Magnetotransport on 2D anisotropic Fermi surfaces

Bachelor's thesis

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Abstract

Knowing the conductivity tensor of a metal can be of great interest in characterizing the material for any practical use. The characterization process would be eased if one could find an analytical expression for the conductivity tensor or some general behaviour of the conductivity from knowing just the Fermi surface of the metal.The aim of this thesis is to calculate the conductivity tensor of normal metals under different conditions by use of the semiclassical Boltzmann equation. First, the Boltzmann equation will be solved in the free electron model for the three cases: no magnetic field, a transverse magnetic field, and a high magnetic field present in accordance with the Drude model [1] and the Hall effect [3, 5].

Next, expressions are found for the conductivity tensor for an arbitrary Fermi surface in both the zero-field and low-field limit of an applied magnetic field **B**, writing out these explicitly to second order in **B** by the method of Jones & Zener [2]. These will then be applied to the tight-binding model, where it will also be examined if the total curvature of the Fermi surface has some relation to the Hall conductivity. We will find that there seems to be no connection between the two.

The last part of the thesis will concentrate on solving the Boltzmann equation for a simple 2D Fermi surface being circular-shaped, like in the free electron model, but with some additional distortion described by a harmonic function weighted with some small factor. This is relying on the method of Smith & Højgaard [3] and will yield a conductivity tensor to exact order in **B**. The method will then be applied to a specific Fermi surface from the tight-binding model.

Contents

1 Introduction

In the semiclassical description of electrons as a gas of electron wave packets, the Boltzmann equation can be used to calculate the conductivity by solving for the distribution function. The characterization of a metal by its Fermi surface in reciprocal space is very useful for this purpose since, as we will see in this thesis, knowing the distribution function at the Fermi energy is sufficient to calculate the conductivity tensor.
This we will use to first derive the conductivity tensor in the free electron model for the three cases: no magnetic field, a transverse magnetic field, and a high magnetic field present. Then we will continue to the more general case of an arbitrary Fermi surface and find expressions for the conductivity tensor in zero magnetic field and in the limit of a low magnetic field, using the method of Jones & Zener [2]. Applying this to the tight-binding model, we will find the conductivity tensor up to second order in the magnetic field as a function of the chemical potential, which in our case determines the shape of the Fermi surface. With the importance of the Fermi surface in mind, one might get the impression that the shape of this constant-energy contour has an influence on the conductivity. In this thesis we will investigate whether the low-field Hall conductivity in the tight-binding model depends on the total curvature of the Fermi surface. Furthermore, we will solve the Boltzmann equation for closed orbits on a simple 2D Fermi surface, parametrized by the length of the wave vector: $k(\varepsilon, \phi) = k_0(\varepsilon) + k_1(\varepsilon)\cos(q\phi)$, ϕ being the azimuthal angle in (k_x, k_y)-plane, ε the energy of the electron, and $q \in \mathbb{N}$. This we will do without making any approximations in the magnetic field, following the method of Smith & Højgaard [3]. Using this approach, we will discover that we can find the conductivity tensor just from knowing the shape of the Fermi surface without having to know the energy function $\varepsilon(\mathbf{k})$. Finally, we will apply this method to a specific Fermi surface in the tight-binding model to find the conductivity to exact order in the magnetic field and compare the high-field limit of this result with the high-field Hall effect.

2 The Boltzmann equation

The central equation throughout this thesis will be the semiclassical Boltzmann equation, which therefore deserves a short introduction. The derivation of the equation can be seen in App. A and we take as a starting point:

$$\frac{\partial f}{\partial t} + \dot{\mathbf{r}} \cdot \frac{\partial f}{\partial \mathbf{r}} + \dot{\mathbf{k}} \cdot \frac{\partial f}{\partial \mathbf{k}} = \left(\frac{\partial f}{\partial t}\right)_{coll}.$$

Here f denotes the non-equilibrium distribution function, $\mathbf{r}$ is the position vector and $\mathbf{k}$ the wave vector of the electron wave packet[1], $\left(\frac{\partial f}{\partial t}\right)_{coll}$ is the collision integral, and dot denotes the derivative with respect to time t. The equilibrium distribution function, f_0, is the Fermi-Dirac distribution function (Eq. A.1, App. A). In the case of a stationary, homogeneous distribution function (that is, $\frac{\partial f}{\partial t} = \frac{\partial f}{\partial \mathbf{r}} = 0$), we have:

$$\dot{\mathbf{k}} \cdot \frac{\partial f}{\partial \mathbf{k}} = \frac{-e}{\hbar}(\mathbf{E} + \mathbf{v} \times \mathbf{B}) \cdot \frac{\partial f}{\partial \mathbf{k}} = \left(\frac{\partial f}{\partial t}\right)_{coll}, \tag{2.1}$$

where $\dot{\mathbf{k}}$ is written in terms of the Lorentz force on an electron with charge $-e$ and velocity $\mathbf{v}$, in an electric field $\mathbf{E}$ and a magnetic field $\mathbf{B}$. Next, we introduce the relaxation time approximation [1, p. 371] (RTA), which says that the collision integral is related to the difference in the

[1] In accordance with the semiclassical approach

distribution function from equilibrium, $g = f - f_0$, and the mean time, τ, between collisions, in the following way:

$$\left(\frac{\partial f}{\partial t}\right)_{coll} = -\frac{g}{\tau}. \tag{2.2}$$

Presuming that $|\mathbf{E}|$ is small so that the response to it is linear [1, p. 365]: $g \propto \mathbf{E}$, the $\mathbf{E}$-term in Eq. 2.1 can be rewritten as:

$$\frac{-e}{\hbar}\mathbf{E}\cdot\frac{\partial f}{\partial \mathbf{k}} = \frac{-e}{\hbar}\mathbf{E}\cdot\frac{\partial f}{\partial \varepsilon}\frac{\partial \varepsilon}{\partial \mathbf{k}} = -e\mathbf{E}\cdot\mathbf{v}\frac{\partial f_0}{\partial \varepsilon}.$$

In the second equality, we have used that $g \propto \mathbf{E}$ to linearise in the electric field since f_0 is independent of $\mathbf{E}$. Throughout this thesis, we will only be working with a constant small electric field. Thus, the stationary, homogeneous Boltzmann equation, in the RTA (Eq. 2.2), reads:

$$-e\mathbf{E}\cdot\mathbf{v}\frac{\partial f_0}{\partial \varepsilon} - \frac{e}{\hbar}(\mathbf{v}\times\mathbf{B})\cdot\frac{\partial f}{\partial \mathbf{k}} = \frac{-g}{\tau}. \tag{2.3}$$

Solving the Boltzmann equation for f, one can calculate the electric current density in a d-dimensional system:

$$\mathbf{j} = \frac{-2e}{(2\pi)^d}\int \mathrm{d}^d\mathbf{k}\,\mathbf{v}f(\mathbf{k}). \tag{2.4}$$

The factor of 2 in the nominator is to include spin. Since the current in thermal equilibrium is zero, we are free to use $g = f - f_0$ instead of f. All calculations in this thesis are done for two-dimensional systems. Once we have found j_μ, the current density in the $\hat{\boldsymbol{\mu}}$-direction due to an electric field in the $\hat{\boldsymbol{\nu}}$-direction, we also know the conductivity tensor $\sigma_{\mu\nu}$.

3 The free electron model

We start by finding the conductivity tensor in Sommerfeld's free electron model [2, p. 62-65] where the valence electrons are considered as free, independent particles with wave functions and corresponding energies:

$$\psi_i(\mathbf{r}) = \mathrm{e}^{i\mathbf{k_i}\cdot\mathbf{r}}, \qquad \varepsilon_{\mathbf{k}_i} = \frac{\hbar^2\mathbf{k}_i^2}{2m}. \tag{3.1}$$

The model completely ignores electron-electron and electron-phonon interactions. In this section, we will use the Boltzmann equation in the form of Eq. 2.3 to find the conductivity from the current density (Eq. 2.4) in three different cases: no magnetic field, a transverse magnetic field, and a high magnetic field present.

3.1 Conductivity in zero magnetic field in the free electron model

In the case of an electric field $\mathbf{E}$ and zero magnetic field ($\mathbf{B} = \mathbf{0}$), the stationary, homogeneous Boltzmann equation in the RTA reads:

$$e\mathbf{E}\cdot\mathbf{v}\Big(-\frac{\partial f_0}{\partial \varepsilon}\Big) = -\frac{g}{\tau}.$$

With this, we can calculate the current density, pursuing from Eq. 2.4:

$$\begin{aligned}\mathbf{j} &= \frac{-2e}{(2\pi)^2}\int \mathrm{d}^2\mathbf{k}\,\mathbf{v}g(\mathbf{k}) = \frac{e^2\tau}{2\pi^2}\int \mathrm{d}^2\mathbf{k}\,\mathbf{v}(\mathbf{E}\cdot\mathbf{v})\Big(-\frac{\partial f_0}{\partial \varepsilon}\Big)\\ &= \frac{e^2\tau}{2\pi^2}\int \mathrm{d}\varepsilon \oint \mathrm{d}k_\parallel\,\frac{1}{\hbar v}\mathbf{v}(\mathbf{E}\cdot\mathbf{v})\Big(-\frac{\partial f_0}{\partial \varepsilon}\Big) \approx \frac{e^2\tau}{2\pi^2}\oint_{k_F} \mathrm{d}k_\parallel\,\frac{1}{\hbar v}\mathbf{v}(\mathbf{E}\cdot\mathbf{v}).\end{aligned} \tag{3.2}$$

In the last equality we have used that $\left(-\frac{\partial f_0}{\partial \varepsilon}\right)$ is almost a delta function around ε_f, so that the integral becomes a line integral over only the $\mathbf{k}$s at the Fermi surface, with a length k_F. For the change of variables from (k_x, k_y) to $(\varepsilon, k_\|)$ see Sec. 4, Eqs. 4.2 to 4.4.
Now we are able to find the components of the conductivity tensor, starting with the element[2] $\sigma_{xx}^{(0)}$:

$$\sigma_{xx}^{(0)} E_x = \frac{e^2\tau}{2\pi^2} \oint_{k_F} \mathrm{d}k_\| \, \frac{1}{\hbar v} v_x (E v_x).$$

Using the free electron model (Eq. 3.1), $\mathbf{v} = \frac{1}{\hbar}\frac{\partial \varepsilon_{\mathbf{k}}}{\partial \mathbf{k}} = \frac{\hbar \mathbf{k}}{m}$, we get the result:

$$\sigma_{xx}^{(0)} E_x = \frac{e^2\tau}{2\pi^2} E \oint_{k_F} \mathrm{d}k_\| \, \frac{1}{\hbar\frac{\hbar k}{m}} \left(\frac{\hbar k_x}{m}\right)^2 = \frac{e^2\tau}{2\pi^2 m} E \int_0^{2\pi} \mathrm{d}\phi \, k_F \frac{k_F^2 cos^2(\phi)}{k_F} = \frac{e^2\tau}{2\pi^2 m} E k_F^2 \pi.$$

Here we have changed the integration variable to be instead the azimuthal angle ϕ in the (k_x, k_y)-plane and employed that k_F is a constant in the free electron model. In the calculation of $\sigma_{yy}^{(0)}$, the only difference is that the integral is now over $\sin^2(\phi)$ instead of $\cos^2(\phi)$ and so $\sigma_{yy}^{(0)} = \sigma_{xx}^{(0)}$. Regarding the off-diagonal terms, they both vanish since they contain the integral $\int_0^{2\pi} \mathrm{d}\phi \, \cos(\phi)\sin(\phi) = 0$. Hence, the conductivity tensor is:

$$\sigma_{\alpha\beta}^{(0)} = \frac{e^2 \tau k_F^2}{2\pi m} \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}.$$

Since we are looking at a 2D material, the number of states, N, is:

$$N = 2\frac{\pi k_F^2}{(\frac{2\pi}{L})^2} = \frac{1}{2\pi} k_F^2 L^2 \quad \Leftrightarrow \quad k_F^2 = 2\pi n, \tag{3.3}$$

where L is the length of the system, n is the electron concentration, and a factor of 2 arises from spin [5]. This means we can rewrite the conductivity as:

$$\sigma_{\alpha\beta}^{(0)} = \frac{e^2 n \tau}{m} \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}, \tag{3.4}$$

which is the well-known Drude model [1, p. 7].

