0^\beta d\lambda e^{-\lambda(\varepsilon_n-\varepsilon_m)} \times \\ &\times \int_0^\infty dt \left\langle f(\varepsilon_m)\left[1 - f(\varepsilon_n)\right] \sum_{mn} \langle n|j_\nu|m\rangle \langle n|j_\mu|m\rangle \, e^{\frac{it}{\hbar}(\hbar\omega + \delta i + \varepsilon_n - \varepsilon_m)} \right\rangle_c\end{aligned} \tag{1.42}$$

Integrating over λ and t we get

$$\sigma_{\mu\nu} = V \sum_{mn} \frac{1 - e^{-\beta(\varepsilon_n-\varepsilon_m)}}{\varepsilon_n - \varepsilon_m} \times \tag{1.43}$$

$$\times \left\langle f(\varepsilon_m)\left[1 - f(\varepsilon_n)\right] \langle n|j_\nu|m\rangle \langle n|j_\mu|m\rangle \frac{i\hbar}{\hbar\omega + \delta i + \varepsilon_n - \varepsilon_m} \right\rangle_c \tag{1.44}$$

We can further simplify this equation by noting that

$$\begin{aligned}\frac{1 - e^{\beta(\varepsilon_n-\varepsilon_m)}}{\varepsilon_n - \varepsilon_m} f(\varepsilon_m)\left[1 - f(\varepsilon_n)\right] &= \frac{1}{\varepsilon_n - \varepsilon_m}\left[f(\varepsilon_m) - f(\varepsilon_m)f(\varepsilon_n) - \right. \\ &\qquad \left. - e^{-\beta(\varepsilon_n-\varepsilon_m)} f(\varepsilon_m)\left[1 - f(\varepsilon_n)\right]\right] \qquad (1.45) \\ &= \frac{1}{\varepsilon_n - \varepsilon_m}\left[f(\varepsilon_m) - \frac{1 + e^{-\beta(\varepsilon_n-\varepsilon_m)} e^{\beta(\varepsilon_n-\mu)}}{(1 + e^{\beta(\varepsilon_n-\mu)}(1 + e^{\beta(\varepsilon_m-\mu)})}\right] \qquad (1.46) \\ &= \frac{f(\varepsilon_m) - f(\varepsilon_n)}{\varepsilon_n - \varepsilon_m}. \qquad (1.47)\end{aligned}$$

We will also limit our attention to the case of static electric field and will therefore set the frequency $\omega = 0$. We thus obtain

$$\sigma_{\mu\nu} = i\hbar V \left\langle \sum_{mn} \frac{f(\varepsilon_m) - f(\varepsilon_n)}{(\varepsilon_n - \varepsilon_m)(\delta i + \varepsilon_n - \varepsilon_m)} \langle n|j_\nu|m\rangle \langle n|j_\mu|m\rangle \right\rangle_c. \tag{1.48}$$

Inserting the completeness relation $\mathbb{I} = \int_{-\infty}^{\infty} d\varepsilon \delta(\varepsilon - H)$ into equation (1.48) we obtain

$$\begin{aligned}\sigma_{\mu\nu} =& i\hbar V \sum_{mn} \int_{-\infty}^{\infty} d\varepsilon \times \\ &\times \left\langle \left(\frac{f(\varepsilon)\delta(\varepsilon - \varepsilon_m)}{(\varepsilon_n - \varepsilon)(\delta i + \varepsilon_n - \varepsilon)} - \frac{f(\varepsilon)\delta(\varepsilon - \varepsilon_n)}{(\varepsilon - \varepsilon_m)(\delta i + \varepsilon - \varepsilon_m)} \right) \langle m|j_\nu|n\rangle \langle n|j_\mu|m\rangle \right\rangle_c.\end{aligned} \tag{1.49}$$

Now we recall, that the δ in the equation is infinitesimal and that we can use the equality of limits:

$$\lim_{\delta\to 0^+} \frac{1}{(\varepsilon_n - \varepsilon)(\varepsilon_n - \varepsilon + i\delta)} = \lim_{\delta\to 0^+} \frac{d}{d\varepsilon} \frac{1}{(\varepsilon_n - \varepsilon + i\delta)}. \tag{1.50}$$

Using the above equality and placing the terms in the equation (1.49) judiciously we have

$$\sigma_{\mu\nu} = i\hbar V \sum_{mn} \int_{-\infty}^{\infty} d\varepsilon f(\varepsilon) \left\langle \left(\langle m|j_\nu|n\rangle \frac{d}{d\varepsilon}\left(\frac{1}{\delta i + \varepsilon_n - \varepsilon}\right) \langle n|j_\mu|m\rangle \delta(\varepsilon - \varepsilon_m) - \right.\right. \\ \left.\left. - \langle m|j_\nu|n\rangle \delta(\varepsilon - \varepsilon_n) \langle n|j_\mu|m\rangle \frac{d}{d\varepsilon}\left(\frac{1}{\delta i + \varepsilon_m - \varepsilon}\right)\right)\right\rangle_c . \tag{1.51}$$

We can rewrite the equation (1.51) using the Green functions. The Green functions are defined as

$$G^{\pm}(\varepsilon) = \lim_{\delta \to 0^+} (\varepsilon - H \pm i\delta)^{-1}. \tag{1.52}$$

Using the Green operators and expressing the current density operators as $j_\mu = -ev_\mu/V$ the equation (1.51) now takes the form

$$\sigma_{\mu\nu} = \frac{ie^2\hbar}{V} \int_{-\infty}^{\infty} d\varepsilon f(\varepsilon) Tr \left\langle v_\nu \frac{d}{d\varepsilon} G^+(\varepsilon) v_\mu \delta(\varepsilon - H) - v_\nu \delta(\varepsilon - H) v_\mu \frac{d}{d\varepsilon} G^-(\varepsilon) \right\rangle_c \tag{1.53}$$

This is the Bastin equation. It connects the conductivity $\sigma_{\mu\nu}$ with the trace of a product of velocity operators, Dirac delta functions of Hamiltonian and derivations of Green functions. The only assumptions needed to derive the equation are the linear response of the system to the perturbation and the use of the independent electron approximation. It is almost simple enough for us to use it in the subsequent computations. However the Dirac delta functions of the Hamiltonian in the energy integral render it very hard to solve numerically. We will therefore have to make one more additional step to obtain a formula for the conductivity which we will be able to use for our computations.

We will first get rid of the Dirac delta functions with the help of identity $\delta(\varepsilon - H) = -\frac{1}{2i\pi}(G^+(\varepsilon) - G^-(\varepsilon))$:

$$\sigma_{\mu\nu} = -\frac{e^2\hbar}{2\pi V} \int_{-\infty}^{\infty} d\varepsilon f(\varepsilon) Tr \left\langle v_\nu \frac{d}{d\varepsilon} G^+(\varepsilon) v_\mu (G^+(\varepsilon) - G^-(\varepsilon)) - \right. \\ \left. - v_\nu (G^+(\varepsilon) - G^-(\varepsilon)) v_\mu \frac{d}{d\varepsilon} G^-(\varepsilon) \right\rangle_c . \tag{1.54}$$

Then we will formally split the integral in two and integrate the first half per partes and keep the second half the same

$$\sigma_{\mu\nu} = \sigma^I_{\mu\nu} + \sigma^{II}_{\mu\nu} \tag{1.55}$$

with

$$\sigma^I_{\mu\nu} = -\frac{e^2\hbar}{4\pi V} \int_{-\infty}^{\infty} d\varepsilon \frac{df(\varepsilon)}{d\varepsilon} Tr \left\langle v_\nu G^+(\varepsilon) v_\mu (G^+(\varepsilon) - G^-(\varepsilon)) - \right. \\ \left. - v_\nu (G^+(\varepsilon) - G^-(\varepsilon)) v_\mu G^-(\varepsilon) \right\rangle_c . \tag{1.56}$$

and

$$\sigma^{II}_{\mu\nu} = -\frac{e^2\hbar}{4\pi V} \int_{-\infty}^{\infty} d\varepsilon f(\varepsilon) Tr \left\langle v_\nu \frac{d}{d\varepsilon} G^+(\varepsilon) v_\mu G^+(\varepsilon) - v_\nu G^+(\varepsilon) v_\mu \frac{d}{d\varepsilon} G^-(\varepsilon) - \right. \\ \left. - v_\nu \frac{d}{d\varepsilon} G^+(\varepsilon) v_\mu G^-(\varepsilon)) + v_\nu G^-(\varepsilon)) v_\mu \frac{d}{d\varepsilon} G^-(\varepsilon) \right\rangle_c . \tag{1.57}$$

This expression can be further simplified by noting that $\frac{dG^{\pm}(\varepsilon)}{d\varepsilon} = -\left(dG^{\pm}(\varepsilon)\right)^2$ and by using the relation $u\hbar v_\mu = [r_\mu, H] = -[r_\mu, G^{-1}]$. Using these relations and integrating per partes once again we arrive at

$$\sigma_{\mu\nu}^{II} = -\frac{e^2\hbar}{4\pi V}\int_{-\infty}^{\infty} d\varepsilon \frac{df(\varepsilon)}{d\varepsilon} Tr\left\langle (G^+(\varepsilon) - G^-(\varepsilon))(r_\mu v_\nu - r_\nu v_\mu)\right\rangle_c . \tag{1.58}$$

Equations (1.55), (1.56) and (1.58) are the Středa equations.

1.5 Anomalous hall effect

Finally we are in a position to take a look at some of the phenomena that give rise to the anomalous Hall effect. Since we are working only with the weak relativistic approximation of the Dirac Hamiltonian (the Pauli Hamiltonian) we will not arrive at all of the phenomena and the picture will thus be incomplete. However in the current state of solid state physics it seems that most of the AHE can be attributed to the three phenomena mentioned in this section.

There are currently three known formalisms in which we can describe the anomalous Hall effect - the Boltzmann formalism, the Kubo formalism and the Keldysh formalism. The Boltzmann formalism is a semiclassical formalism based on the Boltzmann equation. Its main advantage is that it allows us to identify the processes that lead to the anomalous Hall effect. Its disadvantage is that is it impossible to treat the anomalous Hall effect systematically with the Boltzmann formalism and it is possible that we could omit some effects leading to the AHE. The Kubo formalism is based on the Green's functions and it is a fully microscopical theory. It is therefore formally exact within the linear limit and it automatically encompasses all the processes leading to the AHE. However it is more complicated to actually compute exact results in and it does not give much information about the underlining physical processes contributing to the AHE. The Keldysh formalism is also based on the Green's functions. It is possible to calculate nonequilibrium problems with it, however it is even harder to work with, than the Kubo formalism and we will thus not present it in this work.

In this section we will describe the three processes outlined in the Introduction. To describe the processes we will use the language of the Boltzmann formalism. In the next chapter we will show an application of the Kubo formalism to a specific model.

Following Nagaosa et al. (Nagaosa et al., 2010), we will formally divide the AH conductivity into three parts. We will then attribute specific physical processes to these contributions.

The anomalous Hall conductivity can be divided into two parts according to the dependence of the anomalous Hall conductivity on the Bloch state transport lifetime τ. The anomalous hall conductivity can be expressed as a sum of a conductivity independent of the Bloch state transport lifetime $\sigma_{xy} \sim \tau^0$ and a part linearly dependent on the transport lifetime, $\sigma_{xy} \sim \tau^1$. We will call the linearly dependent part the skew-scattering contribution σ_{xy}^{skew}. The part independent of the Bloch transport lifetime can be further divided. We will call the zero frequency (DC) limit of the τ independent anomalous Hall conductivity the intrinsic contribution σ_{xy}^{int}. The third contribution is called the side jump

contribution and is defined as the rest of the anomalous Hall conductivity: $\sigma_{xy}^{sj} = \sigma_{xy} - \sigma_{xy}^{skew} - \sigma_{xy}^{int}$.

Skew-scattering contribution The skew scattering contribution was first recognised by Smit in 1955 and was long considered by the scientific community to be the only origin of the AHE. This is due to the fact that the skew scattering is proportional to the Bloch state transport lifetime and will thus be the dominating contribution in nearly perfect crystals, which were used in the early experiments with the anomalous Hall effect.

The mechanism of the skew scattering can be easily seen from the Lippmann–Schwinger equation:

$$\left|\psi^{\pm}\right\rangle = |\phi\rangle + \frac{1}{E - H_0 \pm i\varepsilon} V \left|\psi^{\pm}\right\rangle \tag{1.59}$$

where $|\psi^{\pm}\rangle$ is the scattered state, $|\phi\rangle$ is the original state, H_0 is the unperturbed Hamiltonian describing the state without the source of scattering and V is the scattering potential. If we take into account the spin orbit interaction, the matrix elements of the impurity scattering potential are (Nagaosa et al., 2010):

$$\langle \mathbf{k}' s' | V | \mathbf{k} s \rangle = \widetilde{V}_{\mathbf{k},\mathbf{k}'} \left(\delta_{s',s} + \frac{i\hbar^2}{4m^2c^2} (\langle s' | \boldsymbol{\sigma} | s \rangle \times \mathbf{k}') \cdot \mathbf{k} \right) \tag{1.60}$$

The second term due to SOI is responsible for the fact that the scattering probability is asymmetrical with respect to the the wave vector $\mathbf{k}$ and it is different for right-handed transitions with respect to the magnetization and for the left-handed ones. This will result in a momentum perpendicular to the magnetization of the sample and to the incidental momentum. As can be seen in the equation (1.60), this effect is also linearly dependent on the incidental momentum of the scattered electron and therefore on the longitudinal current in the sample. The skew-scattering contribution to the anomalous Hall conductivity is also proportional to the potential $\widetilde{V}_{\mathbf{k},\mathbf{k}'}$ and therefore proportional to the Bloch transport lifetime in the sample. Since the longitudinal conductivity is also proportional to the Bloch transport lifetime, the anomalous Hall resistivity originating in the skew scattering will be proportional to the longitudinal resistivity.

Intrinsic contribution The intrinsic contribution was the first contribution described in theory. However it had been discarded for a long time. This was because the anomalous velocity giving rise to the AHE depends on the acceleration of a wave packet $\dot{\mathbf{k}}$ and it was argued that in an equilibrium the acceleration would be zero. However, since the electrons undergo many collisions, there is indeed a non-zero acceleration of the wave packets in the material even if it is in equilibrium and the intrinsic contribution is always present.

The anomalous velocity can be seen, when we consider a semiclassical Lagrangian $\mathcal{L}$ acting on a wave packet $\Psi_{n,\mathbf{k}_c,\mathbf{r}_c}$ in band n with center position $\mathbf{r}_c$ and average wave vector $\mathbf{k}_c$. The wave packet then has the form (Nagaosa et al., 2010):

$$\Psi_{n,\mathbf{k}_c,\mathbf{r}_c} = \frac{1}{\sqrt{V}} \sum_{\mathbf{k}} w_{\mathbf{k}_c,\mathbf{r}_c}(\mathbf{k}) e^{i(\mathbf{k}-\mathbf{k}_c)\cdot\mathbf{a}_n} e^{i(\mathbf{r}-\mathbf{r}_c)\cdot\mathbf{k}} u_{n\mathbf{k}}(\mathbf{r}), \tag{1.61}$$

where $w_{\mathbf{k}_c,\mathbf{r}_c}$ are real coefficients and $\mathbf{a}_n = \langle u_{n,\mathbf{k}} |\, i\partial_{\mathbf{k}} u_{n\mathbf{k}} \rangle$ is a Berry connection of the Bloch state.

The Lagrangian has the form:

$$\mathcal{L} = \langle \Psi_{n,\mathbf{k}_c,\mathbf{r}_c} |\, i\frac{\partial}{\partial t} - H_0 + eV \,| \Psi_{n,\mathbf{k}_c,\mathbf{r}_c} \rangle \tag{1.62}$$

$$= \hbar \mathbf{k}_c \cdot \mathbf{r}_c + \hbar \dot{\mathbf{k}_c} \cdot \mathbf{a}_n(\mathbf{k}_c) - \mathcal{E}(\mathbf{k}_c) + eV(\mathbf{r}_c). \tag{1.63}$$

We can therefore write the Euler-Lagrange conditions as:

$$\hbar \dot{\mathbf{k}_c} = -e\mathbf{E} \tag{1.64}$$

$$\dot{\mathbf{r}_c} = \frac{\partial \mathcal{E}_n(\mathbf{k}_c)}{\partial \mathbf{k}_c} - \hbar \mathbf{k}_c \times \mathbf{b}_n(\mathbf{k}_c). \tag{1.65}$$

where $\mathbf{b}_n(\mathbf{k}_c) = \boldsymbol{\nabla} \times \mathbf{a}_n(\mathbf{k}_c)$ is a Berry curvature of the Bloch state. The second term is the anomalous velocity and it is the origin of the intrinsic contribution to the anomalous Hall conductivity.

The intrinsic contribution is therefore dependent only on the topological properties of the momentum-space of the sample and it is independent of scattering. It is in fact the only term which is finite in scattering-free models. The Hall current created by the intrinsic Hall effect is also dissipationless (Lee et al., 2004).

The anomalous Hall conductivity originating in the intrinsic contribution is dominant in transition metal ferromagnets (Miyasato et al., 2007).

Side jump contribution The side jump contribution has been for a long time a source of great controversies. This is mostly because the side jump is independent of the Bloch state relaxation time, so it is not easily distinguished from the intrinsic contribution. The side jump itself is also very small - in typical metals $\Delta y \sim 10^{-16} m$ and becomes significant only when enhanced through the band structure effects. (Berger, 1970)

The origin of the side jump contribution can be seen from the Lippmann–Schwinger equation (1.59) and the matrix form of the scattering potential. When a wave packet with a wave vector $\mathbf{k}$ is scattered by the potential (1.60) with small enough spin-orbit interaction we can approximate the scattered wave packet in the Born approximation:

$$\Psi_{n,\mathbf{k}_c,\mathbf{r}_c} \sim e^{i\mathbf{r}\cdot\mathbf{k}} + \sum_{k's'} \delta_{ss'} \frac{1}{\mathcal{E} - \mathcal{E}(\mathbf{k}', s') - i\varepsilon} \widetilde{V}_{\mathbf{k},\mathbf{k}'} exp\left(i\frac{\hbar^2}{4m^2c^2} (\sigma_{\mathbf{ss}} \times \mathbf{k}) \cdot \mathbf{k}' \right) \tag{1.66}$$

We can view this scattered wave packet as a new wave packet with the center displaced by:

$$\boldsymbol{\delta} = \frac{\hbar^2}{4m^2c^2} (\boldsymbol{\sigma}_{ss} \times \mathbf{k}). \tag{1.67}$$

We therefore see that in addition to skew scattering the spin-orbit interaction in the scattering potential also causes a shift in the center position of the wave packet, which also leads to the AHE. The displacement is spin-dependent and it is perpendicular to both the spin of the electron and its wave vector.

Both the skew-scattering and the side jump are called extrinsic contributions as they are based on a scattering. It is important to note, that for the intrinsic Hall effect to manifest there has to be an interband hopping available. While for the extrinsic contributions the interband hopping is not necessary, they are both greatly enhanced (by a factor of $\sim 10^4$) by the multiband effects.

2. The models

In this chapter we will introduce two models dealing with the anomalous Hall effect. The models have been devised by Středa and Jonckheere and by Kontani *et al.* Since it is too difficult to make a model that would account for all the effects giving rise to the anomalous Hall conductivity, the models will account for only the intrinsic contribution to the anomalous Hall conductivity.

As we have mentioned in the previous chapter in the recent years there have been numerous experiments suggesting, that the intrinsic anomalous Hall effect is the dominant contribution to the anomalous Hall conductivity in the transition metal ferromagnets in the good metal regime ($\sigma_{xx} \sim 10^4 - 10^6(\Omega cm)^{-1}$). Since these materials represent the biggest group in the ferromagnetic materials, it is worthwhile studying these contributions.

Throughout this chapter we will therefore only deal with ferromagnetic materials. For simplicity we will assume, that the magnetisation $\mathbf{M}$ will be parallel to the z-axis.

We will also restrict ourselves only to crystals with spatial inversion symmetry.

2.1 Středa model

The Středa model is a very simple one. In the paper (Středa and Jonckheere, 2010) Středa argues that the intrinsic contribution to the anomalous Hall conductivity should be obtainable via either the linear response Kubo formula leading to the Berry phase contribution or as a response to a gradient of a chemical potential. Both the approaches should give the same result. Středa therefore uses a model based on the chemical potential difference $\Delta\mu$ and a consequent electric dipole.

We will explain the basic idea behind the Středa model:

Suppose we have a one-dimensional sample with the length L kept at zero temperature. When the sample is in equilibrium with no external forces acting on it, the states with a wave vector $\boldsymbol{k}$ will be in a distribution $f(\boldsymbol{k})$. If we apply an external electric field E in the direction of the y-axis, the distribution will shift along the k_y - axis, as shown in figure 2.1, by $\Delta k = \frac{eE\tau_m}{\hbar}$, with τ_m being the momentum relaxation time. As can be seen from the figure, most of the states deep in the Fermi sea stay the same. However the states near the Fermi-level with $k < 0$ are vacated and more states near the Fermi level with $k > 0$ are filled. These states can be viewed as the sources of current.