3.2 Conductivity in a constant, transverse magnetic field in the free electron model

Now we look at the situation with both an electric field $\mathbf{E}$ and a constant, transverse magnetic field $\mathbf{B} = B\hat{\mathbf{z}}$:

$$-e\mathbf{v}\cdot\mathbf{E}\frac{\partial f_0}{\partial \varepsilon} - \frac{e}{\hbar}\mathbf{v}\times\mathbf{B}\cdot\frac{\partial f}{\partial \mathbf{k}} = \frac{-g}{\tau}. \tag{3.5}$$

This Boltzmann equation is linearised in $\mathbf{E}$ but not in $\mathbf{B}$ as $\mathbf{v}\times\mathbf{B}\cdot\frac{\partial f_0}{\partial \mathbf{k}} = \mathbf{v}\times\mathbf{B}\cdot\mathbf{v}\hbar\frac{\partial f_0}{\partial \varepsilon} = 0$. This also implies that we are free to write instead:

$$e\mathbf{v}\cdot\mathbf{E}\frac{\partial f_0}{\partial \varepsilon} = \frac{g}{\tau} + \frac{eB}{\hbar}\left(v_x\frac{\partial g}{\partial k_y} - v_y\frac{\partial g}{\partial k_x}\right), \tag{3.6}$$

[2] The superscript on σ is to be consistent with the notation later on by indicating that this is independent of B and hence to zeroth order in B.

where in the $\mathbf{v}\times\mathbf{B}$ term we have replaced $\frac{\partial f}{\partial \mathbf{k}}$ with $\frac{\partial g}{\partial \mathbf{k}}$ since adding $-\mathbf{v}\times\mathbf{B}\cdot\frac{\partial f_0}{\partial \mathbf{k}}$ is just adding zero. If we assume free particles ($\mathbf{v} = \frac{\hbar\mathbf{k}}{m}$) and start by considering an $\mathbf{E}$-field along the $\hat{\mathbf{x}}$-direction, we can make the ansatz [3, p. 105] that the solution to g is of the form: $g = ak_x + bk_y$. By insertion into Eq. 3.6, it is seen that this is indeed a solution provided a and b have certain values:

$$\frac{e\hbar}{m}k_x E\frac{\partial f_0}{\partial \varepsilon} = \frac{1}{\tau}(ak_x + bk_y) + \frac{eB}{m}(k_x b - k_y a) \Leftrightarrow$$
$$\frac{1}{\tau}(\tau\eta - a - \tau\omega_c b)k_x + \Big(\omega_c a - \frac{b}{\tau}\Big)k_y = 0.$$

Here $\omega_c = \frac{eB}{m}$ and $\eta = \frac{e\hbar E}{m}\frac{\partial f_0}{\partial \varepsilon}$. Since this must hold for all k_x and k_y, the coefficients in front of these must be zero independently, and so we get that:

$$b = \tau\omega_c a\,, \qquad a = \frac{\tau}{1+(\tau\omega_c)^2}\eta = \frac{\tau}{1+(\tau\omega_c)^2}\frac{e\hbar E}{m}\frac{\partial f_0}{\partial \varepsilon}.$$

We can now to find the conductivity tensor that includes the effects of a non-zero $\mathbf{B}$-field, starting with σ_{xx}:

$$\begin{aligned}
\sigma^B_{xx}E_x &= \frac{-2e}{(2\pi)^2}\int \mathrm{d}^2\mathbf{k}\, v_x g = \frac{-e}{2\pi^2}\int \mathrm{d}^2\mathbf{k}\,\frac{\hbar k_x}{m}a(k_x + \omega_c\tau k_y)\\
&= \frac{e\hbar}{2\pi^2 m}\frac{\tau}{1+(\omega_c\tau)^2}\frac{e\hbar E}{m}\int \mathrm{d}^2\mathbf{k}\Big(-\frac{\partial f_0}{\partial \varepsilon}\Big)k_x^2\\
&= \frac{e^2\hbar^2\tau E}{2\pi^2 m^2}\frac{1}{1+(\omega_c\tau)^2}\int \mathrm{d}\varepsilon \oint \mathrm{d}k_\parallel\,\frac{1}{\hbar v}k_x^2\Big(-\frac{\partial f_0}{\partial \varepsilon}\Big)\\
&= \frac{e^2\hbar^2\tau E}{2\pi^2 m^2}\frac{1}{1+(\omega_c\tau)^2}\oint_{k_F}\mathrm{d}k_\parallel\,\frac{1}{\hbar\frac{\hbar k}{m}}k_x^2\\
&= \frac{e^2\tau E}{2\pi^2 m}\frac{1}{1+(\omega_c\tau)^2}\int_0^{2\pi}\mathrm{d}\phi\, k_F\frac{k_F^2\cos^2(\phi)}{k_F} = \frac{e^2\tau}{2\pi m}k_F^2\frac{1}{1+(\omega_c\tau)^2}E.
\end{aligned} \tag{3.7}$$

The reason why the $k_x k_y$ term in the integrand has been left out already in the second line, is that it is an odd function in ϕ and therefore the integral would just be zero. Using $k_F^2 = 2\pi n$ from Eq. 3.3 we can write the conductivity as:

$$\sigma^B_{xx} = \frac{e^2 n\tau}{m}\frac{1}{1+(\omega_c\tau)^2}.$$

For σ^B_{yx} the only difference is that is has an additional factor $\omega_c\tau$ since the integral is now on the form: $\int \mathrm{d}^2\mathbf{k}\,\omega_c\tau a k_y^2$. If we instead try with an $\mathbf{E}$-field in the $\hat{\mathbf{y}}$-direction and again guess on the solution: $g = ck_x + dk_y$, we get the conditions for the coefficients:

$$\frac{e\hbar}{m}k_y E\frac{\partial f_0}{\partial \varepsilon} = \frac{1}{\tau}(ck_x + dk_y) + \frac{eB}{m}(k_x d - k_y c) \implies$$

$$c = -\omega_c\tau d\,, \qquad d = \frac{\tau}{1+(\omega_c\tau)^2}\eta = a.$$

So for σ^B_{iy} we have:

$$\sigma^B_{iy}E_y = \frac{-e\hbar}{2\pi^2 m}\int d^2\mathbf{k}\, k_i(-bk_x + ak_y),$$

which means $\sigma^B_{xy} = -\sigma^B_{yx}$ and $\sigma^B_{yy} = \sigma^B_{xx}$. Hence, the conductivity tensor in the free electron model, with a transverse **B**-field through the material, is:

$$\sigma^B_{\alpha\beta} = \frac{e^2 n\tau}{m}\begin{bmatrix} \frac{1}{1+(\omega_c\tau)^2} & \frac{-\omega_c\tau}{1+(\omega_c\tau)^2} \\ \frac{\omega_c\tau}{1+(\omega_c\tau)^2} & \frac{1}{1+(\omega_c\tau)^2} \end{bmatrix}. \tag{3.8}$$

The change from the conductivity tensor in the Drude model (Eq. 3.4) to that in Eq. 3.8, in which the conductivity depends on B, is due to the Hall effect.

3.3 High-field Hall effect

When the period, T, of the cyclotron orbit of the electron is much smaller than τ it is possible to neglect the collision effects on the distribution function [3, p. 119]. Then, with an **E**-field in the $\hat{\mathbf{x}}$-direction and a **B**-field in the $\hat{\mathbf{z}}$-direction, the Boltzmann equation 3.5 becomes:

$$-eEv_x\frac{\partial f_0}{\partial \varepsilon} - \frac{eB}{\hbar}\Big(v_y\frac{\partial g}{\partial k_x} - v_x\frac{\partial g}{\partial k_y}\Big) = 0.$$

A solution [3, p. 119] to g is $g = ak_y$ if $a = \frac{E\hbar}{B}\frac{\partial f_0}{\partial \varepsilon}$. This yields a current density in the $\hat{\mathbf{y}}$-direction:

$$j_y = -2e\int \frac{\mathrm{d}^2\mathbf{k}}{(2\pi)^2}\frac{\partial \varepsilon}{\partial k_y}k_y\frac{\partial f_0}{\partial \varepsilon}\frac{E}{B} = \frac{-2eE}{B}\int \frac{\mathrm{d}^2\mathbf{k}}{(2\pi)^2}\,k_y\frac{\partial f_0}{\partial k_y}.$$

Assuming that the Fermi surface is only inside the first Brillouin zone[3], partial integration with respect to k_y yields:

$$\begin{aligned} j_y &= \frac{-2eE}{B}\left(\int \mathrm{d}k_x \overbrace{\left[\frac{1}{(2\pi)^2}k_y f_0\right]_{FBZ}}^{\text{zero as } f_0=0 \text{ at the edge of FBZ}} - \int_{FBZ}\frac{\mathrm{d}^2\mathbf{k}}{(2\pi)^2}\frac{\partial k_y}{\partial k_y}f_0\right) \\ &= \frac{2eE}{B}\int_{FBZ}\frac{\mathrm{d}^2\mathbf{k}}{(2\pi)^2}\,f_0 = \frac{eE}{B}\int_0^\infty \mathrm{d}\varepsilon\,\rho(\varepsilon)f_0 = \frac{en}{B}E, \end{aligned}$$

where $\rho(\varepsilon)$ is the density of states, including spin states. Hence, $\sigma_{yx} = \frac{en}{B}$ in the high-field limit. This is a general result which does not only apply to the free electron model and is derived in App. F. For $\mathbf{E} = E\hat{\mathbf{y}}$, the solution to g is $g = bk_x$ with $b = -a = -\frac{E\hbar}{B}\frac{\partial f_0}{\partial \varepsilon}$ so that $\sigma_{xy} = -\sigma_{yx}$. Regarding the diagonal terms, they are zero as they are integrals of the type:

$$\int_{FBZ}\mathrm{d}k_i\,k_i\int_{FBZ}\mathrm{d}k_j\,\frac{\partial f_0}{\partial k_j} = \int_{FBZ}\mathrm{d}k_i\,k_i\Big[f_0(k_j)\Big]_{k_j=-\pi/a}^{k_j=\pi/a} = 0.$$

Having $T \ll \tau$ corresponds to letting $\omega_c\tau \to \infty$ or equivalently $B \to \infty$. Implying this on the conductivity tensor in Eq. 3.8 indeed yields $-\sigma_{xy} = \sigma_{yx} = \frac{en}{B}$ and $\sigma_{xx} = \sigma_{yy} = 0$.

4 Conductivity in zero magnetic field for an arbitrary Fermi surface

Now that we know how to handle the free electron model, we continue with more complicated Fermi surfaces. We still have the general expression for the current density in absence of a

[3]That is, $-\pi/a < k_F^x, k_F^y > \pi/a$ (FBZ), with a being the lattice constant.

magnetic field:

$$j_i = \frac{e^2\tau}{2\pi^2}\int \mathrm{d}^2\mathbf{k}\Big(-\frac{\partial f_0}{\partial \varepsilon}\Big)v_i v_j E_j. \tag{4.1}$$

As in Eqs. 3.2 and 3.7, we want to change the integration variables from (k_x, k_y) to $(\varepsilon, k_{\|})$. This, we show how to do with a general function $h(\varepsilon)$:

$$\int \mathrm{d}k_x \int \mathrm{d}k_y\, h(\varepsilon) = \int \mathrm{d}\omega \int \mathrm{d}k_x \int \mathrm{d}k_y\, \delta(\omega-\varepsilon)h(\omega). \tag{4.2}$$

We use the rewriting of a δ-function:

$$\delta(f(x)) = \sum_i \frac{\delta(x-x_i)}{\Big|\frac{\partial f}{\partial x}\Big|_{x=x_i}} \qquad \Longrightarrow$$

$$\delta(\omega-\varepsilon) = \sum_i \frac{\delta(\mathbf{k}-\mathbf{k}_i)}{\Big|\frac{\partial \varepsilon}{\partial \mathbf{k}}\Big|_{\mathbf{k}=\mathbf{k}_i}} = \sum_i \frac{\delta(\mathbf{k}-\mathbf{k}_i)}{\hbar v(\mathbf{k}_i)}. \tag{4.3}$$

Here $\mathbf{k}_i(\varepsilon)$ are the roots of $(\omega-\varepsilon)$ that is, the wave vectors with corresponding energy $\varepsilon=\omega$. By inserting Eq. 4.3 into Eq. 4.2 and setting $\omega \equiv \varepsilon$, one gets:

$$\begin{aligned}\int \mathrm{d}k_x \int \mathrm{d}k_y\, h(\varepsilon) &= \int \mathrm{d}\varepsilon \int \mathrm{d}k_x \int \mathrm{d}k_y\, h(\varepsilon)\sum_i \frac{\delta(\mathbf{k}-\mathbf{k}_i)}{\hbar v(\mathbf{k}_i)} \\ &= \int \mathrm{d}\varepsilon \oint \mathrm{d}k_{\|}\,\frac{1}{\hbar v}h(\varepsilon). \end{aligned}\tag{4.4}$$

In the last line we have used that, since $\mathbf{k}_i(\varepsilon)$ are the wave vectors corresponding to the energy $\varepsilon=\omega$, the δ-function, for every ε, picks out only the $\mathbf{k}$s with that particular energy, that is, only the $\mathbf{k}_{\|}$s at that energy contour.
So we are ready to rewrite Eq. 4.1 in terms of the new variables:

$$\begin{aligned} j_i = \frac{e^2\tau}{2\pi^2}\int \mathrm{d}\varepsilon \oint \mathrm{d}k_{\|}\,\frac{1}{\hbar v}\Big(-\frac{\partial f_0}{\partial \varepsilon}\Big)v_i v_j E_j &= \frac{e^2\tau}{2\pi^2}\oint_{k_F} \mathrm{d}k_{\|}\,\frac{1}{\hbar v}v_i v_j E_j \\ \Longrightarrow \qquad \sigma_{ij}^{(0)} = \frac{e^2\tau}{2\pi^2\hbar^3}\oint_{k_F}\mathrm{d}k_{\|}\,\frac{1}{v}\frac{\partial \varepsilon}{\partial k_i}\frac{\partial \varepsilon}{\partial k_j}, \end{aligned}\tag{4.5}$$

employing $\Big(-\frac{\partial f_0}{\partial \varepsilon}\Big) \approx \delta(\varepsilon-\varepsilon_f)$. Furthermore, if the Fermi surface is symmetric around the k_i-axis, where $i = x, y$, components $\sigma_{ij}^{(0)}$ with $i \neq j$ will be zero due to the anti-symmetry of the function $\frac{\partial \varepsilon}{\partial k_j}$ and we get a δ_{ij}.[4] This zero-field result is also called the longitudinal conductivity [4].

5 Conductivity in a constant, transverse, weak magnetic field for an arbitrary Fermi surface

Putting on a constant $\mathbf{B}$-field, the Boltzmann equation reads, as in Eq. 2.3:

$$\frac{-e}{\hbar}(\mathbf{E}+\mathbf{v}\times\mathbf{B})\cdot\nabla_{\mathbf{k}}f(\mathbf{k}) = \frac{-g(\mathbf{k})}{\tau} \quad \Longrightarrow$$

[4]This can be realized by letting the axis of symmetry be eg. the $\mathbf{k_x}$-axis and recognize that for every $\mathbf{v}$ underneath the $\mathbf{k_x}$-axis there is a corresponding $\mathbf{v}'$ above the $\mathbf{k_x}$-axis with $v_x = v'_x$ and $v_y = -v'_y$.

$$-e\mathbf{E}\cdot\mathbf{v}\Big(\frac{\partial f_0}{\partial\varepsilon}\Big)-\frac{e}{\hbar}\mathbf{v}\times\mathbf{B}\cdot\nabla_{\mathbf{k}}g(\mathbf{k})=\frac{-g(\mathbf{k})}{\tau},\tag{5.1}$$

where we have linearised in $\mathbf{E}$ and used $-\mathbf{v}\times\mathbf{B}\cdot\nabla_{\mathbf{k}}f_0(\mathbf{k})=0$. This we will now solve using the method of Jones & Zener [2, p. 501][4]. Introducing the operator Q:

$$Q=\frac{-e\tau}{\hbar^2}(\nabla_{\mathbf{k}}\varepsilon)\times\mathbf{B}\cdot\nabla_{\mathbf{k}},$$

and inserting this into Eq. 5.1, one gets:

$$(1+Q)g(\mathbf{k})=\underbrace{\frac{-e\tau}{\hbar}\mathbf{E}\cdot(\nabla_{\mathbf{k}}\varepsilon)\Big(-\frac{\partial f_0}{\partial\varepsilon}\Big)}_{g_0(\mathbf{k})}.$$

Writing $g(\mathbf{k})$ as a geometric row:

$$g(\mathbf{k})=\frac{g_0(\mathbf{k})}{1+Q}=\sum_{n=0}^{\infty}(-Q)^n g_0(\mathbf{k})=g_0-Qg_0+Q^2g_0-Q^3g_0+\ldots,$$

the current density can be written:

$$\begin{aligned}\mathbf{j}&=-2e\int\frac{\mathrm{d}^2\mathbf{k}}{(2\pi)^2}\,\frac{1}{\hbar}(\nabla_{\mathbf{k}}\varepsilon)g(\mathbf{k})\\&=\frac{-e}{2\pi^2\hbar}\sum_{n=0}^{\infty}\int\mathrm{d}^2\mathbf{k}\,(\nabla_{\mathbf{k}}\varepsilon)\Big(\frac{e\tau}{\hbar^2}(\nabla_{\mathbf{k}}\varepsilon)\times\mathbf{B}\cdot\nabla_{\mathbf{k}}\Big)^n\Big(\frac{-e\tau}{\hbar}\mathbf{E}\cdot(\nabla_{\mathbf{k}}\varepsilon)\Big(-\frac{\partial f_0}{\partial\varepsilon}\Big)\Big)\\&=\frac{e^2\tau}{2\pi^2\hbar^2}\int\mathrm{d}^2\mathbf{k}\,(\nabla_{\mathbf{k}}\varepsilon)\mathbf{E}\cdot(\nabla_{\mathbf{k}}\varepsilon)\Big(-\frac{\partial f_0}{\partial\varepsilon}\Big)\\&+\frac{e^3\tau^2}{2\pi^2\hbar^4}\int\mathrm{d}^2\mathbf{k}\,(\nabla_{\mathbf{k}}\varepsilon)\Big((\nabla_{\mathbf{k}}\varepsilon)\times\mathbf{B}\cdot\nabla_{\mathbf{k}}\Big)\Big(\mathbf{E}\cdot(\nabla_{\mathbf{k}}\varepsilon)\Big(-\frac{\partial f_0}{\partial\varepsilon}\Big)\Big)+\ldots,\end{aligned}\tag{5.2}$$

where only terms up to first order in $\mathbf{B}$ are written explicitly. The current density can also be written in tensor notation:

$$\begin{aligned}j_\alpha&=\frac{e^2\tau}{2\pi^2\hbar^2}\int\mathrm{d}^2\mathbf{k}\,\Big(-\frac{\partial f_0}{\partial\varepsilon}\Big)\frac{\partial\varepsilon}{\partial k_\alpha}\frac{\partial\varepsilon}{\partial k_\beta}E_\beta\\&+\frac{e^3\tau^2}{2\pi^2\hbar^4}\int\mathrm{d}^2\mathbf{k}\,\Big(-\frac{\partial f_0}{\partial\varepsilon}\Big)\frac{\partial\varepsilon}{\partial k_\alpha}\epsilon_{\mu\delta\gamma}\frac{\partial\varepsilon}{\partial k_\delta}B_\gamma E_\beta\frac{\partial}{\partial k_\mu}\Big(\frac{\partial\varepsilon}{\partial k_\beta}\Big)+\ldots\\&=\sigma^{(0)}_{\alpha\beta}E_\beta+\sigma^{(1)}_{\alpha\beta\gamma}B_\gamma E_\beta+\ldots\end{aligned}$$

It is seen that $\sigma^{(0)}_{\alpha\beta}$ is just the zeroth-order conductivity found in Eq. 4.5. For small $\mathbf{B}$-fields, we can approximate the magnetoconductivity: $\sigma^B_{\alpha\beta}\simeq\sigma^{(1)}_{\alpha\beta\gamma}B_\gamma$. If we take $\mathbf{B}\parallel\hat{\mathbf{z}}$, the magnetoconductivity is:

$$\begin{aligned}\sigma^B_{\alpha\beta}&\simeq\frac{e^3\tau^2B}{2\pi^2\hbar^2}\int\mathrm{d}^2\mathbf{k}\,\Big(-\frac{\partial f_0}{\partial\varepsilon}\Big)v_\alpha\epsilon_{\mu\delta z}v_\delta\frac{\partial^2\varepsilon}{\partial k_\mu\partial k_\beta}\\&=\frac{e^3\tau^2B}{2\pi^2}\int\mathrm{d}\varepsilon\oint\mathrm{d}k_\parallel\,\frac{1}{\hbar v}\Big(-\frac{\partial f_0}{\partial\varepsilon}\Big)v_\alpha\epsilon_{\mu\delta z}v_\delta m^{-1}_{\mu\beta}\\&=\frac{e^3\tau^2B}{2\pi^2\hbar}\oint_{k_F}\mathrm{d}k_\parallel\,\frac{1}{v}v_\alpha\epsilon_{\mu\delta z}v_\delta m^{-1}_{\mu\beta}\\&=\frac{e^3\tau^2B}{2\pi^2\hbar}\oint_{k_F}\mathrm{d}k_\parallel\,\frac{1}{v}v_\alpha m^{-1}_{\beta\mu}\epsilon_{\mu\delta}v_\delta.\end{aligned}\tag{5.3}$$

Here, $m^{-1}_{\beta\mu}$ is the inverse mass tensor and $\epsilon_{\mu\delta}$ is the Levi-Cività symbol where we have suppressed the z-component in the last line since this is unnecessary as we are only letting μ and δ be x and y. If the Fermi surface has a symmetry axis along the k_x or k_y-axis, the corresponding $\sigma^{(1)}_{ii} = \sigma^{(0)}_{iiz}B_z$, where $i = x$ or $i = y$ respectively, will be zero. This is due to the anti-symmetric functions in the integral:

$$\sigma^{(1)}_{ii} \sim \oint_{k_F} \mathrm{d}k_\parallel \frac{1}{v}\frac{\partial\varepsilon}{\partial k_i}\Big(\frac{\partial^2\varepsilon}{\partial k_i^2}\frac{\partial\varepsilon}{\partial k_j} - \frac{\partial^2\varepsilon}{\partial k_i\partial k_j}\frac{\partial\varepsilon}{\partial k_i}\Big), i \neq j$$

If the Fermi surface is symmetric about both the k_x and the k_y-axis, the diagonal terms are both zero. The off-diagonal elements are called the Hall conductivity [4].

5.1 Magnetoconductivity to second order in B

Improving our expression for the conductivity, we can continue by looking at the term of second order in B in Eq. 5.2:

$$\mathbf{j}(\mathscr{O}(B^2)) = \frac{-e}{2\pi^2\hbar}\int \mathrm{d}^2\mathbf{k}(\nabla_\mathbf{k}\varepsilon)\Big(\frac{e\tau}{\hbar^2}(\nabla_\mathbf{k}\varepsilon)\times\mathbf{B}\cdot\nabla_\mathbf{k}\Big)^2\Big(\frac{-e\tau}{\hbar}\mathbf{E}\cdot(\nabla_\mathbf{k}\varepsilon)\Big(-\frac{\partial f_0}{\partial\varepsilon}\Big)\Big).$$

We can write this in tensor notation as:

$$\begin{aligned} j_\alpha(\mathscr{O}(B^2)) &= \frac{e^4\tau^3}{2\pi^2\hbar^6}\int \mathrm{d}^2\mathbf{k}\Big(-\frac{\partial f_0}{\partial\varepsilon}\Big)\frac{\partial\varepsilon}{\partial k_\alpha}\Big(\epsilon_{\zeta\eta\gamma}\frac{\partial\varepsilon}{\partial k_\eta}B_\gamma\frac{\partial}{\partial k_\zeta}\Big)\Big(\epsilon_{\lambda\nu\delta}\frac{\partial\varepsilon}{\partial k_\nu}B_\delta\frac{\partial}{\partial k_\lambda}\Big)\Big(E_\beta\frac{\partial\varepsilon}{\partial k_\beta}\Big) \\ &= \frac{e^4\tau^3}{2\pi^2\hbar^6}B_\gamma B_\delta E_\beta\int \mathrm{d}^2\mathbf{k}\Big(-\frac{\partial f_0}{\partial\varepsilon}\Big)\frac{\partial\varepsilon}{\partial k_\alpha}\Big(\epsilon_{\zeta\eta\gamma}\frac{\partial\varepsilon}{\partial k_\eta}\frac{\partial}{\partial k_\zeta}\Big)\Big(\epsilon_{\lambda\nu\delta}\frac{\partial\varepsilon}{\partial k_\nu}\frac{\partial^2\varepsilon}{\partial k_\lambda\partial k_\beta}\Big). \end{aligned}$$

Letting as usual $\mathbf{B} \parallel \hat{\mathbf{z}}$:

$$\begin{aligned} \sigma^{(2)}_{\alpha\beta} &= \frac{e^4\tau^3B^2}{2\pi^2\hbar^6}\int \mathrm{d}^2\mathbf{k}\Big(-\frac{\partial f_0}{\partial\varepsilon}\Big)\frac{\partial\varepsilon}{\partial k_\alpha}\epsilon_{\zeta\eta}\epsilon_{\lambda\nu}\frac{\partial\varepsilon}{\partial k_\eta}\Big(\frac{\partial^2\varepsilon}{\partial k_\zeta\partial k_\nu}\frac{\partial^2\varepsilon}{\partial k_\lambda\partial k_\beta} + \frac{\partial\varepsilon}{\partial k_\nu}\frac{\partial^3\varepsilon}{\partial k_\zeta\partial k_\lambda\partial k_\beta}\Big) \\ &= \frac{e^4\tau^3B^2}{2\pi^2\hbar^2}\oint_{k_F}\mathrm{d}k_\parallel\frac{1}{v}v_\alpha v_\eta\epsilon_{\zeta\eta}\epsilon_{\lambda\nu}\Big(\hbar m^{-1}_{\zeta\nu}m^{-1}_{\lambda\beta} + v_\nu\frac{\partial}{\partial k_\zeta}m^{-1}_{\lambda\beta}\Big). \end{aligned} \tag{5.4}$$

As in Eq. 5.3 we have suppressed the z-index on the Levi-Cività symbols, letting all indices be only x or y.

Having an $\mathbf{E}$-field in a direction making an angle θ with the $\hat{\mathbf{k_x}}$-direction as illustrated in Fig. 1, the current density in an angle Θ reads:

$$j_\Theta = E\cos(\Theta)(\sigma_{xx}\cos(\theta) + \sigma_{xy}\sin(\theta)) + E\sin(\Theta)(\sigma_{yx}\cos(\theta) + \sigma_{yy}\sin(\theta)). \tag{5.5}$$

To second order in $\mathbf{B}$, σ_{ij} can be replaced by the expressions found in this and the previous two sections.

6 The tight-binding model

We now want to apply the results of Secs. 4 and 5 to the tight-binding model [5, p. 235] in which the energy is given by:

$$\varepsilon_\mathbf{k} = -2t(\cos(ak_x) + \cos(ak_y)), \tag{6.1}$$

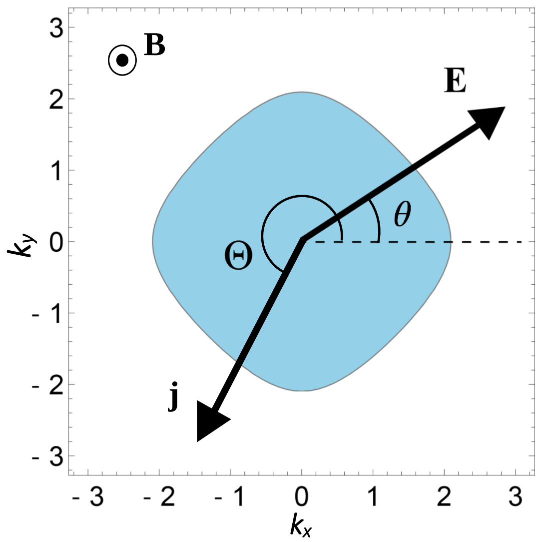

Figure 1: Sketch of a Fermi surface in $\mathbf{k}$-space together with a vector $\mathbf{E}$, representing the electric field, which makes an angle θ with the $\hat{\mathbf{k_x}}$-vector. Introducing also a magnetic field $\mathbf{B}$ in the $\hat{\mathbf{z}}$-direction, the current density $\mathbf{j}$ in an angle Θ is given by Eq. 5.5.

where t is the overlap energy, assumed to be equal in the $\hat{\mathbf{x}}$ and $\hat{\mathbf{y}}$-direction, and a is the lattice spacing. A contour plot of the energy for $(k_x, k_y) \in [-\pi, \pi]$, $a = t = 1$ is shown in Fig. 2. The contours correspond to Fermi surfaces at different values of the chemical potential μ which is equal to the Fermi energy as we are working at temperatures $Tk_B \ll \varepsilon_F$, where k_B is the Boltzmann constant and ε_F is the Fermi energy. Fig. 2 shows that as the chemical potential is increased, the Fermi surfaces evolve from being approximately circular, like in the free electron model, into becoming square-like (the Fermi surface is a perfect square at $\mu = 0$), before developing into shapes that enable hole-like orbits in the presence of a magnetic field. However, the Fermi surface always possesses C_4-symmetry, which simplifies the zeroth-order (Eq. 4.5) and first-order (Eq. 5.3) conductivity to the longitudinal and Hall conductivity respectively.