We can describe this shift in the distribution $f(\boldsymbol{k})$ of the wave vectors with the help of quasi-Fermi levels $F^{\pm}$. We can define the positive quasi-Fermi level F^+ as the Fermi level of the electrons moving in the same direction as the applied electric field E. In the same way we define the negative quasi-Fermi level F^- as the Fermi level of the electrons moving in the opposite direction as that of the applied electric field E. As can be seen in the figure 2.1 the negative quasi-Fermi level is lower than the positive quasi-Fermi level: $F^- < F^+$. Since the negative quasi-Fermi level is lower than the positive one, for every state with $k_y < 0$ we can find a state with the opposite velocity and the current contributions from these two states cancel out. So the only states that contribute to the current

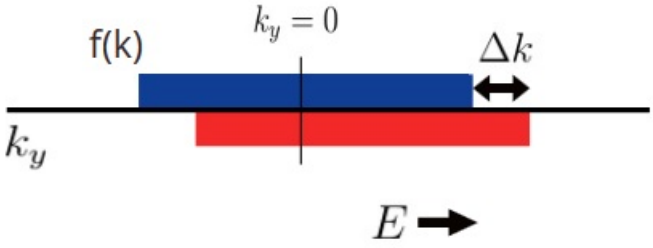

Figure 2.1: Shift of the distribution $f(\boldsymbol{k})$ with an external electric field E applied. The blue rectangle above the axis represents the original distribution $f(\boldsymbol{k})$. The red rectangle below the axis represents the shifted distribution.

are the states with $k_y > 0$ with the energy between the positive and negative quasi-Fermi levels - we will call these states the k^+ states.

We can now evaluate the current created with the k^+ states. Electron gas moving with the velocity v with the density n has a contribution to the current $j = env$. Since in this case the density of electrons associated with the state k is $1/L$, we can express the current created by the k^+ states as:

$$j = \sum_{k^+} \frac{e}{L} v(k) \tag{2.1}$$

where we have summed over all the k^+ states. We can now change the sum over the k states into an integral $\sum_k \longrightarrow \frac{L}{\pi} \int_k dk$ and express the group velocity of the electrons as $\mathbf{v}_\alpha(\mathbf{k}) = \frac{1}{\hbar} \nabla_{\mathbf{k}} \mathcal{E}_\alpha(\mathbf{k})$ (see e.g. Ashcroft and Mermin (1976)):

$$j = \frac{2e}{h} \int_{k^+} \frac{d\mathcal{E}}{dk} dk = -\frac{2e}{h} \int_{k^+} dE, \tag{2.2}$$

where we integrate over the k^+ states. Since the k^+ states occupy all the k states between F^+ and F^- we have:

$$j = \frac{2e}{h}(F^+ - F^-). \tag{2.3}$$

The difference between the quasi-Fermi levels is the chemical potential difference between the states at the Fermi surface $\Delta\mu(k_F)$. We can therefore rewrite the equation (2.3) as

$$j = \frac{2e}{h} \Delta\mu(k_F). \tag{2.4}$$

In order to find the conductivity we therefore need to find the relationship between the chemical potential difference $\Delta\mu(k_F)$ and the electric field E.

In the model we will use the independent electron approximation and assume that the properties of the material can be described by a Pauli-like single electron Hamiltonian:

$$H = \frac{p^2}{2m} + V(\mathbf{r}) + H_{so} + H_z \tag{2.5}$$

where $\mathbf{p}$ is the momentum of the electron, m is the free electron mass, $V(\mathbf{r})$ is the crystalline potential and H_{so} is the Hamiltonian of the spin-orbit interaction and H_z is the Hamiltonian of Zeeman effect:

$$H_{so} = \frac{\lambda_c^2}{4\hbar}\boldsymbol{\sigma} \cdot [\nabla V(\mathbf{r}) \times \mathbf{p}] = \frac{\lambda_c^2}{4\hbar}\mathbf{p} \cdot [\boldsymbol{\sigma} \times \nabla V(\mathbf{r})] \tag{2.6}$$

$$H_z = -\mu_B \mathbf{B}_{eff} \cdot \boldsymbol{\sigma} \tag{2.7}$$

with λ_c being an effective Compton wavelength $\lambda_c = \frac{h}{mc}$, $\boldsymbol{\sigma}$ is the vector of Pauli matrices introduced in equation (1.2), μ_B is the Bohr magneton and $\mathbf{B}_{eff}$ is the effective magnetic field.

Eigenvectors of this Hamiltonian are two-component spinors and, since the Hamiltonian is translation-invariant in the lattice vectors, we can express them in the Bloch form $|\alpha, \mathbf{k}\rangle$:

$$\Psi_{\alpha,\mathbf{k}}(\mathbf{r}) \equiv \langle \mathbf{r}|\alpha, \mathbf{k}\rangle = \frac{e^{i\mathbf{k}\cdot\mathbf{r}}}{\sqrt{8\pi^3}} u_\alpha(\mathbf{k}, \mathbf{r}) \tag{2.8}$$

with $u_\alpha(\mathbf{k}, \mathbf{r})$ being periodic in the lattice vectors, $\mathbf{k}$ being the wave vector and $\alpha = (n, m, l, s)$ being the band index comprising of n - principal quantum number, m - orbital quantum number, l - azimuthal quantum number and s - the spin number. We will suppose that the material is ferromagnetic, with the effective magnetic field $\mathbf{B}_{eff}$ in the direction of the z-axis. The spin number will therefore be a good quantum number.

The velocity operator corresponding to the Hamiltonian (2.5) is:

$$\mathbf{v} = \frac{1}{i\hbar}[H, \mathbf{r}] = \frac{\mathbf{p}}{m} + \frac{\lambda_c^2}{4\hbar}\boldsymbol{\sigma} \times \nabla V(\mathbf{r}). \tag{2.9}$$

A typical feature accompanying the spin orbit interaction is the mass-center separation along the y-axis $\Delta Y_\alpha(k_x)$ of the states $|\alpha, k_x\rangle$ and $|\alpha, -k_x\rangle$ (with $k_x > 0$). This mass-center separation can also be seen as the source of the anomalous hall effect. We can calculate the mass center separation via the requirement that in the stationary state the force

$$F_y \equiv \frac{1}{ih}[p_y, H] \tag{2.10}$$

is zero. Equating the force to zero will then yield the formula for the mass-center separation.

If we apply an external electric field E_y in the direction of the y-axis the states $|\alpha, k_x\rangle$ and $|\alpha, -k_x\rangle$ with opposite velocities will acquire a chemical potential difference $\Delta\mu$ between them:

$$\Delta\mu = -E_y e \Delta Y_\alpha(k_F). \tag{2.11}$$

with $\Delta Y_\alpha(k_F)$ being the mass-center separation of the eigenstates with the wave vector from the Fermi surface.We can now employ the equation (2.4) to find the current contribution $J_x^\alpha(\mu)$ of the α band:

$$J_x^\alpha(\mu) = -\frac{2e^2}{h}\Delta Y_\alpha(k_F) E_y. \tag{2.12}$$

From this equation we can easily identify the contribution of the band α to the anomalous Hall conductivity as:

$$\sigma_{xy}^{\alpha} = -\frac{2e^2}{h}\Delta Y_{\alpha}(k_F) \tag{2.13}$$

The anomalous Hall conductivity will then simply be the sum of the contributions of all the bands α:

$$\sigma_{xy} = \sum_{\alpha} \sigma_{xy}^{\alpha} \tag{2.14}$$

We can therefore identify the Hall conductivity with the mass-center separation $\Delta Y_{\alpha}(k_F)$.

For the purposes of the next chapter we need to generalise this model to two-dimensional systems. The conductivity contribution expressed in the equation (2.13) is the contribution of the states $|\alpha, k_x\rangle$ and $|\alpha, -k_x\rangle$. In order to take into account the whole Fermi surface we need to integrate over all the states at the Fermi surface with $k_x > 0$. The total anomalous Hall conductivity will then be:

$$\sigma_{xy} = -\frac{2e^2}{h}\int dk \delta(k^2 - k_F^2)\Delta Y_{\alpha}(k). \tag{2.15}$$

Středa also gives a simple example model in (Středa and Jonckheere, 2010) to show the current . The simple model will be a linear chain of atomic orbitals along the x-axis, with the separation a. The potential $V(\mathbf{r})$ of the chain will be:

$$V(x, y) = -V_0 cos(2\pi x/a) + m\Omega^2 y^2/2, \tag{2.16}$$

with the harmonic oscillator potential in the y-direction. In the Figure 2.2, we can see the current densities $j_x^{\alpha}(k_x, x, y) = ev_x^{\alpha}(k_x, x, y)$ obtained by Středa by tight binding approximation for a set of parameters mentioned in the description below the figure.

In the case of the simple example the force will be

$$F_y = -m\Omega^2 y + 2s\frac{\lambda_c^2 m\Omega^2}{4\hbar}p_x \tag{2.17}$$

which, with the help of relation (2.9) gives the mass-center separation is

$$\Delta Y_{\alpha}(k_x) = 2s\frac{\lambda_c^2 m}{2\hbar}\left[1 - \left(\frac{\lambda_c^2 m}{4\hbar}\right)^2 \Omega^2\right]^{-1} 2v_x^{\alpha}(k_x). \tag{2.18}$$

This leads to the Hall conductivity

$$\sigma_{xy}^{\alpha} = -\frac{e^2}{h}\frac{s\lambda_c^2 m}{\hbar}\left[1 - \left(\frac{\lambda_c^2 m}{4\hbar}\right)^2 \Omega^2\right]^{-1} 2v_x^{\alpha}(k_F). \tag{2.19}$$

We can see from the equation (2.19) that the anomalous Hall conductivity are approaching zero as the spin-orbit interaction vanishes. This is exactly the expected behaviour. We also see that when $\left(\frac{\lambda_c^2 m}{4\hbar}\right)^2 \Omega^2 \longrightarrow 1$ the anomalous Hall