6.1 Longitudinal conductivity for the tight-binding model

Using Eq. 4.5 with the energy function given in Eq. 6.1, the longitudinal conductivity (or equivalently, the conductivity in absence of an external magnetic field) is:

$$\sigma_{ii}^{(0)} = \frac{e^2 \tau t a}{\pi^2 \hbar^2} \oint_{k_F} \mathrm{d}k_\parallel \frac{\sin^2(ak_i)}{\sqrt{\sin^2(ak_x) + \sin^2(ak_y)}}.$$

Expressing the ks at the Fermi surface with energy μ as: $k_x = k_F(\mu, \phi)\cos(\phi)$ and $k_y = k_F(\mu, \phi)\sin(\phi)$, the conductivity becomes:

$$\sigma_{ii}^{(0)}(\mu) = \frac{e^2 \tau t a}{\pi^2 \hbar^2} \int_0^{2\pi} \mathrm{d}\phi\, k_F(\mu, \phi) \frac{\sin^2(ak_i)}{\sqrt{\sin^2(ak_F(\mu, \phi)\cos(\phi)) + \sin^2(ak_F(\mu, \phi)\sin(\phi))}}. \quad (6.2)$$

In Fig. 3 the integral in Eq. 6.2 is plotted as a function of the chemical potential for both $\sigma_{xx}^{(0)}$ and $\sigma_{yy}^{(0)}$ which coincide as one would expect due to the equivalence of the $\hat{\mathbf{x}}$ and $\hat{\mathbf{y}}$-direction.

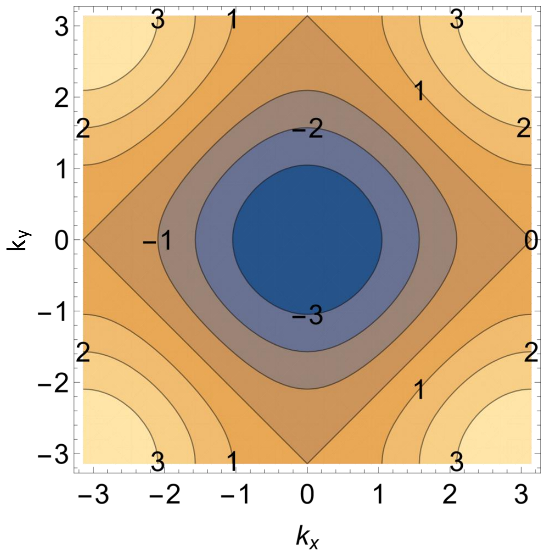

Figure 2: Energy contour plot for the tight-binding model $\varepsilon_{\mathbf{k}} = -2t(\cos(ak_x) + \cos(ak_y))$ in the range $(k_x, k_y) \in [-\pi, \pi]$ with $a = t = 1$.

The longitudinal conductivities grows with increasing chemical potential μ which is no surprise since the Fermi surface becomes larger as $\mu \to 0^-$, meaning a larger electron number density.

6.2 Hall conductivity for the tight-binding model

As mentioned, the Fermi surfaces have fourfold symmetry and so the magnetoconductivity contains no diagonal terms to first order in B. The off-diagonal terms, ie. the Hall conductivity components, are:

$$
\begin{aligned}
\sigma^H_{yx} &= \frac{e^3\tau^2 B}{2\pi^2\hbar} \oint_{k_F} \mathrm{d}k_\parallel \, \frac{1}{v} v_y m^{-1}_{x\mu} \epsilon_{\mu\delta} v_\delta \\
&= \frac{e^3\tau^2 B}{2\pi^2\hbar} \oint_{k_F} \mathrm{d}k_\parallel \, \frac{1}{v} v_y (m^{-1}_{xx} \epsilon_{xy} v_y + m^{-1}_{xy} \epsilon_{yx} v_x) \\
&= \frac{e^3\tau^2 B}{2\pi^2\hbar^4} \oint_{k_F} \mathrm{d}k_\parallel \, \frac{\hbar}{\sqrt{(\frac{\partial\varepsilon}{\partial k_x})^2 + (\frac{\partial\varepsilon}{\partial k_y})^2}} \frac{1}{\hbar} \frac{\partial\varepsilon}{\partial k_y} \Big(\frac{\partial^2\varepsilon}{\partial k_x^2} \frac{\partial\varepsilon}{\partial k_y} - \frac{\partial^2\varepsilon}{\partial k_x \partial k_y} \frac{\partial\varepsilon}{\partial k_x} \Big).
\end{aligned}
$$

$$
\frac{\partial\varepsilon}{\partial k_i} = 2ta\sin(ak_i)\,, \qquad \frac{\partial^2\varepsilon}{\partial k_i \partial k_j} = 0, i \neq j\,, \qquad \frac{\partial^2\varepsilon}{\partial k_i^2} = 2ta^2\cos(ak_i) \implies
$$

$$
\begin{aligned}
\sigma^H_{yx} &= \frac{e^3\tau^2 B}{2\pi^2\hbar^4} \oint_{k_F} \mathrm{d}k_\parallel \, \frac{2ta\sin(ak_y)}{2ta\sqrt{\sin^2(ak_x) + \sin^2(ak_y)}} 2ta^2\cos(ak_x) 2ta\sin(ak_y) \\
&= \frac{e^3\tau^2 B}{\pi^2\hbar^4} 2t^2a^3 \oint_{k_F} \mathrm{d}k_\parallel \, \frac{\sin^2(ak_y)\cos(ak_x)}{\sqrt{\sin^2(ak_x) + \sin^2(ak_y)}}. \qquad (6.3)
\end{aligned}
$$

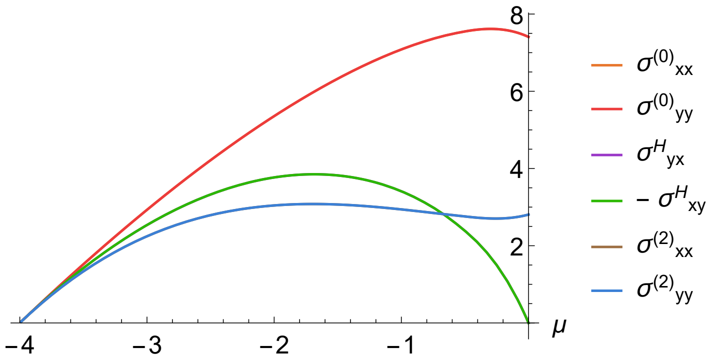

Figure 3: The integral in the expression for: the longitudinal conductivities $\sigma_{xx}^{(0)}$ and $\sigma_{yy}^{(0)}$ (orange and red (coincide)), the Hall conductivities σ_{yx}^{H} and $-\sigma_{xy}^{H}$ (purple and green (coincide)), and the second-order conductivities $\sigma_{xx}^{(2)}$ and $\sigma_{yy}^{(2)}$ (brown and blue (coincide)), all plotted as functions of the chemical potential μ for the tight-binding model. The conductivities are only plotted for $\mu < 0$ since for $\mu > 0$, we just have $\sigma_{ii}^{(0)}(\mu) = \sigma_{ii}^{(0)}(-\mu)$, $\sigma_{ij}^{(1)}(\mu) = -\sigma_{ij}^{(1)}(-\mu)$, and $\sigma_{ii}^{(2)}(\mu) = \sigma_{ii}^{(2)}(-\mu)$ as shown in App. B.

Similarly, the xy-component is:

$$\sigma_{xy}^{H} = \frac{-e^3\tau^2 B}{\pi^2\hbar^4} 2t^2a^3 \oint_{k_F} \mathrm{d}k_{\parallel} \frac{\sin^2(ak_x)\cos(ak_y)}{\sqrt{\sin^2(ak_x) + \sin^2(ak_y)}}. \tag{6.4}$$

The integral in Eq. 6.3 is plotted together with the integral in Eq. 6.4 times (-1) in Fig.3, both as functions of μ, where they are seen to coincide. The opposite sign arises from the handedness of the electrons orbiting the Fermi surface. Another thing worth noticing is that $\sigma_{yx}^{H} \to 0$ as $\mu \to 0$, which indicate that as the corners of the Fermi surface become more distinct, the electrons, when moving around on the energy contour, meet a larger resistance which goes towards infinity when the Fermi surface is a square. The calculation of second-order terms is done in App. C and shows that only $\sigma_{xx}^{(2)}$ and $\sigma_{yy}^{(2)}$ are non-zero. These are also plotted in Fig. 3 and are seen to coincide as well.

6.3 Curvature of the Fermi surface

From Fig. 2 it appears that as $\mu \to 0^-$, some parts of the Fermi surface become more curved while other parts are straightened out. Since the Hall conductivity to first order in B contains the mass tensor, which expresses the curvature of the Fermi surface, one might get the idea that energy contours with a high total curvature have a larger $\sigma_{\alpha\beta}^{H}$ than contours with a low total curvature. To get a more precise measure of "total curvature", we first look at the general expression for curvature: For a curve which can be parametrized by the arch length l and has a tangent vector $\mathbf{T}$, the curvature in a point P on the curve is:

$$\kappa_P = \left|\frac{\partial \hat{\mathbf{T}}}{\partial l}\right|_P.$$

This is a very intuitive expression for the curvature, κ, since it states that κ is given by the rate of change of the unit tangent vector $\hat{\mathbf{T}}$ along the curve parametrized by l. In the case of

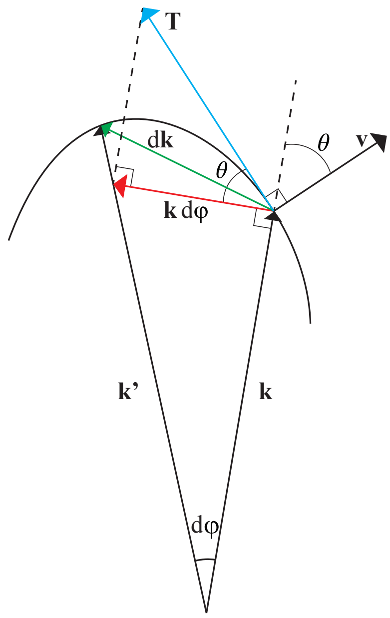

Figure 4: Sketch to explain the infinitesimals dl, dϕ, and d$\mathbf{k}$. As the angle d$\phi \to 0$, the vector d$\mathbf{k}$ (green) approaches the tangent vector $\mathbf{T}$ (blue) and $|\mathrm{d}\mathbf{k}| = \mathrm{d}l$. Thus, the small line segment dl will be: $\mathrm{d}l = \frac{k\mathrm{d}\phi}{\cos(\theta)}$, where θ is the angle between the $\mathbf{k}$-vector and the velocity vector $\mathbf{v}$. Courtesy of M. F. Olsen.

the Fermi surface, which is parametrized by the Fermi vector $k_F(\mu, \phi)$, an infinitesimal part of the arch length is: $\mathrm{d}l = \frac{k_F(\mu,\phi)}{\cos(\theta)}\mathrm{d}\phi$, θ being the angle between $\mathbf{k}$ and $\mathbf{v}$ (see Fig. 4), which means the curvature is:

$$\kappa = \left|\frac{\partial \hat{\mathbf{T}}}{\partial l}\right| = \left|\frac{\partial \hat{\mathbf{T}}}{\partial \phi}\frac{\partial \phi}{\partial l}\right| = \frac{\cos(\theta)}{k_F(\mu,\phi)}\left|\frac{\partial \hat{\mathbf{T}}}{\partial \phi}\right|.$$

As $\mathbf{v} = \frac{1}{\hbar}\frac{\partial \varepsilon}{\partial \mathbf{k}}$, the velocity vector is always perpendicular to the Fermi surface and so the unit tangent vector must be:

$$\hat{\mathbf{T}} = \frac{1}{v}\begin{pmatrix} -v_y \\ v_x \end{pmatrix}.$$

It is then possible to numerically find the function $\kappa(\mu, \phi)$ which for $\mu = -0.5$ is plotted in Fig. 9 in App. D in agreement with Fig. 2. Now we can define the measure of "total curvature" as the integral:

$$\kappa(\mu) = \int_0^{2\pi} \mathrm{d}\phi\, \kappa(\mu, \phi).$$

This is plotted in Fig. 5 together with the ratio $\kappa(\mu)/A(\mu)$ of κ to the area, A, of the Fermi surface. This ratio is of some relevance in that with growing μ, the Fermi surface gets larger, meaning a larger area, which leads to a higher number density of conduction electrons. From Fig. 5, it appears that the total curvature of the Fermi surface is largest at a low chemical potential. Comparing this with the Hall conductivities $\sigma^H_{yx}(\mu)$ and $-\sigma^H_{xy}(\mu)$ in Fig. 3 (green graph), there seems to be no connection between the curvature of the Fermi surface and the Hall conductivity, at least not for the tight-binding model.

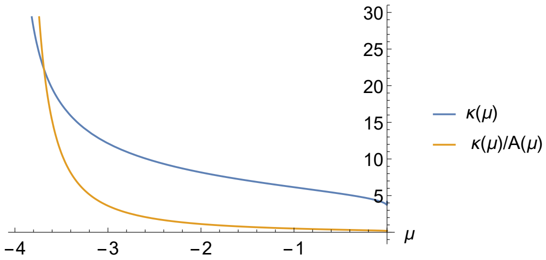

Figure 5: The total curvature of the Fermi surface in the tight-binding model as a function of the chemical potential μ in ratio to 1 (blue graph) an to the area of the Fermi surface $A(\mu)$ (orange graph).