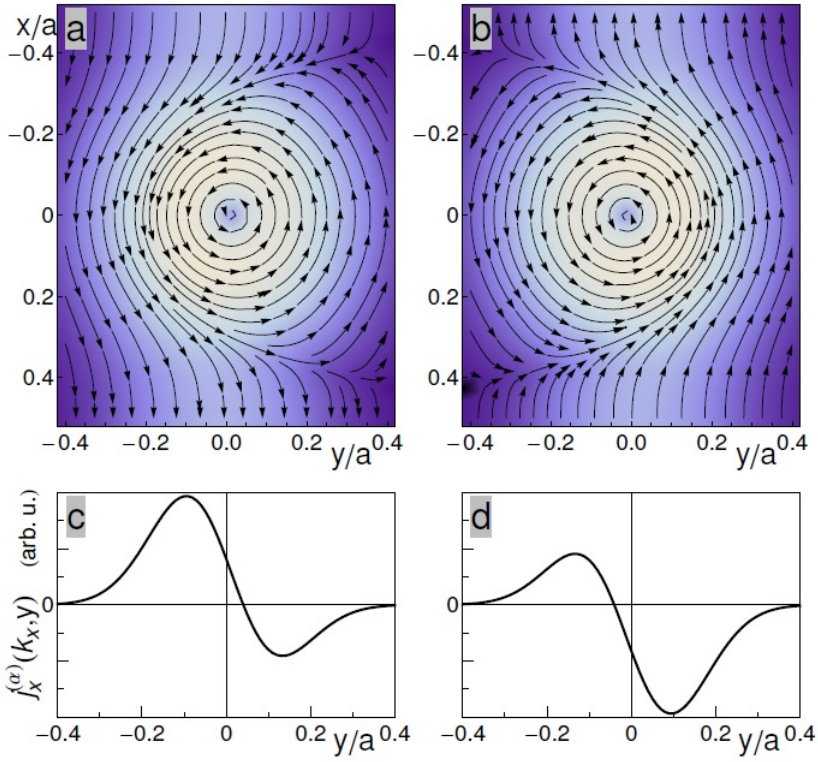

Figure 2.2: Current distributions for an energy band in the chain-potential model given by Středa. The current distributions were computed for a set of parameters: $2ma^2V_0/\hbar^2 = 75.0$, $m\Omega^2a^2/(4\pi^2V_0) = 1.4$ and $\pi\lambda_c^2/a^2 = 0.015$ with $s_z = 1/2$ and $m = -1$. For figures (a) and (c) $k_x = 1.5/a$. For figures (b) and (d) $k_x = -1.5/a$. In figures (a) and (b) there are current distributions with arrows indicating the direction of the current and the lighter the background is the larger the current magnitude. In figures (c) and (d) there are current densities averaged over the x and y coordinates. We can see that there is a clear spatial separation of the states with the opposite velocities.

conductivity goes to infinity. This is also an expected behaviour as the aforementioned parameter should be much less than one in the weak relativistic limit and in the case that $\left(\frac{\lambda_c^2 m}{4\hbar}\right)^2 \Omega^2 \longrightarrow 1$ the weak relativistic limit would break down.

Středa also shows, that the conductivity obtained via the the equation (2.11) is equivalent to the conductivity obtained from the Berry phase of the momentum-space and therefore to the intrinsic anomalous Hall conductivity (Středa and Jonckheere, 2010).

In table 2.1 we have summed up all the assumptions implied by the Středa model.

Table 2.1: **Assumptions implied by the Středa model**

Independent electron approximation
Linear response approximation
Zero temperature
Ferromagnetic material with $\mathbf{M}\|\|\hat{z}$
Space inversion symmetry

2.2 Kontani model

The Kontani model is a bit more complicated. It studies the intrinsic anomalous Hall effect in the tight binding model of the interaction between the d-orbitals. Since in the ferromagnets the anomalous Hall effect comes about due to the spin-orbit interaction with the Hamiltonian (in the simplified case of ferromagnet with pure $s_z = \pm 1/2$ spin states) $H_{so} = \lambda \boldsymbol{\sigma} \cdot \boldsymbol{L} = \lambda s_z l_z$, we can restrict ourselves to the d-orbitals, for which $\langle d_\alpha | l_z | d_\beta \rangle$ is non-zero. This condition reduces the orbitals to d_{xz}, d_{yz}, d_{xy} and $d_{x^2-y^2}$. Furthermore, since the anomalous Hall effect comes from the interband hopping, we can also neglect the orbitals d_{xy} and $d_{x^2-y^2}$, as the energy splitting between them is about 1eV, while the d_{xz} and d_{yz} orbitals are degenerate - this means that the frequency of hopping between the d_{xy} and $d_{x^2-y^2}$ is exponentially smaller, than that of the hopping between the d_{xz} and d_{yz} orbitals. We will therefore concern ourselves only with the d_{xz} and d_{yz} orbitals.

In this model we will describe the system with the Hamiltonian $H = H_0 + H_{SO}$ consisting of a part H_0 which will describe the system without a spin interaction and a part H_{SO} which will describe the spin-orbit interaction. We will express the Hamiltonian H_0 with the use of creation and annihilation operators for the electron on the orbital d_α: $c_{\mathbf{k}}^{\alpha\dagger}$ and $c_{\mathbf{k}}^{\alpha}$. To make the notation a bit less unwieldy we will write an index x when referring to the d_{xz} orbital and y when referring to the d_{yz} orbital.

$$H_0 = \sum_{\mathbf{k}} \hat{c}_{\mathbf{k}}^\dagger \hat{h}_{\mathbf{k}}^0 \hat{c}_{\mathbf{k}} \tag{2.20}$$

with

$$\hat{h}_{\mathbf{k}}^0 = \begin{pmatrix} \xi_{\mathbf{k}}^x & \xi_{\mathbf{k}}^{xy} \\ \xi_{\mathbf{k}}^{yx} & \xi_{\mathbf{k}}^y \end{pmatrix}, \; \hat{c}_{\mathbf{k}}^\dagger = \begin{pmatrix} c_{\mathbf{k}}^{x\dagger}, c_{\mathbf{k}}^{y\dagger} \end{pmatrix} \tag{2.21}$$

where $\xi_{\mathbf{k}}^x = -2t \cos k_x$, $\xi_{\mathbf{k}}^y = -2t \cos k_y$ $\xi_{\mathbf{k}}^{xy} = 4t' \sin k_x \sin k_y$. Here t and t' are the hopping integrals between the nearest and the next-nearest lattice points as shown in figure 2.3.

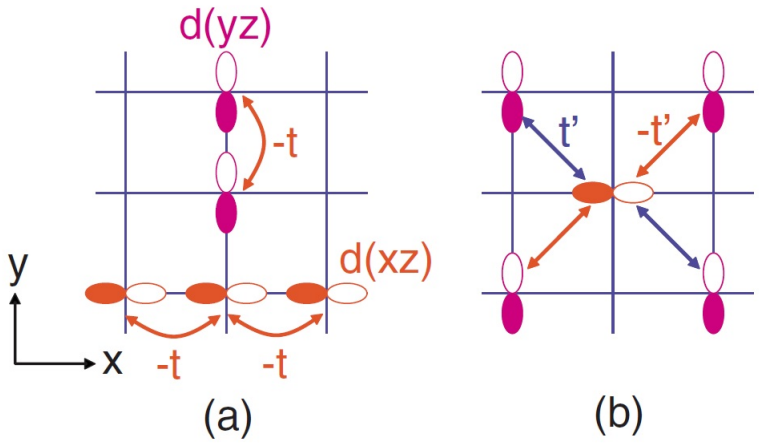

Figure 2.3: (a) - figure of hopping integrals between the same orbitals. (b) - figure of hopping integrals between different orbitals. Figure a courtesy of (Kontani et al., 2007).

The spin-orbit interaction part H_{SO} is given by the equation (1.7). We will however express it with the help of creation and annihilation operators as

$$H_{SO} = \sum_{k} \hat{c}^{\dagger}_{\mathbf{k}} \hat{h}^{\lambda} \hat{c}_{\mathbf{k}}. \tag{2.22}$$

In the basis of eigenvectors $|l, l_z\rangle$ of L^2 and L_z, $\beta = \{ |2, -2\rangle, |2, -1\rangle, |2, 0\rangle, |2, 1\rangle, |2, 2\rangle \}$, we have the matrix representation of L_z:

$$\langle l, m|L_z|l', m'\rangle \overset{\beta}{=} \begin{pmatrix} -2 & 0 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 2 \end{pmatrix}, \tag{2.23}$$

and the d_{xz} and d_{yz} states have the representation

$$|x, z\rangle = -\frac{1}{\sqrt{2}} \left(|2, 1\rangle - |2, -1\rangle\right) \overset{\beta}{=} \frac{1}{\sqrt{2}} \begin{pmatrix} 0 \\ -1 \\ 0 \\ 1 \\ 0 \end{pmatrix} \tag{2.24}$$

and

$$|y, z\rangle = -\frac{i}{\sqrt{2}} \left(|2, 1\rangle + |2, -1\rangle\right) \overset{\beta}{=} \frac{i}{\sqrt{2}} \begin{pmatrix} 0 \\ 1 \\ 0 \\ 1 \\ 0 \end{pmatrix}. \tag{2.25}$$

We therefore see, that in our basis $\beta' = \{d_{xz}, d_{yz}\}$ the representation of the spin-orbit interaction is

$$\hat{h}^{\lambda} = sgn(s_z)\lambda\sigma_y \tag{2.26}$$

with σ_y being the Pauli matrix given in the equation (1.2).

The velocity operator corresponding to the Hamiltonian is given by $\mathbf{v}_\alpha(\mathbf{k}) = \frac{1}{\hbar}\nabla_{\mathbf{k}}\mathcal{E}_\alpha(\mathbf{k})$. We therefore have

$$v_x = \frac{1}{\hbar}\begin{pmatrix} 2t\sin k_x & 4t'\cos k_x \sin k_y \\ 4t'\cos k_x \sin k_y & 0 \end{pmatrix} \tag{2.27}$$

$$v_y = \frac{1}{\hbar}\begin{pmatrix} 0 & 4t'\sin k_x \cos k_y \\ 4t'\sin k_x \cos k_y & 2t\sin k_y \end{pmatrix} \tag{2.28}$$

In order to use the Kubo-Středa equation we will also need to express the Green functions corresponding to the Hamiltonian H. The Green functions are defined by the equation (1.52). We will express the Green function in the matrix form in which it has the form $\hat{G}(\omega) = (\omega + \mu - \hat{h}^0_{\mathbf{k}} - \hat{h}^\lambda)^{-1}$

$$\begin{pmatrix} G_{xx} & G_{xy} \\ G_{xy} & G_{yy} \end{pmatrix} = \frac{1}{d(\omega)}\begin{pmatrix} \omega + \mu - \xi^y_{\mathbf{k}} & \alpha_{\mathbf{k}} \\ \alpha^*_{\mathbf{k}} & \omega + \mu - \xi^x_{\mathbf{k}}, \end{pmatrix} \tag{2.29}$$

with $\alpha_{\mathbf{k}} = \xi^{xy}_{\mathbf{k}} + i\lambda sgn(s_z)$ and $d(\omega) = (\omega + \mu - \xi^x_{\mathbf{k}})(\omega + \mu - \xi^y_{\mathbf{k}}) - |\alpha_{\mathbf{k}}|^2$. We can also express $d(\omega)$ as

$$d(\omega) = (\omega + \mu - E^+_{\mathbf{k}})(\omega + \mu - E^-_{\mathbf{k}}), \tag{2.30}$$

where $E^\pm_{\mathbf{k}}$ is the quasiparticle dispersion relation:

$$E^\pm_{\mathbf{k}} = \frac{1}{2}(\xi^x_{\mathbf{k}} + \xi^y_{\mathbf{k}} \pm \sqrt{(\xi^x_{\mathbf{k}} - \xi^y_{\mathbf{k}})^2 + 4|\alpha_{\mathbf{k}}|^2}). \tag{2.31}$$

In order to model the ferromagnetic state, we will assume that in the d-orbitals are only electrons with spin $s_z = -1/2$.