7 Solving the Boltzmann equation for closed orbits on a simple 2D Fermi surface

The results for the conductivity tensor in the tight-binding model in Fig. 3, Sec. 6 were accomplished because we knew the energy function $\varepsilon(k_x, k_y)$. However, putting on a transverse magnetic field, we could only solve the Boltzmann equation by approximating a small **B**-field. The purpose of this section is to try and find a solution to the Boltzmann equation for an electron in a periodic potential, moving in both an electric field and a homogeneous magnetic field, and in this way be able to write an expression for the conductivity, without having to make the approximation of small $|\mathbf{B}|$. The method is the one explained in Smith & Højgaard [3, p. 123-134]. To describe the motion of an electron in 2D, we introduce the modified Boltzmann equation:

$$\hbar \frac{\mathrm{d}\mathbf{k}}{\mathrm{d}\tilde{t}} = -e\mathbf{v} \times \mathbf{B}. \tag{7.1}$$

with coordinates $(\varepsilon, \tilde{t})$. The $\tilde{t}$ is a parametrization of constant energy curves in k-space and is also the physical time if the only force experienced by the electron is the magnetic force. Taking the length of the vectors on both sides and integrating, we get:

$$\hbar|\mathrm{d}\mathbf{k}| = \hbar \mathrm{d}l = e|-\mathbf{v} \times \mathbf{B}|\mathrm{d}\tilde{t} \implies$$

$$\frac{\hbar}{eB} \oint \mathrm{d}l \, \frac{1}{v} = \int_0^T \mathrm{d}\tilde{t} = T = \frac{2\pi}{\omega_c}, \tag{7.2}$$

where $\mathbf{B}$ is assumed as usual to point in the $\hat{\mathbf{z}}$-direction, perpendicular to the Fermi surface, T is the period of the electron orbit, and l is the length travelled by the electron along the energy contour, see Fig. 4. The part of the originally formulated Boltzmann equation (Eq. 2.3), involving the **B**-field, can be expressed in terms of this $\tilde{t}$:

$$\frac{\partial f}{\partial \tilde{t}} = \frac{\partial f}{\partial \mathbf{k}} \frac{\partial \mathbf{k}}{\partial \tilde{t}} = \frac{-e}{\hbar} \mathbf{v} \times \mathbf{B} \cdot \frac{\partial f}{\partial \mathbf{k}}.$$

Hence, the stationary, homogeneous Boltzmann equation in the RTA reads:

$$-e\mathbf{E} \cdot \mathbf{v} \frac{\partial f_0}{\partial \varepsilon} + \frac{\partial f}{\partial \tilde{t}} = \frac{-g}{\tau}. \tag{7.3}$$

Since we now have the Boltzmann equation formulated in terms of $\tilde{t}$, we will need to make a change of variables in the expression for the current density, that is, from variables (k_x, k_y) to

$(\varepsilon, \tilde{t})$:

$$\int\int \mathrm{d}k_x \mathrm{d}k_y = \int\oint \mathrm{d}\varepsilon \mathrm{d}l \frac{1}{\hbar v} = \int\int \mathrm{d}\varepsilon \frac{1}{\hbar}\frac{eB}{\hbar}\mathrm{d}\tilde{t}.$$

The first equality follows from Eq. 4.4 and the second from Eq. 7.2. The current density is then:

$$\mathbf{j} = \frac{-e}{2\pi^2}\frac{eB}{\hbar^2}\int\int \mathrm{d}\varepsilon \mathrm{d}\tilde{t}\, \mathbf{v} g, \tag{7.4}$$

where the integration limits depend on whether the orbit is closed or open.

Considering two adjacent, closed orbits with energies ε and $\varepsilon + \Delta\varepsilon$, where $\Delta\varepsilon = \hbar v \Delta k$, the difference in the area covered in k-space is:

$$\Delta A = \oint \mathrm{d}l\, \Delta k = \frac{\Delta\varepsilon}{\hbar}\oint \mathrm{d}l\, \frac{1}{v} = \frac{\Delta\varepsilon}{\hbar}\frac{2\pi}{\omega_c}\frac{eB}{\hbar} = \Delta\varepsilon\frac{2\pi eB}{\hbar^2\omega_c}, \tag{7.5}$$

where we have used Eq. 7.2. Since for Bloch electrons [3, p. 124], $\Delta\varepsilon = \varepsilon_{n+1} - \varepsilon_n = \hbar\omega_c$, we have that: $A(\varepsilon_{n+1}) - A(\varepsilon_n) = \frac{2\pi eB}{\hbar}$. Applying Eq. 7.5 we write the cyclotron mass as:

$$m_c = \frac{eB}{\omega_c} = \frac{\hbar^2}{2\pi}\frac{\partial A}{\partial\varepsilon}. \tag{7.6}$$

7.1 A solution to the Boltzmann equation

The constant-energy contours in a simple 2D model can be parametrized by $k(\varepsilon, \phi) = k_0(\varepsilon) + k_1(\varepsilon)Y(\phi)$ where $k_0(\varepsilon)$ is a perfect circular surface and $Y(\phi)$ is a function of the azimuthal angle in the (k_x, k_y)-plane, weighted by $k_1(\varepsilon)$. As a measure of the distortion of the energy contours relative to circles, we introduce the constants: $\beta = \frac{k_1(\varepsilon_F)}{k_0(\varepsilon_F)}$ and $\gamma = \frac{k_1'(\varepsilon_F)}{k_0'(\varepsilon_F)}$ where prime denotes the derivative with respect to energy. We choose for $Y(\phi)$ the harmonic function $Y(\phi) = \cos(4\phi)$ so that the Fermi surface possesses C_4-symmetry and write: $k(\varepsilon_F, \phi) = k_0(\varepsilon_F)(1 + \beta\cos(4\phi))$. With this parametrization, we want to find the distribution function from Eq. 7.3, using that we can replace f with g in the term concerning the magnetic field:

$$\begin{aligned} -e\mathbf{E}\cdot\mathbf{v}\frac{\partial f_0}{\partial\varepsilon} + \frac{\partial g}{\partial\tilde{t}} = \frac{-g}{\tau} \implies \\ \Big(\omega_c\frac{\partial}{\partial\tilde{\phi}} + \frac{1}{\tau}\Big)g = e\mathbf{E}\cdot\mathbf{v}\frac{\partial f_0}{\partial\varepsilon}. \end{aligned} \tag{7.7}$$

In the second line, we have introduced the variable $\tilde{\phi}$ defined by $\frac{d\tilde{\phi}}{d\tilde{t}} = \omega_c$. Finding the relation between ϕ and $\tilde{\phi}$ and writing $\mathbf{v}(\varepsilon_F)$ in terms of ϕ, will enable us to solve the Boltzmann equation at the Fermi level which is what we need to find the conductivity tensor. The first step involves the identity:

$$\frac{\partial k}{\partial k_x} = \frac{\partial k}{\partial\varepsilon}\frac{\partial\varepsilon}{\partial k_x} + \frac{\partial k}{\partial\phi}\frac{\partial\phi}{\partial k_x}. \tag{7.8}$$

By inserting:

$$\frac{\partial k}{\partial k_x} = \frac{\partial}{\partial k_x}\sqrt{k_x^2 + k_y^2} = \frac{k_x}{k}, \qquad \frac{\partial\phi}{\partial k_x} = \frac{\partial}{\partial k_x}\arctan\Big(\frac{k_y}{k_x}\Big) = \frac{-k_y}{k^2},$$

we can use Eq. 7.8 to write the velocity at the Fermi level[5] as:

$$\frac{k_x}{k} = \frac{\partial k}{\partial \varepsilon}\frac{\partial \varepsilon}{\partial k_x} - \frac{\partial k}{\partial \phi}\frac{k_y}{k^2} = (k_0' + k_1'\cos(4\phi))\frac{\partial \varepsilon}{\partial k_x} + k_1 4\sin(4\phi)\frac{k_y}{k^2} \implies$$

$$\frac{\partial \varepsilon}{\partial k_x}\Big|_{\varepsilon_F} = \frac{1}{k_0'(1+\gamma\cos(4\phi))}\Big(\cos(\phi) - k_0 4\beta\sin(4\phi)\frac{\sin(\phi)}{k}\Big).$$

Since $\frac{1}{k} = \frac{1}{k_0(1+\beta\cos(4\phi))} \approx \frac{1}{k_0}(1-\beta\cos(4\phi))$ we can for $\frac{\partial\varepsilon}{\partial k_x}\Big|_{\varepsilon_F}$ to linear order in β set $\frac{1}{k} \approx \frac{1}{k_0}$:

$$\frac{\partial \varepsilon}{\partial k_x}\Big|_{\varepsilon_F} = \frac{1}{k_0'(1+\gamma\cos(4\phi))}\big(1 - 4\beta\tan(\phi)\sin(4\phi)\big)\cos(\phi). \tag{7.9}$$

Similarly for $v_y(\varepsilon_F)$:

$$\frac{k_y}{k} = (k_0' + k_1'\cos(4\phi))\frac{\partial \varepsilon}{\partial k_y} - k_1 4\sin(4\phi)\frac{k_x}{k^2} \implies$$

$$\frac{\partial \varepsilon}{\partial k_y}\Big|_{\varepsilon_F} = \frac{1}{k_0'(1+\gamma\cos(4\phi))}\big(1 + 4\beta\cot(\phi)\sin(4\phi)\big)\sin(\phi). \tag{7.10}$$

To find the relation between $\tilde{\phi}$ and ϕ, we will need the following expression for the mass, $m_0 = \frac{eB}{\omega_c}$, at the Fermi level. From 7.6 we know that:

$$\begin{aligned} m_0 &= \frac{\hbar^2}{2\pi}\frac{\partial A}{\partial \varepsilon}\Big|_{\varepsilon_F} = \frac{\hbar^2}{2\pi}\Big[\frac{\partial}{\partial\varepsilon}\int_0^{2\pi} \mathrm{d}\phi \int_0^{k_0} \mathrm{d}\tilde{k_0}\,\tilde{k_0}(1+\beta\cos(4\phi))\Big]\Big|_{\varepsilon_F} \\ &= \frac{\hbar^2}{2\pi}\Big[\frac{\partial}{\partial\varepsilon}\Big(\frac{1}{2}k_0^2\Big(2\pi + \frac{\beta}{4}\sin(4\phi)\Big|_0^{2\pi}\Big)\Big)\Big]\Big|_{\varepsilon_F} = \hbar^2 k_0' k_0|_{\varepsilon_F}. \end{aligned} \tag{7.11}$$

Using the definition of $\tilde{\phi}$ together with Eq. 7.2, we get that at the Fermi level: $\mathrm{d}\tilde{\phi} = \omega_c\,\mathrm{d}\tilde{t} = \omega_c\frac{\hbar}{eB}\frac{1}{v}\,\mathrm{d}l = \frac{\hbar\,\mathrm{d}l}{m_0 v}$. Fig. 4 shows that $\mathrm{d}l\cos(\theta) = k\,\mathrm{d}\phi \implies \mathrm{d}l = \frac{vk}{\mathbf{v}\cdot\mathbf{k}}k\,\mathrm{d}\phi$, allowing us to write:

$$\frac{\mathrm{d}\tilde{\phi}}{\mathrm{d}\phi} = \frac{\hbar\,\mathrm{d}l}{m_0 v}\frac{vk}{\mathbf{v}\cdot\mathbf{k}}k\frac{1}{\mathrm{d}l} = \frac{\hbar}{m_0}\frac{k^2}{\mathbf{v}\cdot\mathbf{k}}.$$

Applying Eqs. 7.9 and 7.10:

$$\begin{aligned} \mathbf{v}\cdot\mathbf{k} &= v_x k_x + v_y k_y \\ &= \frac{k}{\hbar}\Big[\frac{(1-4\beta\tan(\phi)\sin(4\phi))\cos^2(\phi)}{k_0'(1+\gamma\cos(4\phi))} + \frac{(1+4\beta\cot(\phi)\sin(4\phi))\sin^2(\phi)}{k_0'(1+\gamma\cos(4\phi))}\Big] \\ &= \frac{1}{\hbar}\frac{k}{k_0'(1+\gamma\cos(4\phi))} \implies \end{aligned} \tag{7.12}$$

$$\frac{\mathrm{d}\tilde{\phi}}{\mathrm{d}\phi} = \frac{\hbar}{\hbar^2 k_0' k_0}\frac{k^2\hbar k_0'(1+\gamma\cos(4\phi))}{k} = \frac{k}{k_0}(1+\gamma\cos(4\phi)) = (1+\beta\cos(4\phi))(1+\gamma\cos(4\phi)). \tag{7.13}$$

Now we are ready to tackle the Boltzmann equation in the form of Eq. 7.7, starting with an **E**-field in the $\hat{\mathbf{x}}$-direction:

$$\Big(\omega_c\frac{\partial\phi}{\partial\tilde{\phi}}\frac{\partial}{\partial\phi} + \frac{1}{\tau}\Big)g = \frac{eE}{\hbar}\frac{\partial f_0}{\partial\varepsilon}\frac{\partial\varepsilon}{\partial k_x}. \tag{7.14}$$

[5] As we are only working at the Fermi level, we will from now on just write $k = k_0(1+\beta\cos(\phi))$ without specifying that this only applies at ε_F.

Due to the term $\frac{\partial f_0}{\partial \varepsilon}$ we will as usual get a $\delta(\varepsilon-\varepsilon_F)$ in the computation of the current density. Hence, we can restrict ourselves to using only $\frac{\partial \varepsilon}{\partial k_x}\Big|_{\varepsilon_F}$. Writing this as a Fourier series with coefficients $\lambda_{m'}$ and employing Eq. 7.13, we get:

$$\Big(\omega_c\frac{\partial}{\partial\phi}+\frac{1}{\tau}(1+\beta\cos(4\phi))(1+\gamma\cos(4\phi))\Big)g=\underbrace{\frac{eE}{\hbar}\frac{\partial f_0}{\partial\varepsilon}}_{\tilde{E}}(1+\beta\cos(4\phi))(1+\gamma\cos(4\phi))\sum_{m'}\lambda_{m'}\mathrm{e}^{im'\phi}.$$

It seems that we can find a solution for g at the Fermi level as a Fourier series, $g(\phi)=\sum_n g_n\mathrm{e}^{in\phi}$:

$$\Big(\omega_c\frac{\partial}{\partial\phi}+\sum_k l_k\mathrm{e}^{ik\phi}\Big)\sum_n g_n\mathrm{e}^{in\phi}=\tilde{E}\sum_m r_m^{(x)}\mathrm{e}^{im\phi}. \tag{7.15}$$

Here we have written $\frac{1}{\tau}(1+\beta\cos(4\phi))(1+\gamma\cos(4\phi))$ as a Fourier series with $l_0=\frac{2+\beta\gamma}{2\tau}$, $l_{\pm4}=\frac{\beta+\gamma}{2\tau}$, $l_{\pm8}=\frac{\beta\gamma}{4\tau}$ and absorbed $(1+\beta\cos(4\phi))(1+\gamma\cos(4\phi))$ on the RHS into the sum which runs from $m=-9$ to $m=9$ with $r_m^{(x)}=0$ for m even. Rewriting the LHS, we get a set of linear equations:

$$\sum_n i\omega_c n g_n\mathrm{e}^{in\phi}+\sum_{k,n}l_k g_n\mathrm{e}^{i(n+k)\phi}=\tilde{E}\sum_m r_m^{(x)}\mathrm{e}^{im\phi}.$$

To compare exponents, we change the indices on the LHS: $n\to m$ in the first sum and $k\to m-n$ in the second one:

$$\sum_m i\omega_c m g_m\mathrm{e}^{im\phi}+\sum_m\Big(\sum_n l_{m-n}g_n\Big)\mathrm{e}^{im\phi}=\tilde{E}\sum_m r_m^{(x)}\mathrm{e}^{im\phi}\implies$$

$$i\omega_c m g_m+\sum_n l_{m-n}g_n=\sum_n\underbrace{\Big(i\omega_c m\delta_{mn}+l_{m-n}\Big)}_{A_{mn}}g_n=\tilde{E}r_m^{(x)}.$$

From eg. Eq. 7.15, we see that the Fourier series of g must consist of terms $g_n\mathrm{e}^{in\phi}$ with $n=-9,...,9$ and $g_n=0$ for n even. Hence, $\underline{\underline{A}}$ being a 19×19-matrix and $\mathbf{g}=(g_{-9},...,g_9)$, $\mathbf{r}^{(x)}=(r_{-9}^{(x)},...,r_9^{(x)})$ being vectors of length 19, we can write the solution to the Boltzmann equation for this simple Fermi surface with $\mathbf{E}=E\hat{\mathbf{x}}$, very compressed as:

$$g^{(x)}(\phi)=\mathbf{g}\cdot\mathbf{e},\qquad\qquad \mathbf{g}=\tilde{E}\underline{\underline{A}}^{-1}\mathbf{r}^{(x)},\qquad\qquad \mathbf{e}=\begin{pmatrix}\mathrm{e}^{-i9\phi}\\ \mathrm{e}^{-i8\phi}\\ \vdots\\ \mathrm{e}^{i9\phi}\end{pmatrix}.$$

For an $\mathbf{E}$-field in the $\hat{\mathbf{y}}$-direction, we will have the exact same equations only with a different $\mathbf{r}^{(y)}$: $\sum_m r_m^{(y)}\mathrm{e}^{im\phi}=(1+\beta\cos(4\phi))(1+\gamma\cos(4\phi))\sum_{m'}\xi_{m'}\mathrm{e}^{im'\phi}$.