In order to account for the scattering of the quasiparticles Kontani uses retarded and advanced Green functions with quasiparticle damping rate $\gamma = \hbar/2\tau$:

$$G^R_{\alpha\beta}(\omega) = G_{\alpha\beta}(\omega + i\gamma) \tag{2.32}$$

$$G^A_{\alpha\beta}(\omega) = G_{\alpha\beta}(\omega - i\gamma) \tag{2.33}$$

We can now employ the Kubo-Středa formula to calculate the anomalous Hall conductivity. We will use the equations (1.55), (1.56) and (1.57) in which we have explicitly written out the traces as the sums over the orbitals:

$$\sigma^{AH}_{xy} = \sigma^I_{xy} + \sigma^{II}_{xy}, \tag{2.34}$$

$$\sigma^I_{xy} = \sum_{\mathbf{k},\alpha\alpha',\beta\beta'} \frac{e^2\hbar}{4\pi\Omega}\int d\epsilon v^{\alpha'\alpha}_x v^{\beta'\beta}_y \left(-\frac{df}{d\epsilon}\right)\left[G^R_{\alpha\beta'}G^A_{\beta\alpha'} - \frac{1}{2}(G^R_{\alpha\beta'}G^R_{\beta\alpha'} + G^A_{\alpha\beta'}G^A_{\beta\alpha'})\right] \tag{2.35}$$

$$\begin{aligned}\sigma^{II}_{xy} = -\frac{1}{2}\sum_{\mathbf{k},\alpha\alpha',\beta\beta'} \frac{e^2\hbar}{4\pi\Omega}\int d\epsilon v^{\alpha'\alpha}_x v^{\beta'\beta}_y f(\epsilon)\times \\ \times\left[\frac{\partial}{\partial\epsilon}G^R_{\alpha\beta'}G^R_{\beta\alpha'} - G^R_{\alpha\beta'}\frac{\partial}{\partial\epsilon}G^R_{\beta\alpha'} - \frac{\partial}{\partial\epsilon}G^A_{\alpha\beta'}G^A_{\beta\alpha'} + G^A_{\alpha\beta'}\frac{\partial}{\partial\epsilon}G^A_{\beta\alpha'}\right]\end{aligned} \tag{2.36}$$

We will now simplify the expressions. First we will sum over the greek indices. We see that the only combinations of the indices for which the velocities are odd in both k_x and k_y and non-zero are $(\alpha\alpha', \beta\beta') = (xxxy), (xxyx), (xyyy)$ and $(yxyy)$. All the other combinations of indices are either trivially zero, or are odd in k_x, k_y or both and will therefore vanish after summation over all $\mathbf{k}$. Since the model has a square lattice symmetry, the expressions (2.35) and (2.36) are both invariant to permutation of k_x and k_y. We can therefore write the sum over the greek indices as a single component

$$\sigma_{xy}^{I} = \sum_{\mathbf{k}} \frac{e^2\hbar}{4\pi\Omega} \int d\epsilon v_x v_y \left(-\frac{df}{d\epsilon}\right) \left[G_{xx}^R G_{yx}^R - \frac{1}{2}(G_{xx}^R G_{yx}^R + G_{xx}^A G_{yx}^A)\right] \tag{2.37}$$

$$\begin{aligned}\sigma_{xy}^{II} = -\frac{1}{2}\sum_{\mathbf{k}} \frac{e^2\hbar}{4\pi\Omega} \int d\epsilon v_x v_y f(\epsilon) \Bigg[&\frac{\partial}{\partial\epsilon} G_{xx}^R G_{yx}^R - G_{xx}^R \frac{\partial}{\partial\epsilon} G_{yx}^R - \\ &- \frac{\partial}{\partial\epsilon} G_{xx}^A G_{yx}^A + G_{xx}^A \frac{\partial}{\partial\epsilon} G_{yx}^A\Bigg]\end{aligned} \tag{2.38}$$

where $v_x v_y \equiv v_x^{xx} v_y^{xy} = 8tt' \sin^2 k_x \cos k_y$.

The Green functions can be simplified into (Kontani et al., 2007):

$$\sigma_{xy}^{I} = \sum_{\mathbf{k}} \frac{e^2\hbar}{4\pi\Omega} \int d\epsilon v_x v_y \left(-\frac{df}{d\epsilon}\right) \frac{4\gamma}{d^R(\epsilon) d^A(\epsilon)} \tag{2.39}$$

$$\sigma_{xy}^{II} = -\frac{1}{2}\sum_{\mathbf{k}} \frac{e^2\hbar}{4\pi\Omega} \int d\epsilon v_x v_y f(\epsilon) \left[\left(\frac{1}{d^R(\epsilon)}\right)^2 - \left(\frac{1}{d^A(\epsilon)}\right)^2\right] \tag{2.40}$$

In the limit of $T \to 0K$ the Fermi-Dirac distribution becomes a step function $f(\epsilon) \to \theta(\epsilon - \mu)$ and with its derivative a Dirac delta function $df/d\epsilon \to \delta(\epsilon - \mu)$. We can use these relations along with the table integral

$$\int_{-\infty}^{\mu} \frac{dx}{(x-a)^2(x-b)^2} = \frac{-(2\mu - a - b)}{(a-b)^2(\mu-a)(\mu-b)} - \frac{2}{(a-b)^3} \ln\left(\frac{a-\mu}{b-\mu}\right) \tag{2.41}$$

to evaluate the integrals in equations (2.39) and (2.40). Using these relations we arrive at a set of three contributions to the anomalous conductivity

$$\sigma_{xy} = \sigma_{xy}^{I} + \sigma_{xy}^{IIa} + \sigma_{xy}^{IIb} \tag{2.42}$$

$$\sigma_{xy}^{I} = \frac{2\lambda}{\pi} \sum_{\mathbf{k}} v_x v_y \frac{\gamma}{[(\mu - E_{\mathbf{k}}^{+})^2 + \gamma^2][(\mu - E_{\mathbf{k})^2}^{-} + \gamma^2]} \tag{2.43}$$

$$\sigma_{xy}^{IIa} = \frac{2\lambda}{\pi} \sum_{\mathbf{k}} \frac{v_x v_y}{(E_{\mathbf{k}}^{+} - E_{\mathbf{k}}^{-})^2} Im\left\{\frac{2\mu - E_{\mathbf{k}}^{+} - E_{\mathbf{k}}^{-} + 2i\gamma}{(\mu - E_{\mathbf{k}}^{+} + i\gamma)(\mu - E_{\mathbf{k}}^{-} + i\gamma)}\right\}, \tag{2.44}$$

$$\sigma_{xy}^{IIb} = \frac{4\lambda}{\pi} \sum_{\mathbf{k}} \frac{v_x v_y}{(E_{\mathbf{k}}^{+} - E_{\mathbf{k}}^{-})^3} Im\left\{\ln\left(\frac{E_{\mathbf{k}}^{+} - \mu - i\gamma}{E_{\mathbf{k}}^{-} - \mu - i\gamma)}\right)\right\}. \tag{2.45}$$

These relations are valid even for finite damping rates γ. In order to account only for the intrinsic anomalous Hall effect we will take the limit of the damping rate going to zero. In this case we get the contributions to the anomalous Hall effect as (Kontani et al., 2007):

$$\sigma_{xy}^{I} = \lambda \frac{e^2\hbar}{\Omega} \sum_{\mathbf{k}} v_x v_y \frac{\delta(\mu - E_{\mathbf{k}}^{+}) + \delta(\mu - E_{\mathbf{k}}^{-})}{(E_{\mathbf{k}}^{+} - E_{\mathbf{k}}^{-})^2} \tag{2.46}$$

$$\sigma_{xy}^{IIa} = -\lambda \frac{e^2\hbar}{\Omega} \sum_{\mathbf{k}} v_x v_y \frac{\delta(\mu - E_{\mathbf{k}}^{+}) + \delta(\mu - E_{\mathbf{k}}^{-})}{(E_{\mathbf{k}}^{+} - E_{\mathbf{k}}^{-})^2} \tag{2.47}$$

$$\sigma_{xy}^{IIb} = 2\lambda \frac{e^2\hbar}{\Omega} \sum_{\mathbf{k}} v_x v_y \frac{-\theta(\mu - E_{\mathbf{k}}^{+}) + \theta(\mu - E_{\mathbf{k}}^{-})}{(E_{\mathbf{k}}^{+} - E_{\mathbf{k}}^{-})^3} \tag{2.48}$$

The fist contribution σ_{xy}^{I} is the Fermi surface term. The second and the third terms σ_{xy}^{IIa} and σ_{xy}^{IIb} are Fermi sea terms, although the term σ_{xy}^{IIa} is in the case of no scattering nonzero only on the Fermi surface. In the limit of no scattering ($\gamma \to 0$) the first contribution σ_{xy}^{I} is of the same magnitude as the σ_{xy}^{IIa} and they cancel each other out. (This nullification of the two terms however occurs only in the intrinsic limit.) In the case of no scattering and zero temperature the only contribution to the anomalous Hall conductivity therefore comes from the last term σ_{xy}^{IIb}. This term has been recognised as the term coming from the Berry curvature (Onoda and Nagaosa, 2002).

All the contributions to the conductivity are linear $v_x v_y = 8tt' \sin^2 k_x \cos k_y$. This implies that should the hopping integral t' between different bands be zero the anomalous Hall conductivity would vanish. This corresponds to the fact that the d_{xz} orbital does not allow the transport in the y direction and the d_{yz} does not allow transport in the x direction. Therefore wee need the interband hopping in order to achieve the anomalous Hall current.

In the table 2.2 we have summed up the assumptions implied in this model. The first four assumptions come from the use of the Kubo-Středa formula.

Table 2.2: **Assumptions implied by the Kontani model**

Independent electron approximation
Linear response approximation
Zero temperature
Zero frequency
Tight binding model with only d_{xz} and d_{yz} orbitals
Ferromagnetic material with $\mathbf{M}\|\|\hat{z}$

3. Model comparison

In this chapter we make an attempt to compare the two models described in the previous chapter. We calculate the anomalous Hall conductivity predicted by the two models and in order to compare the two models we need to calculate the conductivity for the same material under the same conditions.

We have chosen the material to be Strontium ruthenate (Sr_2RuO_4) as the shape of the Fermi surface in Sr_2RuO_4 is very favourable for computation. In the Figure 3.1 there is a depiction of the Fermi surface of Sr_2RuO_4 calculated in (Eremin et al., 2004). Another reason for choosing Sr_2RuO_4 is that the material has shown many interesting properties such as Spin-Triplet Superconductivity (Maeno et al., 2012) and it is relatively easy to produce high-quality crystals (Lichtenberg, 2002). It is therefore a focal point of great interest in the solid state physics and it is worthwhile to compute some of its properties.

We will further assume that the temperature approaches 0K and that the magnetisation $\mathbf{M}$ of the material is parallel to the z-axis.

Unless explicitly stated otherwise, in this chapter we will use the Hartree atomic units for which the electron mass m, the elementary charge e, the reduced Planck's constant $\hbar$ and the Coulomb's constant k_e are defined as identity.

With all these presumptions in mind we can now proceed to the calculations and the comparison of the models.

3.1 Adjusting the Středa model

The Středa model is easier to adjust to a different setting than the Kontani model. We will therefore adjust the Středa model to the conditions of the Kontani model. We will use the same Hamiltonian as before:

$$H = \frac{p^2}{2m} + V(\mathbf{r}) + H_{so} + H_z \tag{3.1}$$

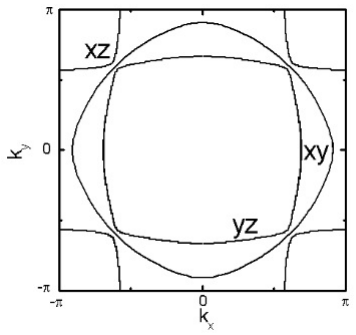

Figure 3.1: Fermi surface of Strontium ruthenate (Sr_2RuO_4) obtained by Eremin *et al.*

with

$$H_{so} = \frac{\lambda_c^2}{4\hbar}\boldsymbol{\sigma} \cdot [\nabla V(\mathbf{r}) \times \mathbf{p}] \tag{3.2}$$

$$H_z = -\mu_B \mathbf{B}_{eff} \cdot \boldsymbol{\sigma}. \tag{3.3}$$

However we will have to change the potential $V(\mathbf{r})$ to reflect on the fact that in the Kontani model we use a tight-binding Hamiltonian. In the tight-binding approximation we assume, that in the vicinity of the atom we can take the Hamiltonian of the atom as the nearly complete Hamiltonian of the system. Hence in the vicinity of the atom the potential is spherically symmetric. We will therefore assume the potential near the atom to be a function of the magnitude of distance from the center of the atom squared

$$V(\mathbf{r}) = f(r^2). \tag{3.4}$$

This is clearly not the case for the potential in the Sr_2RuO_4 crystal, nevertheless, since we are already using the tight-binding approximation in the Kontani model, we can assume that this approximation is reasonably accurate for the purpose of comparing the two models. If we chose some more general potential the calculations would likely become unmanageable and we would have to fill in too many details.

We can now express the spin-orbit interaction as

$$H_{so} = \frac{\lambda_c^2}{4\hbar}\boldsymbol{\sigma} \cdot [\nabla V(\mathbf{r}) \times \mathbf{p}] \tag{3.5}$$

$$= \frac{\lambda_c^2}{4\hbar}\frac{r}{r} f'(r^2)\boldsymbol{\sigma} \cdot [\mathbf{r} \times \mathbf{p}] \tag{3.6}$$

$$= \frac{\lambda_c^2}{4\hbar} f'(r^2)\boldsymbol{\sigma} \cdot \mathbf{L}, \tag{3.7}$$

where $f'(r^2) \equiv \left.\frac{df(u)}{du}\right|_{u=r^2}$. If we compare the last expression (3.7) with the equation (1.7) we see that

$$\frac{\lambda_c^2}{4\hbar} f'(r^2) = \lambda, \tag{3.8}$$

which has the same meaning as λ in the Kontani model.

The velocity expectation values are

$$\mathbf{v} = \frac{1}{i\hbar}[H, \mathbf{r}] \tag{3.9}$$

$$= \frac{\mathbf{p}}{m} + \frac{\lambda_c^2}{4\hbar}\boldsymbol{\sigma} \times \nabla V(\mathbf{r}) \tag{3.10}$$

$$= \frac{\mathbf{p}}{m} + \frac{\lambda_c^2}{4\hbar} f'(r^2)\boldsymbol{\sigma} \times \boldsymbol{r}. \tag{3.11}$$

From equation (3.11) we can express the x and y components of momentum as

$$p_x = mv_x - 2\lambda(\sigma_y z - \sigma_y y) \tag{3.12}$$

$$p_z = mv_z - 2\lambda(\sigma_x y - \sigma_y x) \tag{3.13}$$

In order to evaluate the force F_y we will evaluate commutation relations of each term in the Hamiltonian with the momentum in the y-direction p_y:

$$\left[p_y, \frac{p^2}{2m}\right] = 0 \tag{3.14}$$

$$[p_y, H_z] = 0 \tag{3.15}$$

$$[p_y, H_{so}] = \frac{\lambda_c^2}{4\hbar}[p_y, f'(r^2)\boldsymbol{\sigma}\cdot\mathbf{L}] \tag{3.16}$$

$$= \frac{\lambda_c^2}{4\hbar}\{[p_y, f'(r^2)]\sigma\cdot\mathbf{L} + f'(r^2)\sigma\cdot[p_y, \mathbf{L}]\} \tag{3.17}$$

$$= \frac{\lambda_c^2}{4\hbar}\{-i\hbar y f''(r^2)\boldsymbol{\sigma}\cdot\mathbf{L} + i\hbar f'(r^2)(\sigma_z p_x - \sigma_x p_z)\} \tag{3.18}$$

$$= -\frac{i\hbar y f''(r^2)\lambda_c^2}{4\hbar}\boldsymbol{\sigma}\cdot\mathbf{L} + i\hbar\lambda(\sigma_z p_x - \sigma_x p_z) \tag{3.19}$$

$$[p_y, V(\mathbf{r})] = -2i\hbar y f'(r^2) \tag{3.20}$$

$$= \frac{-8iy\hbar^2\lambda}{\lambda_c^2} \tag{3.21}$$

Putting it all together and using equations (3.12) - (3.13) we get

$$F_y = \frac{1}{i\hbar}[p_y, H] \tag{3.22}$$

$$= \frac{-8y\hbar\lambda}{\lambda_c^2} - \frac{y f''(r^2)\lambda_c^2}{4\hbar}\boldsymbol{\sigma}\cdot\mathbf{L} + \lambda(\sigma_z p_x - \sigma_x p_z) \tag{3.23}$$

$$= \frac{-8y\hbar\lambda}{\lambda_c^2} - \frac{y f''(r^2)\lambda_c^2}{4\hbar}\boldsymbol{\sigma}\cdot\mathbf{L} + \lambda\sigma_z[mv_x - 2\lambda(\sigma_y z - \sigma_y y)] - \\ - \lambda\sigma_x[mv_z - 2\lambda(\sigma_x y - \sigma_y x)] \tag{3.24}$$

Now, as we are only interested in movement in the $x-y$ plane, we will restrict the movement along the z axis. This means that we will set the expectation values of z and v_z to zero.

Since λ_c is of the order of 10^{-2}Bohrs and $\hbar = 1$ in the Hartree atomic units, and the second term in the equation (3.24) is approximately λ_c^4 times smaller than the first one, we will neglect the term completely.

Using the multiplication rules for the Pauli matrices we thus arrive at the expression for force:

$$F_y = y\left[4\lambda^2 - \frac{8\hbar\lambda}{\lambda_c^2}\right] + \lambda\sigma_z m v_x - i\lambda^2\sigma_z m x \tag{3.25}$$

In the static case the force is zero. From the real part of equation (3.25) we therefore obtain the equation for the mass-center separation $\Delta Y_\alpha(k_x)$:

$$\Delta Y_\alpha(k_x) = \left[\frac{8\hbar}{\lambda_c^2} - 4\lambda\right]^{-1}\sigma_z m v_x(k_x) \tag{3.26}$$

By inserting the mass-center separation (3.26) into the equation (2.13) we obtain the contribution of the α state to the anomalous Hall conductivity:

$$\sigma_{xy}^\alpha = -\frac{2e^2}{h}\left[\frac{8\hbar}{\lambda_c^2} - 4\lambda\right]^{-1}\sigma_z m v_x(k_F) \tag{3.27}$$

We obtain the anomalous Hall conductivity by summing over the contributions from all the states. In the case of our model we take into consideration two states - d_{yz} and d_{xz} orbitals. The velocities corresponding to these states are $v^{xz}(k_x, k_y) = 0$ and $v^{xz}(k_x, k_y) = 2t \sin k_x$. Therefore in the Středa model there will be non-zero contribution to the anomalous Hall conductivity only from the d_{xz} orbital.

Furthermore, since we assume our model to be two-dimensional, we need to integrate the conductivity over half of the Fermi surface with $k_x > 0$ to get the total conductivity. We therefore have:

$$\sigma_{xy}^{\alpha} = -\frac{e^2}{h} \frac{4\sigma_z mt}{\frac{8\hbar}{\lambda_c^2} - 4\lambda} \int dk\ \theta(k_x)\delta(k^2 - k_F^2) \sin k_x. \tag{3.28}$$

As a final touch we can use the equation (3.8) to adjust the denominator in the expression for the anomalous Hall conductivity:

$$\sigma_{xy}^{\alpha} = -\frac{e^2}{h} \frac{\lambda\sigma_z mt}{2f'(r^2) - 4\lambda^2} \int dk\ \theta(k_x)\delta(k^2 - k_F^2) \sin k_x. \tag{3.29}$$

The parameter $f'(r^2)$ is completely at our disposal, so we will determine its value by the requirement that the anomalous Hall conductivity obtained through the Středa model be comparable with the Kontani model.