7.2 Conductivity for the simple 2D Fermi surface

We are now fully equipped to work out the current density from Eq. 7.4, allowing ourselves to express v and g only as how they look at the Fermi energy with reference to the $\delta(\varepsilon-\varepsilon_F)$ that will appear:

$$\begin{aligned}
j_\mu &= \frac{-e^2B}{2\pi^2\hbar^2}\int\int \mathrm{d}\varepsilon \mathrm{d}\tilde{t}\, v_\mu g^{(\nu)} \\
&= \frac{-e^2B}{2\pi^2\hbar^2}\frac{1}{\hbar\omega_c}\int\int \mathrm{d}\varepsilon \mathrm{d}\phi\, \frac{\mathrm{d}\tilde{\phi}}{\mathrm{d}\phi}\tilde{E}\Big(\sum_{m'}\zeta_{m'}\mathrm{e}^{im'\phi}\Big)(\underline{\underline{A^{-1}}}\mathbf{r}^{(\nu)})\cdot\mathbf{e} \\
&= \frac{e^3BE}{2\pi^2\hbar^4\omega_c}\int \mathrm{d}\varepsilon\left(\frac{-\partial f_0}{\partial\varepsilon}\right)\int \mathrm{d}\phi\,(1+\beta\cos(4\phi))(1+\gamma\cos(4\phi))\Big(\sum_{m'}\zeta_{m'}\mathrm{e}^{im'\phi}\Big)(\underline{\underline{A^{-1}}}\mathbf{r}^{(\nu)})\cdot\mathbf{e} \\
&= \frac{e^3BE}{2\pi^2\hbar^4\omega_c}\int_0^{2\pi}\mathrm{d}\phi\Big(\sum_m r_m^{(\mu)}\mathrm{e}^{im\phi}\Big)(\underline{\underline{A^{-1}}}\mathbf{r}^{(\nu)})\cdot\mathbf{e}.
\end{aligned}$$

Here $\zeta_{m'}$ can be either $\lambda_{m'}$ or $\xi_{m'}$ depending on the direction $\mu = x, y$ of the current density. This integral we can solve using:

$$\int_0^{2\pi}\mathrm{d}\phi\,\mathrm{e}^{i(m+n)\phi} = 2\pi\delta_{-nm} \implies$$

$$j_{\mu\nu} = \frac{e^3BE}{\pi\hbar^4\omega_c}(\underline{\underline{A^{-1}}}\mathbf{r}^{(\nu)})\cdot\tilde{\mathbf{r}}^{(\mu)},$$

where we have introduced the vector: $\tilde{\mathbf{r}}^{(x)} = (r_9^{(x)}, ..., r_{-9}^{(x)})$. This means the conductivity tensor components are:

$$\sigma_{\mu\nu} = \frac{e^3B}{\pi\hbar^4\omega_c}(\underline{\underline{A^{-1}}}\mathbf{r}^{(\nu)})\cdot\tilde{\mathbf{r}}^{(\mu)}. \tag{7.16}$$

With the help of the computer program Wolfram Mathematica, Eq. 7.16 can be solved to second order in β and γ and to first order in $\beta\gamma$:

$$\begin{aligned}
\sigma_{xx}(\beta,\gamma) = \sigma_{yy}(\beta,\gamma) = \sigma_0\Big[&\frac{1}{1+\alpha^2} + \frac{1+13\alpha^2}{2(1+\alpha^2)(1+34\alpha^2+225\alpha^4)}\gamma^2 \\
&+ \frac{-1+57\alpha^2+349\alpha^4+675\alpha^6}{2(1+\alpha^2)(1+34\alpha^2+225\alpha^4)}\gamma\beta + \frac{16+319\alpha^2+675\alpha^4}{2(1+\alpha^2)(1+9\alpha^2)(1+25\alpha^2)}\beta^2\Big].
\end{aligned} \tag{7.17}$$

$$\begin{aligned}
\sigma_{yx}(\beta,\gamma) = -\sigma_{xy}(\beta,\gamma) = \sigma_0\Big[&\frac{\alpha}{1+\alpha^2} + \frac{3\alpha+15\alpha^3}{2(1+\alpha^2)(1+34\alpha^2+225\alpha^4)}\gamma^2 \\
&- \frac{4(4\alpha+61\alpha^3+105\alpha^5)}{(1+2\alpha^2+\alpha^4)(1+34\alpha^2+225\alpha^4)}\gamma\beta + \frac{16\alpha-131\alpha^3+225\alpha^5}{2(1+\alpha^2)(1+9\alpha^2)(1+25\alpha^2)}\beta^2\Big].
\end{aligned} \tag{7.18}$$

Here $\alpha = \omega_c\tau$, and the factor σ_0 in front of the parentheses is:

$$\frac{e^3B}{\pi\hbar^4\omega_c}\frac{\tau}{2k_0'^2} = \frac{e^3\tau B}{2\pi\hbar^4\omega_c}\frac{\hbar^4k_0^2}{m_0^2} = \frac{e^3\tau Bk_0^2}{2\pi m_0^2}\frac{m_0}{eB} = \frac{k_0^2}{2\pi}\frac{e^2\tau}{m_0} = \frac{n_0e^2\tau}{m_0} = \sigma_0,$$

where we have invoked Eq. 7.11 and introduced $n_0 = k_0^2/2\pi$, the electron concentration for the non-distorted Fermi surface. The actual electron concentration is: $n = \frac{1}{2\pi^2}4\int_0^{\pi/2}\mathrm{d}\phi\,k^2(\phi)/2 = \frac{k_0^2}{\pi^2}\int_0^{\pi/2}\mathrm{d}\phi\,(1+\beta\cos(4\phi))^2 = n_0(1+\beta^2/2)$. Eqs. 7.17 and 7.18 are plotted as functions of β, γ in Fig. 6, which shows that the longitudinal conductivity grows with increasing γ and β. The transverse, on the other hand, becomes larger with increasing β but decreases with γ. Also, the values of β and γ have a larger effect on the longitudinal conductivity than on the transverse

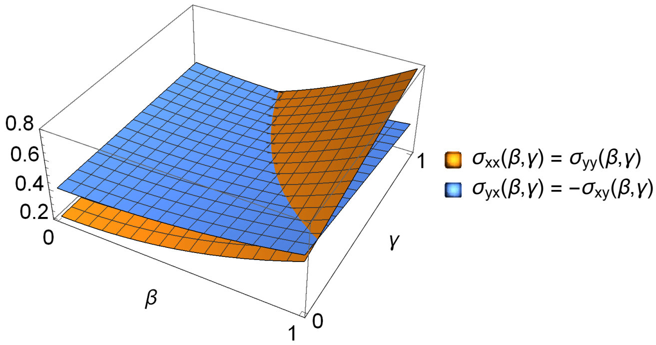

Figure 6: The longitudinal (orange) and transverse (blue) conductivity as functions of β and γ with $\sigma_0 = 1$, $\alpha = 2$ for the Fermi surface described by $k(\varepsilon_F) = k_0(\varepsilon_F)(1 + \beta\cos(4\phi))$. The values of β and γ shows to have a larger influence on the longitudinal conductivity than on the transverse.

which is slightly surprising as $\sigma_{yx}(\beta, \gamma)$ exactly describes the electron transport on the Fermi surface which is modulated by the very same β and γ.

Going through the calculations with an **E**-field in an arbitrary direction, making an angle θ with the $\mathbf{k_x}$-axis, one simply gets that:

$$\sigma_{\mu\theta} = \sigma_{\mu x}\cos(\theta) + \sigma_{\mu y}\sin(\theta).$$

If one instead chooses a harmonic function $Y(\phi) = \cos(q\phi)$ with $q \in \mathbb{N}$, the conductivity will still be in the form of Eq. 7.16, only now the components of $\mathbf{r}$ will range from $r_{m=-2q-1}$ to $r_{m=2q+1}$) with non-zero components for $m = \pm 2q \pm 1, \pm q \pm 1, \pm 1$ (similarly for $\tilde{\mathbf{r}}$ only arranged in the opposite order) and $\mathbf{e} = (\mathrm{e}^{-2q-1}, \ldots, \mathrm{e}^{2q+1})$. The Fourier coefficients l_k will still be: $l_0 = \frac{2+\beta\gamma}{2\tau}, l_{\pm q} = \frac{\beta+\gamma}{2\tau}, l_{\pm 2q} = \frac{\beta\gamma}{4\tau}$.
If we had made all the calculations with $\gamma = \frac{k_1'(\varepsilon_F)}{k_0'(\varepsilon_F)} = 0$ we would have got expressions $\sigma_{xx}(\beta)$ and $\sigma_{yx}(\beta)$ which are shown in App. E. Taking the high-field limit of $\sigma_{yx}(\beta)$ as is done in Eq. E.7, one gets $\sigma_{yx}(\beta) \simeq \frac{ne}{B}$ just like in the high-field expansion in App. F and the high-field Hall effect in the free electron model Sec. 3.3.

7.3 Applying the method to the tight-binding model

The method presented in the previous sections has the advantage that we do not need to make any approximations in the magnetic field. The disadvantage is that we have no information about the energy function $\varepsilon(k)$ or even $k(\varepsilon)$ which we could do without as we were only doing calculations at ε_F. However, the mass tensor remains unknown as it requires either both the first and second derivatives of $\varepsilon(\mathbf{k})$ with respect to $\mathbf{k}$ or the first and second derivatives of $k(\varepsilon, \phi)$ with respect to both ε and ϕ, depending on whether we are given $\varepsilon(\mathbf{k}, \phi)$ or $k(\varepsilon, \phi)$.
To get around this, we now try and create a test function $k(\varepsilon, \phi)$, with known $k_0(\varepsilon)$ and $k_1(\varepsilon)$, which at a certain energy looks like a specific Fermi surface in the tight-binding model, for which we know the energy function. This way, we can find the conductivity for this chemical potential in the tight-binding model to exact order in B while still knowing the mass tensor from either the test function or the energy function of the tight-binding model. In Fig. 7 the Fermi surface for the tight binding-model at the chemical potential $\mu = -1$ is plotted together with a test function $k(\varepsilon, \phi) = c(\varepsilon + b\varepsilon^2\cos(4\phi))$ with $c = 20, b = 0.5$ for $\varepsilon = 0.1$. As they practically

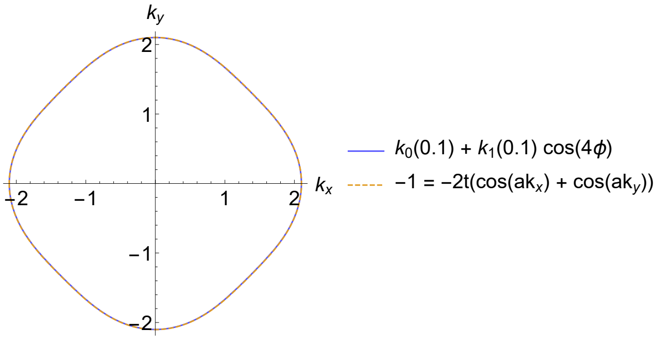

Figure 7: The Fermi surface for the test function $k(\varepsilon, \phi) = c(\varepsilon + b\varepsilon^2 \cos(4\phi))$ with $c = 20, b = 0.5$ for $\varepsilon = 0.1$ (blue), plotted together with the Fermi surface for the tight-binding model $\varepsilon_{\mathbf{k}} = -2t(\cos(ak_x) + \cos(ak_y))$ with $t = a = 1$ and the chemical potential $\mu = -1$ (orange). The two Fermi surfaces coincide completely.

coincide completely, it seems only fair that the test function can be used to calculate σ_{xx} and σ_{yx} from Eqs. 7.17 and 7.18 for a system described by the tight-binding model with a chemical potential $\mu = -1$.