3.2 Kontani model

There is no need to alter the Kontani model in any way. We are comparing only the intrinsic contribution to the anomalous Hall effect, so we will use the equations (2.46 - 2.48):

$$\sigma_{xy}^{I} = \lambda \frac{e^2\hbar}{\Omega} \sum_{\mathbf{k}} v_x v_y \frac{\delta(\mu - E_{\mathbf{k}}^{+}) + \delta(\mu - E_{\mathbf{k}}^{-})}{(E_{\mathbf{k}}^{+} - E_{\mathbf{k}}^{-})^2} \tag{3.30}$$

$$\sigma_{xy}^{IIa} = -\lambda \frac{e^2\hbar}{\Omega} \sum_{\mathbf{k}} v_x v_y \frac{\delta(\mu - E_{\mathbf{k}}^{+}) + \delta(\mu - E_{\mathbf{k}}^{-})}{(E_{\mathbf{k}}^{+} - E_{\mathbf{k}}^{-})^2} \tag{3.31}$$

$$\sigma_{xy}^{IIb} = 2\lambda \frac{e^2\hbar}{\Omega} \sum_{\mathbf{k}} v_x v_y \frac{-\theta(\mu - E_{\mathbf{k}}^{+}) + \theta(\mu - E_{\mathbf{k}}^{-})}{(E_{\mathbf{k}}^{+} - E_{\mathbf{k}}^{-})^3} \tag{3.32}$$

Since the terms σ^{I} and σ^{IIa} cancel each other out we do need to compute only the term σ^{IIb}. In order to perform the calculations we will change the sum over the wave vectors k into the integral:

$$\sigma_{xy}^{IIb} = 2\lambda \frac{e^2\hbar 4\pi^2}{a} \int_{BZ} dk\ v_x v_y \frac{-\theta(\mu - E_{\mathbf{k}}^{+}) + \theta(\mu - E_{\mathbf{k}}^{-})}{(E_{\mathbf{k}}^{+} - E_{\mathbf{k}}^{-})^3}, \tag{3.33}$$

where we integrate over the first Brillouin zone.

3.3 Results

In order to obtain the results we first need to fill in a few constants. We have used the length of the unit cell $a = 4\mathring{A}$ and the ratio $t/t' = 0.1$. Both the constants were chosen to represent Strontium Ruthenate - Sr_2RuO_4.

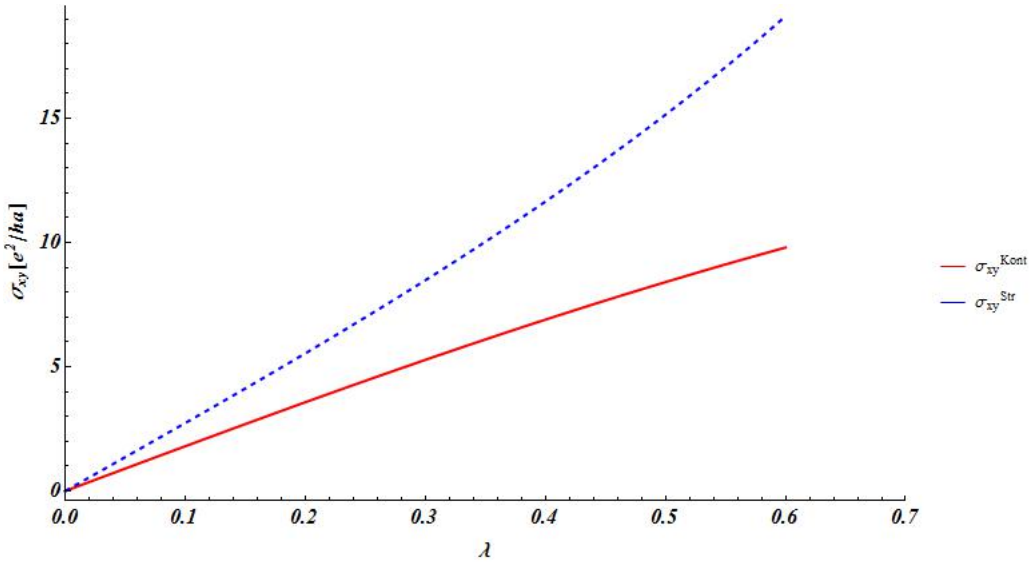

Figure 3.2: Calculated anomalous Hall conductivities as a function of spin-orbit coupling constant λ for density of states $n = 0.4$. The dashed line represents the conductivity obtained through the Středa model, the full line represents the conductivity obtained through the Kontani model.

In the Středa model we need to fix the derivation of the potential, so that it suits our calculations. We therefore chose $f'(r^2) = 10E_h/a_0$, so that the conductivity calculated via the Středa model is comparable with the conductivity calculated via the Kontani model.

We have used Mathematica to numerically evaluate the integrals and to graphically present the obtained results.

In figures 3.2 to 3.5 are calculated anomalous Hall conductivities as functions of the spin-orbit coupling constant λ for values of state densities $n = 0.4$ 0.8 1.2 and 1.6.

In figures 3.6-3.8 are calculated anomalous Hall conductivities as functions of the density of states n for values of the spin-orbit interaction $\lambda = 0.05$ 0.2 and 0.4.

Evaluation of the results We can see from the graphs that the conductivities calculated via the Středa model and via the Kontani model have generally very similar behaviour. This is not surprising as the (non-zero) conductivity contributions in both the models have been recognised as the contributions coming from the Berry curvature and it is to be expected that they behave similarly.

There are however some differences which we presume come out due to the fact that we are applying two theoretical models made with different assumptions to the same conditions. In this case we had to bend the conditions for the Středa model to be able to calculate the conductivity it predicts.

Let us now briefly review the basic premises of the two models. In the Středa model the anomalous velocity comes about from the different chemical potentials of the states in the same band with the opposite velocity in x-direction. The Středa model therefore takes into account the Fermi surface contribution to the

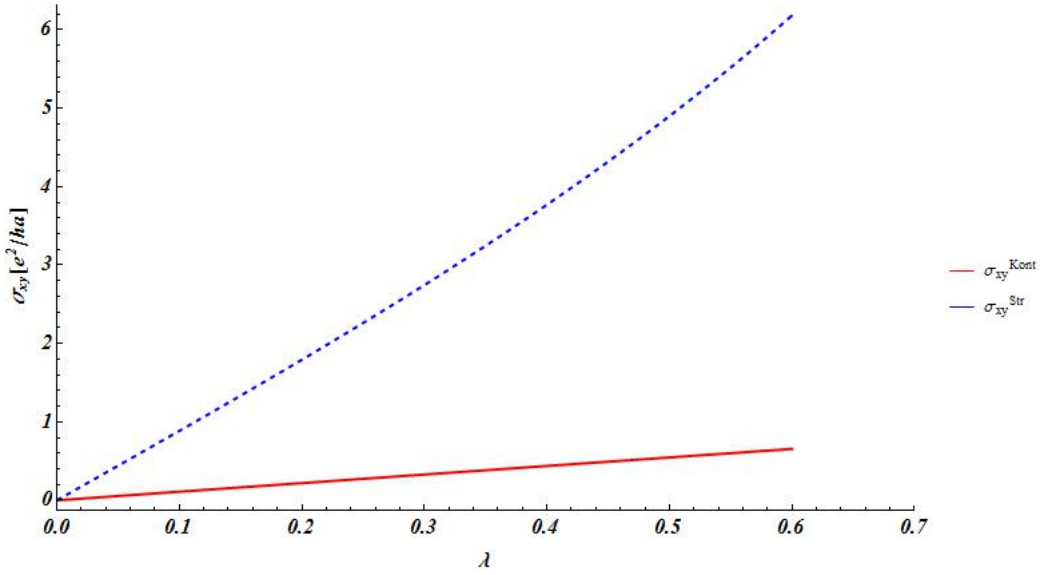

Figure 3.3: Calculated anomalous Hall conductivities as a function of spin-orbit coupling constant λ for density of states $n = 0.8$. The dashed line represents the conductivity obtained through the Středa model, the full line represents the conductivity obtained through the Kontani model.

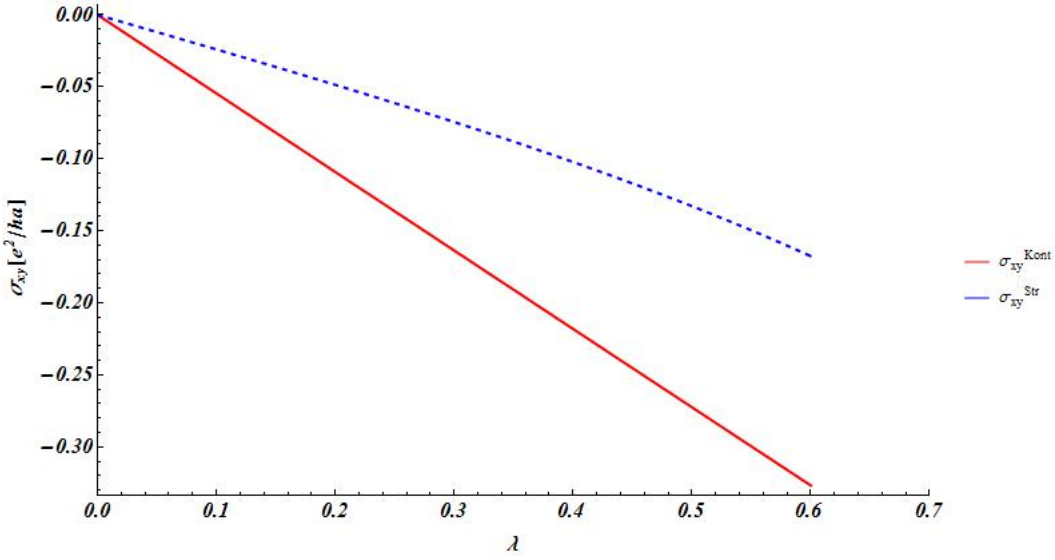

Figure 3.4: Calculated anomalous Hall conductivities as a function of spin-orbit coupling constant λ for density of states $n = 1.2$. The dashed line represents the conductivity obtained through the Středa model, the full line represents the conductivity obtained through the Kontani model.