Having $k_0'(\varepsilon) = c$ and $k_1'(\varepsilon) = 2cb\varepsilon$ so that $\beta = be|_{\varepsilon_F=0.1} = 0.05$ and $\gamma = 2b\varepsilon|_{\varepsilon_F=0.1} = 0.1$, Eqs. 7.17 and 7.18 become:

$$\begin{aligned}\sigma_{xx} = \frac{e^3 B\tau}{2\pi\hbar^4\omega_c}\frac{1}{20^2}\Big[&\frac{1}{1+\alpha^2} + \frac{1+13\alpha^2}{2(1+\alpha^2)(1+34\alpha^2+225\alpha^4)}0.01 \\ &+ \frac{-1+57\alpha^2+349\alpha^4+675\alpha^6}{2(1+\alpha^2)(1+34\alpha^2+225\alpha^4)}0.005 + \frac{16+319\alpha^2+675\alpha^4}{2(1+\alpha^2)(1+9\alpha^2)(1+25\alpha^2)}0.0025\Big].\end{aligned}$$

$$\begin{aligned}\sigma_{yx} = \frac{e^3 B\tau}{2\pi\hbar^4\omega_c}\frac{1}{20^2}\Big[&\frac{\alpha}{1+\alpha^2} + \frac{3\alpha+15\alpha^3}{2(1+\alpha^2)(1+34\alpha^2+225\alpha^4)}0.01 \\ &- \frac{4(4\alpha+61\alpha^3+105\alpha^5)}{(1+2\alpha^2+\alpha^4)(1+34\alpha^2+225\alpha^4)}0.005 + \frac{16\alpha-131\alpha^3+225\alpha^5}{2(1+\alpha^2)(1+9\alpha^2)(1+25\alpha^2)}0.0025\Big].\end{aligned} \tag{7.19}$$

Expanding σ_{yx} to order B^{-1}, ie. considering the high-field limit, we get:

$$\sigma_{yx} \simeq \frac{e^2\tau m_0}{2\pi\hbar^4}\frac{1}{c^2}\frac{1}{\alpha}(1+\beta^2/2) = \frac{e}{2\pi B}\frac{1}{c^2}\frac{m_0^2}{\hbar^4}(1+\beta^2/2) = \frac{e}{2\pi B}\cdot 4.025,$$

where $m_0 = \frac{\hbar^2}{2\pi}\frac{\partial A}{\partial\varepsilon}\Big|_{\varepsilon_F}$ and A is the area of the Fermi surface: $A = \int_0^{2\pi} \mathrm{d}\phi\, \frac{1}{2}(c\varepsilon + cb\varepsilon^2\cos(4\phi))^2$. We can compare this result with that of the high-field expansion in Eq. F, App. F:

$$\sigma_{yx} = \frac{en}{B} = \frac{e}{2\pi^2 B}A = \frac{e}{2\pi B}c^2\varepsilon^2(1+\frac{b^2\varepsilon^2}{2}) = \frac{e}{2\pi B}\cdot 4.005.$$

Indeed we see that the high-field limit of Eq. 7.19 is in accordance with the usual high-field Hall effect, also mentioned in Sec. 3.3.

8 Conclusion

Throughout this thesis, we have thoroughly exploited the Boltzmann equation to find the conductivity tensor in several different cases. First, we worked within the free electron model to find the Drude and Hall conductivity tensors together with the high-field Hall effect $\sigma_{yx} = \frac{en}{B}$. Handling a more general case, we then also found expressions for the conductivity in zero magnetic field for an arbitrary Fermi surface and used the method of Jones & Zener [2, p. 501] to find the conductivity tensor in a constant, transverse, weak magnetic field for an arbitrary Fermi surface to second order in B, all in agreement with Paaske and Khveshchenko [4]. Applying this to the tight-binding model, we got the results in Fig. 3 for the conductivity tensors as functions of the chemical potential: $\sigma_{ij}^{(n)}(\mu)$ where $i, j = x, y$ and $n = 0, 1, 2$ is the order of the magnetic field B. Motivated by the inverse mass term $m_{\mu\nu}^{-1}$ in the expression for the Hall conductivity σ_{xy}^H, we then investigated whether the total curvature of the Fermi surface has an influence on the Hall conductivity for tight-binding model. Comparing the functions $\kappa(\mu)$ and $\sigma_{xy}^H(\mu)$, there seemed to be no connection between the two.

Afterwards, we turned to a different approach for solving the Boltzmann equation, which relied on the method of Smith & Højgaard [3]. Here we introduced the modified Boltzmann equation $\hbar\frac{\mathrm{d}\mathbf{k}}{\mathrm{d}\tilde{t}} = -e\mathbf{v}\times\mathbf{B}$ with $\tilde{t}$ parametrizing curves of constant energy in k-space. Having also constant-energy contours described by the function $k(\varepsilon, \phi) = k_0(\varepsilon) + k_1(\varepsilon)\cos(q\phi)$ with ϕ the azimuthal angle in the (k_x, k_y)-plane and $q \in \mathbb{N}$, it was possible to solve the Boltzmann equation for $g = f - f_0$ leading to a conductivity tensor: $\sigma_{\mu\nu} = \frac{e^3 B}{\pi\hbar^4\omega_c}(\underline{\underline{A^{-1}}}\mathbf{r}^{(\nu)}) \cdot \tilde{\mathbf{r}}^{(\mu)}$. Here $\underline{\underline{A^{-1}}}$ is a matrix of dimension $4q + 3$ and $\mathbf{r}^{(\nu)}$, $\tilde{\mathbf{r}}^{(\mu)}$ are vectors of length $4q + 3$, all consisting of the coefficients of known Fourier series, as presented in Sec. 7.1. This led to the conductivity tensor elements $\sigma_{\mu\nu}(\beta, \gamma)$ which are functions of $\beta = \frac{k_1(\varepsilon_F)}{k_0(\varepsilon_F)}$, $\gamma = \frac{k_1'(\varepsilon_F)}{k_0'(\varepsilon_F)}$ and are plotted for the case $q = 4$ in Fig. 6. Finally, we applied the method to the tight-binding model to find the conductivity to exact order in the magnetic field for the specific case of $\mu = -1$ and saw that the high-field limit of this was in accordance with the high-field Hall effect.

As a suggestion for further work, it would be interesting to see how widely the method of Smith & Højgaard in Sec. 7 could be applied to other types of Fermi surfaces than the tight-binding model. Also, it was slightly surprising that the curvature of the Fermi surface in the tight-binding model seemingly had nothing to do with the Hall conductivity, seeing that the mass tensor entered the expression for it. Other methods to investigate whether that result is true for any model, other than the one presented in this thesis, would indeed be intriguing.

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Appendices

A Derivation of the Boltzmann equation

The derivation of the semiclassical Boltzmann equation assumes that the mean free path[6] l of the electrons in the crystal is much longer than their de Broglie wavelength such that they can be considered collectively as a semiclassical gas.[1, p. 361] The distribution function in thermal equilibrium, ie. when $k_B T \ll \varepsilon_F$, will then be given by the Fermi-Dirac distribution function:

$$f_0 = \frac{1}{\mathrm{e}^{(\varepsilon_{\mathbf{k}}-\mu)/k_B T}+1}. \tag{A.1}$$

Here, $\varepsilon_{\mathbf{k}}$ is the energy of an electron wave packet with wave vector $\mathbf{k}$, μ is the chemical potential, k_B is the Boltzmann constant, T is the temperature of the electron gas, and ε_F is the Fermi energy. Since we consider the electrons as a semiclassical gas, we can write up the continuity equation in phase space for the non-equilibrium distribution function [3, p. 2] $f(\mathbf{r}, \mathbf{p}, t)$:

$$\frac{\partial f}{\partial t} + \partial_{x_\mu}(v_\mu f) = \Big(\frac{\partial f}{\partial t}\Big)_{coll} \quad ; \qquad \partial_{x_\mu} = (\frac{\partial}{\partial \mathbf{r}}, \frac{\partial}{\partial \mathbf{p}}), \qquad v_\mu = (\dot{\mathbf{r}}, \dot{\mathbf{p}}). \tag{A.2}$$

The right-hand side, $\big(\frac{\partial f}{\partial t}\big)_{coll}$, is the collision integral which is zero in absence of collisions and otherwise amounts to the difference in the particle number $N(\mathbf{r}, \mathbf{k}, t)$ due to the difference in inscattering and outscattering. If $\mathbf{r}, \mathbf{p}$ obey the Hamilton equations: $\dot{\mathbf{r}} = \frac{\partial H}{\partial \mathbf{p}}, \dot{\mathbf{p}} = -\frac{\partial H}{\partial \mathbf{r}}$, we have that in:

$$\partial_{x_\mu}(v_\mu f) = v_\mu \frac{\partial f}{\partial x_\mu} + f\frac{\partial v_\mu}{\partial x_\mu}, \tag{A.3}$$

the second term on the RHS is equal to zero as:

$$\frac{\partial \dot{\mathbf{p}}}{\partial \mathbf{p}} = \frac{\partial}{\partial \mathbf{p}}\Big(-\frac{\partial H}{\partial \mathbf{r}}\Big) = -\frac{\partial}{\partial \mathbf{r}}\dot{\mathbf{r}} \implies \qquad f\frac{\partial v_\mu}{\partial x_\mu} = f\frac{\partial \dot{\mathbf{r}}}{\partial \mathbf{r}} + f\frac{\partial \dot{\mathbf{p}}}{\partial \mathbf{p}} = 0. \tag{A.4}$$

Hence, the continuity equation A.2 becomes:

$$\frac{\partial f}{\partial t} + v_\mu \frac{\partial f}{\partial x_\mu} = \boxed{\frac{\partial f}{\partial t} + \dot{\mathbf{r}}\cdot\frac{\partial f}{\partial \mathbf{r}} + \dot{\mathbf{p}}\cdot\frac{\partial f}{\partial \mathbf{p}} = \Big(\frac{\partial f}{\partial t}\Big)_{coll}} \tag{A.5}$$

This is the Boltzmann equation [3].

B The conductivity tensor for $\varepsilon > 0$ in models with energy functions anti-symmetric around $\varepsilon = 0$

To ease calculations of the conductivity tensor in models with an energy function symmetric around $\varepsilon = 0$, we show here that $\sigma_{ii}^{(0)}(\varepsilon) = \sigma_{ii}^{(0)}(-\varepsilon)$, $\sigma_{ij}^{(1)}(\varepsilon) = -\sigma_{ij}^{(1)}(-\varepsilon)$, and $\sigma_{ij}^{(2)}(\varepsilon) = \sigma_{ij}^{(2)}(-\varepsilon)$. We start by introducing the vector $\mathbf{p}$ related to the wave vector $\mathbf{k}$ in the following way:

$$\mathbf{k} = \begin{cases} (\pi, \pi) - \mathbf{p} & \text{in the first quadrant} \\ (-\pi, \pi) - \mathbf{p} & \text{in the second quadrant} \\ (-\pi, -\pi) - \mathbf{p} & \text{in the third quadrant} \\ (\pi, -\pi) - \mathbf{p} & \text{in the fourth quadrant} \end{cases}$$

[6] That is, the average length travelled by the particles between collisions.

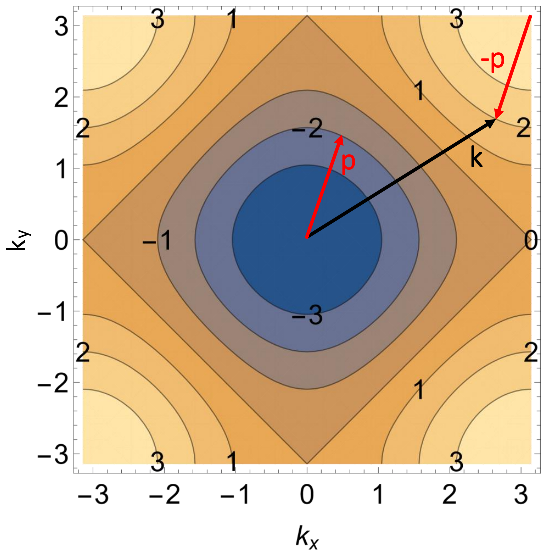


Figure 8: Energy contour plot for the tight-binding model to illustrate the definition of the vector $\mathbf{p}$ which has energy $\varepsilon_{\mathbf{p}} = -\varepsilon_{\mathbf{k}}$.

Also, $\varepsilon_{\mathbf{k}} = -\varepsilon_{\mathbf{p}}$, see Fig. 8. Thus $\mathrm{d}\mathbf{p} = -\mathrm{d}\mathbf{k}$, meaning that:

$$\begin{aligned}
\frac{\partial \varepsilon_{\mathbf{k}}}{\partial k_\alpha} &= \frac{\partial \varepsilon_{\mathbf{k}}}{\partial p_\alpha}\frac{\partial p_\alpha}{\partial k_\alpha} = -\frac{\partial \varepsilon_{\mathbf{p}}}{\partial p_\alpha}(-1) = \frac{\partial \varepsilon_{\mathbf{p}}}{\partial p_\alpha} \\
\frac{\partial^2 \varepsilon_{\mathbf{k}}}{\partial k_\alpha \partial k_\beta} &= \frac{\partial}{\partial k_\alpha}\Big(\frac{\partial \varepsilon_{\mathbf{p}}}{\partial p_\beta}\Big) = \frac{\partial^2 \varepsilon_{\mathbf{p}}}{\partial p_\alpha \partial p_\beta}\frac{\partial p_\alpha}{\partial k_\alpha} = -\frac{\partial^2 \varepsilon_{\mathbf{p}}}{\partial p_\alpha \partial p_\beta} \\
\frac{\partial^3 \varepsilon_{\mathbf{k}}}{\partial k_\alpha \partial k_\beta \partial k_\gamma} &= \frac{\partial}{\partial k_\alpha}\Big(-\frac{\partial^2 \varepsilon_{\mathbf{p}}}{\partial p_\beta \partial p_\gamma}\Big) = -\frac{\partial^3 \varepsilon_{\mathbf{p}}}{\partial p_\alpha \partial p_\beta \partial p_\gamma}\frac{\partial p_\alpha}{\partial k_\alpha} = \frac{\partial^3 \varepsilon_{\mathbf{p}}}{\partial p_\alpha \partial p_\beta \partial p_\gamma},
\end{aligned}$$

and so on.