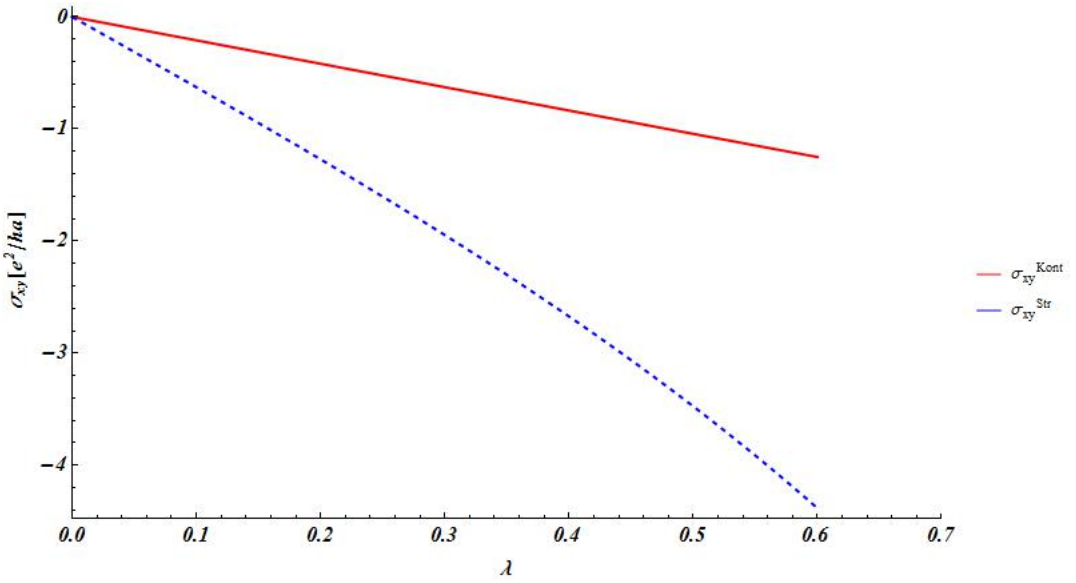

Figure 3.5: Calculated anomalous Hall conductivities as a function of spin-orbit coupling constant λ for density of states $n = 1.6$. The dashed line represents the conductivity obtained through the Středa model, the full line represents the conductivity obtained through the Kontani model.

conductivity and it does not need the interband hopping to emerge. On the other hand in the Kontani model the anomalous velocity comes about from the interband hopping and it is related to the Fermi sea. The models are therefore very different in terms of the basic assumptions which are implied in either of them.

From the graphs of the anomalous Hall conductivities as functions of the spin-orbit coupling constant λ we see that the magnitudes of the conductivities grow monotonically with the spin-orbit coupling constant λ. This is to be expected as the anomalous Hall effect is caused by the spin-orbit coupling.

From the graphs of the anomalous Hall conductivities as functions of the electron densities we also see that the conductivities change the sign near the unit electron density. This is in accordance with both the results obtained by Kontani (Kontani et al., 2007) and the experimental results (Fang et al., 2003).

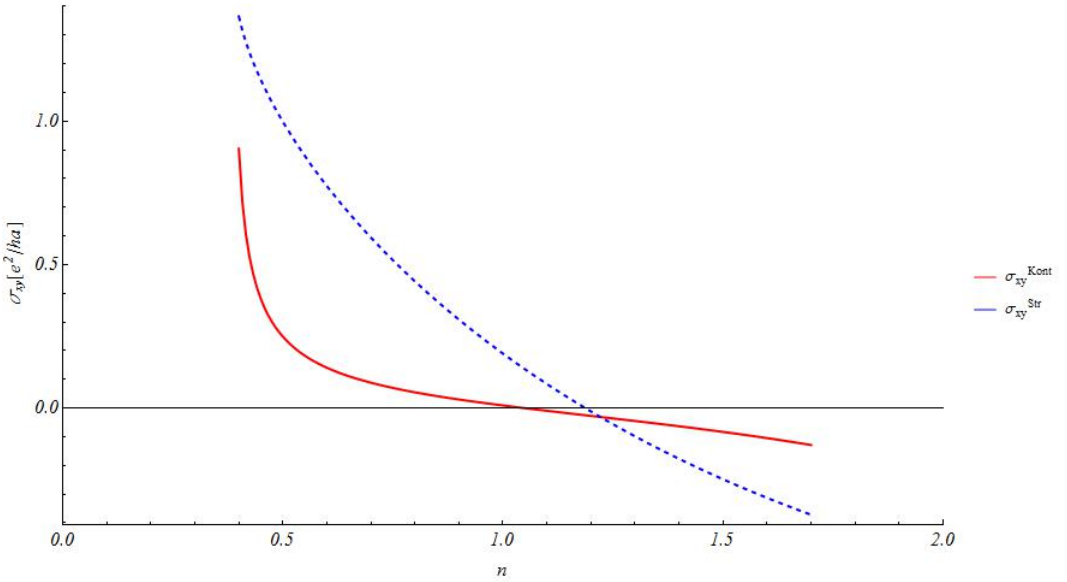

Figure 3.6: Calculated anomalous Hall conductivities in dependence on density of states n for spin-orbit coupling constant $\lambda = 0.05$. The dashed line represents the conductivity obtained through the Středa model, the full line represents the conductivity obtained through the Kontani model.

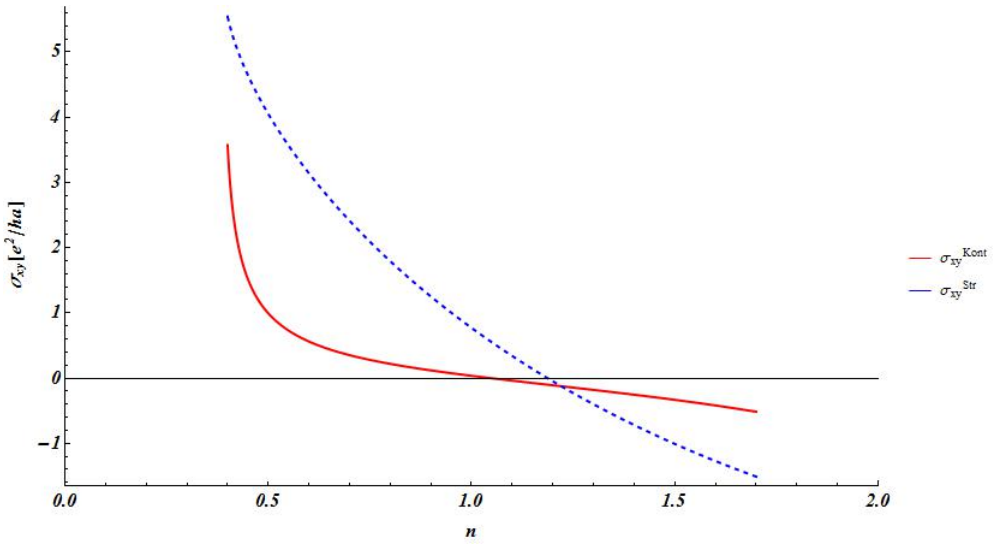

Figure 3.7: Calculated anomalous Hall conductivities in dependence on density of states n for spin-orbit coupling constant $\lambda = 0.2$. The dashed line represents the conductivity obtained through the Středa model, the full line represents the conductivity obtained through the Kontani model.

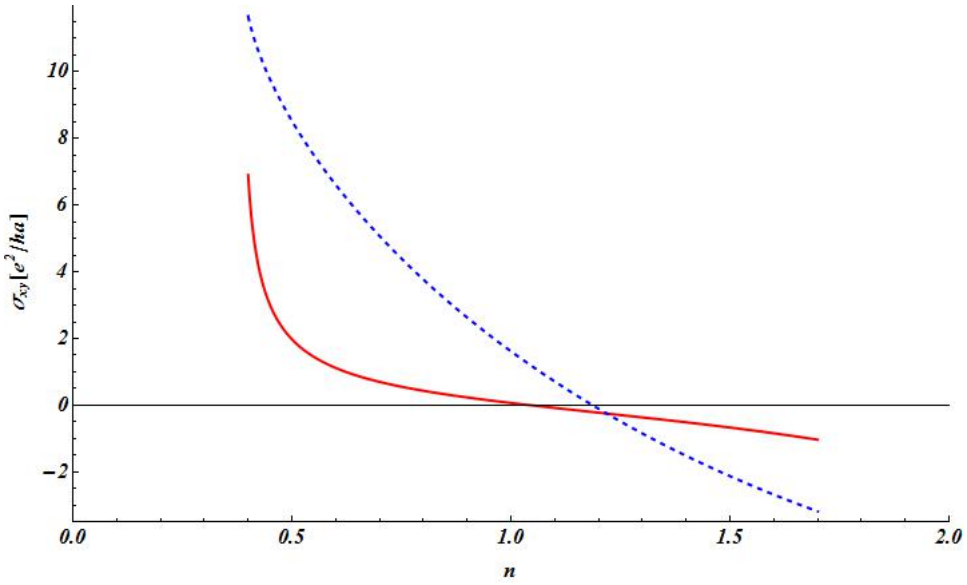

Figure 3.8: Calculated anomalous Hall conductivities in dependence on density of states n for spin-orbit coupling constant $\lambda = 0.4$. The dashed line represents the conductivity obtained through the Středa model, the full line represents the conductivity obtained through the Kontani model.

Conclusions

The objective of this work was to introduce one of the many effects that have their origin in the spin-orbit interaction. Our effect of choice was the anomalous Hall effect. This effect is an interesting topic of research since for a long time it has been mired in controversy and even now there are very few good models describing it. The anomalous Hall effect is also of growing importance in the solid state physics due to the advent of spintronics.

In the first chapter we have shortly summarised all the necessary approximations and frameworks for the description of the intrinsic anomalous Hall effect. We have chosen to describe the AHE with the help of the Kubo-Středa formula. We have also discussed the description of the AHE in the language of the Boltzmann formalism and the different types of the contributions to the anomalous Hall conductivity - we have described the intrinsic, skew-scattering and the side jump contributions.

In the second chapter we have introduced two models dealing with intrinsic anomalous Hall effect - the Středa model and the Kontani model. We have derived both the models using the formalism laid out in the first chapter. The models are very different in terms of the underlying assumptions.

In Středa model the anomalous Hall conductivity comes about from the spacial separation of the states with the opposite longitudinal velocities and from a consequent chemical potential difference. In the Kontani model the anomalous Hall conductivity originates from the interband hopping between the d_{xz} and d_{yz} orbitals. The Kontani model is more general and its assumptions are closer to reality, while the Středa model is simple and readily applicable to a wider class of materials.

In the third chapter we have compared the two models. Despite the different structure of the models, for example the different number of orbitals in the basis and the different form of the anomalous Hall conductance formula, the models recover similar trends regarding the dependence on the magnitude of spin-orbit interaction and electron occupancy. This is important especially regarding the applicability of the Středa model, which can be doubted because of its more simple structure with only one orbital involved in the calculation.

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