Starting with the longitudinal conductivity tensor, we have:

$$\sigma^{(0)}_{\alpha\alpha}(\varepsilon) \sim \oint_{k_F} \mathrm{d}k_\parallel \,\frac{1}{v}\Big(\frac{\partial \varepsilon_{\mathbf{k}}}{\partial k_\alpha}\Big)^2 = \int_{k_\parallel(\phi=0)}^{k_\parallel(\phi=\pi/2)} \mathrm{d}k_\parallel \,\frac{1}{v}\Big(\frac{\partial \varepsilon_{\mathbf{k}}}{\partial k_\alpha}\Big)^2 + \int_{k_\parallel(\phi=\pi/2)}^{k_\parallel(\phi=\pi)} \ldots + \int_{k_\parallel(\phi=\pi)}^{k_\parallel(\phi=3\pi/2)} \ldots + \int_{k_\parallel(\phi=3\pi/2)}^{k_\parallel(\phi=2\pi)} \ldots$$

Changing integration variable from $k_\parallel$ to $p_\parallel$ yields:

$$\begin{aligned}
\sigma^{(0)}_{\alpha\alpha}(\varepsilon) &\sim \int_{p_\parallel(\phi=\pi/2)}^{p_\parallel(\phi=0)} (-\mathrm{d}p_\parallel)\,\frac{1}{v}\Big(\frac{\partial \varepsilon_{\mathbf{p}}}{\partial p_\alpha}\Big)^2 + \int_{p_\parallel(\phi=\pi)}^{p_\parallel(\pi/2)} \ldots + \int_{p_\parallel(\phi=3\pi/2)}^{p_\parallel(\phi=\pi)} \ldots + \int_{p_\parallel(\phi=2\pi)}^{p_\parallel(\phi=3\pi/2)} \ldots \\
&= \int_{p_\parallel(\phi=2\pi)}^{p_\parallel(\phi=0)} (-\mathrm{d}p_\parallel)\,\frac{1}{v}\Big(\frac{\partial \varepsilon_{\mathbf{p}}}{\partial p_\alpha}\Big)^2 = \int_{p_\parallel(\phi=0)}^{p_\parallel(\phi=2\pi)} \mathrm{d}p_\parallel\,\frac{1}{v}\Big(\frac{\partial \varepsilon_{\mathbf{p}}}{\partial p_\alpha}\Big)^2 \implies
\end{aligned}$$

$$\sigma^{(0)}_{\alpha\alpha}(\varepsilon) = \sigma^{(0)}_{\alpha\alpha}(-\varepsilon).$$

The change of limits on the integrals when going from $\mathrm{d}k_\parallel$ to $\mathrm{d}p_\parallel$ as the integration variable, can be realized by considering Fig. 8. Similarly for the Hall conductivity:

$$\begin{aligned}
\sigma^H_{\alpha\beta}(\varepsilon) &\sim \int_{k_\parallel(\phi=0)}^{k_\parallel(\phi=2\pi)} \mathrm{d}k_\parallel \, \frac{\partial \varepsilon_{\mathbf{k}}}{\partial k_\alpha}\epsilon_{\alpha\beta}\frac{\partial^2\varepsilon_{\mathbf{k}}}{\partial k_\beta \partial k_\mu}\epsilon_{\mu\delta}\frac{\partial \varepsilon_{\mathbf{k}}}{\partial k_\delta}\frac{1}{v} + \int_{k_\parallel(\phi=\pi/2)}^{k_\parallel(\phi=\pi)} \ldots + \int_{k_\parallel(\phi=\pi)}^{k_\parallel(\phi=3\pi/2)} \ldots + \int_{3\pi/2}^{2\pi} \ldots \\
&= \int_{p_\parallel(\phi=\pi/2)}^{p_\parallel(\phi=0)} (-\mathrm{d}p_\parallel) \, \frac{\partial \varepsilon_{\mathbf{p}}}{\partial p_\alpha}\epsilon_{\alpha\beta}\Big(\frac{-\partial^2\varepsilon_{\mathbf{p}}}{\partial p_\beta \partial p_\mu}\Big)\epsilon_{\mu\delta}\frac{\partial \varepsilon_{\mathbf{p}}}{\partial p_\delta}\frac{1}{v} + \int_{p_\parallel(\phi=\pi)}^{p_\parallel(\pi/2)} \ldots + \int_{p_\parallel(\phi=3\pi/2)}^{p_\parallel(\phi=\pi)} \ldots + \int_{p_\parallel(\phi=2\pi)}^{p_\parallel(\phi=3\pi/2)} \ldots
\end{aligned}$$

Proceeding the same way as for the longitudinal conductivity, we get:

$$\sigma^H_{\alpha\beta}(\varepsilon) = -\sigma^H_{\alpha\beta}(-\varepsilon).$$

This result is no surprise, as we know from the Lorentz force that electrons on a Fermi surface enclosing states of higher energy ($\varepsilon > 0$), cycles in the opposite sense (clockwise) of the electrons on a surface enclosing states of lower energy ($\varepsilon < 0$), when exposed to an external **B**-field in the $\hat{\mathbf{z}}$-direction. Finally, for the second-order conductivity:

$$\begin{aligned}
\sigma^{(2)}_{\alpha\beta}(\varepsilon) &\sim \int_{k_\parallel(\phi=0)}^{k_\parallel(\phi=\pi/2)} \mathrm{d}k_\parallel \, \frac{1}{v}\frac{\partial \varepsilon_{\mathbf{k}}}{\partial k_\alpha}\frac{\partial \varepsilon_{\mathbf{k}}}{k_\eta}\epsilon_{\zeta\eta}\epsilon_{\lambda\nu}\Big(\frac{\partial^2\varepsilon_{\mathbf{k}}}{\partial k_\zeta \partial k_\nu}\frac{\partial^2\varepsilon_{\mathbf{k}}}{\partial k_\lambda \partial k_\beta} + \frac{\partial \varepsilon_{\mathbf{k}}}{\partial k_\nu}\frac{\partial^3\varepsilon_{\mathbf{k}}}{\partial k_\zeta \partial k_\lambda \partial k_\beta}\Big) + \ldots \\
&= \int_{p_\parallel(\phi=\pi/2)}^{p_\parallel(\phi=0)} (-\mathrm{d}p_\parallel) \, \frac{1}{v}\frac{\partial \varepsilon_{\mathbf{p}}}{\partial p_\alpha}\frac{\partial \varepsilon_{\mathbf{p}}}{p_\eta}\epsilon_{\zeta\eta}\epsilon_{\lambda\nu}\Big(\frac{\partial^2\varepsilon_{\mathbf{p}}}{\partial p_\zeta \partial p_\nu}\frac{\partial^2\varepsilon_{\mathbf{p}}}{\partial p_\lambda \partial p_\beta} + \frac{\partial \varepsilon_{\mathbf{p}}}{\partial p_\nu}\frac{\partial^3\varepsilon_{\mathbf{p}}}{\partial p_\zeta \partial p_\lambda \partial p_\beta}\Big) + \ldots \implies
\end{aligned}$$

$$\sigma^{(2)}_{\alpha\beta}(\varepsilon) = \sigma^{(2)}_{\alpha\beta}(-\varepsilon).$$

C Magnetoconductivity with terms of second order in B for the tight-binding model

Here, we find $\sigma^{(2)}_{\alpha\beta}$ as presented in Eq. 5.4, Sec. 5.1 for the tight-binding model with $\alpha, \beta = x, y$ and B small, pointing in the $\hat{\mathbf{z}}$-direction. Remember that in the tight-binding model:

$$\varepsilon = -2t(\cos(ak_x) + \cos(ak_y))\,, \qquad \frac{\partial \varepsilon}{\partial k_i} = 2ta\sin(ak_i)\,,$$

$$\frac{\partial^2 \varepsilon}{\partial k_i \partial k_j} = 0,\, i \neq j\,, \qquad \frac{\partial^2 \varepsilon}{\partial k_i^2} = 2ta^2\cos(ak_i)\,, \qquad \frac{\partial^3 \varepsilon}{\partial k_i^3} = -2ta^3\sin(ak_i).$$

We start with the conductivity tensor element $\sigma^{(2)}_{yx}$ of second order in B due to a magnetic field in $\hat{\mathbf{z}}$-direction:

$$\begin{aligned}
\sigma^{(2)}_{yx} &= \frac{e^4\tau^3B^2}{2\pi^2\hbar^7}\oint_{k_F}\mathrm{d}k_\parallel \, \frac{1}{v}\frac{\partial \varepsilon}{\partial k_y}\frac{\partial \varepsilon}{\partial k_\eta}\epsilon_{\zeta\eta}\epsilon_{\lambda\nu}\Big(\frac{\partial^2\varepsilon}{\partial k_\zeta \partial k_\nu}\frac{\partial^2\varepsilon}{\partial k_\lambda \partial k_x} + \frac{\partial \varepsilon}{\partial k_\nu}\frac{\partial^3\varepsilon}{\partial k_\zeta \partial k_\lambda \partial k_x}\Big) \\
&= \frac{e^4\tau^3B^2}{2\pi^2\hbar^7}\oint_{k_F}\mathrm{d}k_\parallel \, \frac{1}{v}\frac{\partial \varepsilon}{\partial k_y}\frac{\partial \varepsilon}{\partial k_\eta}\epsilon_{\zeta\eta}\epsilon_{xy}\Big(\frac{\partial^2\varepsilon}{\partial k_\zeta \partial k_y}\frac{\partial^2\varepsilon}{\partial k_x^2} + \frac{\partial \varepsilon}{\partial k_y}\frac{\partial^3\varepsilon}{\partial k_\zeta \partial k_x^2}\Big) \\
&= \frac{e^4\tau^3B^2}{2\pi^2\hbar^7}\oint_{k_F}\mathrm{d}k_\parallel \, \frac{1}{v}\frac{\partial \varepsilon}{\partial k_y}\Big(\epsilon_{xy}\frac{\partial \varepsilon}{\partial k_y}\frac{\partial \varepsilon}{\partial k_y}\frac{\partial^3\varepsilon}{\partial k_x^3} + \epsilon_{yx}\frac{\partial \varepsilon}{\partial k_x}\frac{\partial^2\varepsilon}{\partial k_y^2}\frac{\partial^2\varepsilon}{\partial k_x^2}\Big) && \text{(C.1)} \\
&= \frac{e^4\tau^3B^2}{2\pi^2\hbar^7}\oint_{k_F}\mathrm{d}k_\parallel \, \frac{-2^4t^4a^6\sin(ak_y)}{v}\big(\sin^2(ak_y)\sin(ak_x) + \sin(ak_x)\cos(ak_y)\cos(ak_x)\big) \\
&= \frac{-4e^4\tau^3B^2t^3a^5}{\pi^2\hbar^6}\oint_{k_F}\mathrm{d}k_\parallel \, \frac{\sin(ak_y)\sin(ak_x)}{\sqrt{\sin^2(ak_x) + \sin^2(ak_y)}}\big(\sin^2(ak_y) + \cos(ak_x)\cos(ak_y)\big). && \text{(C.2)}
\end{aligned}$$

Changing integration variable from $\mathrm{d}k_\parallel$ to $(\mathrm{d}k_x, \mathrm{d}k_y)$ with some transformation factor, one can see that this is an integral over odd functions in both k_x and k_y and will therefore be zero. The same applies to $\sigma_{xy}^{(2)}$, calculated below by starting from Eq. C.1 and interchanging $(x \leftrightarrow y)$:

$$\begin{aligned}\sigma_{xy}^{(2)} &= \frac{e^4\tau^3B^2}{2\pi^2\hbar^7}\oint_{k_F}\mathrm{d}k_\parallel\,\frac{1}{v}\frac{\partial\varepsilon}{\partial k_x}\epsilon_{yx}\Big(\epsilon_{yx}\frac{\partial\varepsilon}{\partial k_x}\frac{\partial\varepsilon}{\partial k_x}\frac{\partial^3\varepsilon}{\partial k_y^3}+\epsilon_{xy}\frac{\partial\varepsilon}{\partial k_y}\frac{\partial^2\varepsilon}{\partial k_x^2}\frac{\partial^2\varepsilon}{\partial k_y^2}\Big)\\ &= \frac{-4e^4\tau^3B^2t^3a^5}{\pi^2\hbar^6}\oint_{k_F}\mathrm{d}k_\parallel\,\frac{\sin(ak_x)\sin(ak_y)}{\sqrt{\sin^2(ak_x)+\sin^2(ak_y)}}\big(\sin^2(ak_x)+\cos(ak_x)\cos(ak_y)\big).\end{aligned}\tag{C.3}$$

On the contrary, $\sigma_{xx}^{(2)}$ and $\sigma_{yy}^{(2)}$ are integrals over even functions in k_x and k_y and thus yields non-zero conductivity components:

$$\sigma_{xx}^{(2)} = \frac{-4e^4\tau^3B^2t^3a^5}{\pi^2\hbar^6}\oint_{k_F}\mathrm{d}k_\parallel\,\frac{\sin^2(ak_x)}{\sqrt{\sin^2(ak_x)+\sin^2(ak_y)}}\big(\sin^2(ak_y)+\cos(ak_x)\cos(ak_y)\big).\tag{C.4}$$

$$\sigma_{yy}^{(2)} = \frac{-4e^4\tau^3B^2t^3a^5}{\pi^2\hbar^6}\oint_{k_F}\mathrm{d}k_\parallel\,\frac{\sin^2(ak_y)}{\sqrt{\sin^2(ak_x)+\sin^2(ak_y)}}\big(\sin^2(ak_x)+\cos(ak_x)\cos(ak_y)\big).\tag{C.5}$$

These are plotted as functions of the chemical potential μ in Fig. 3 which reveals that $\sigma_{xx}^{(2)}$ and $\sigma_{yy}^{(2)}$ coincide as they ought to because of the fourfold symmetry of the Fermi surface.

D Curvature of the Fermi surface in the tight-binding model

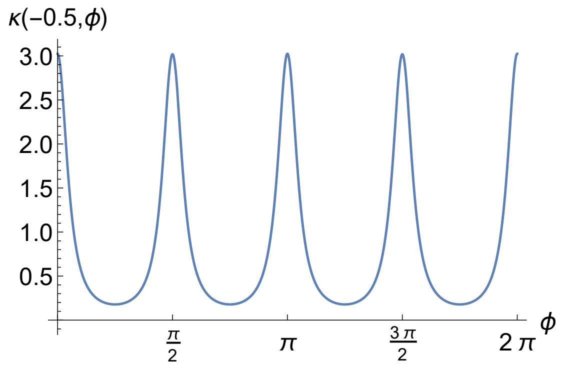
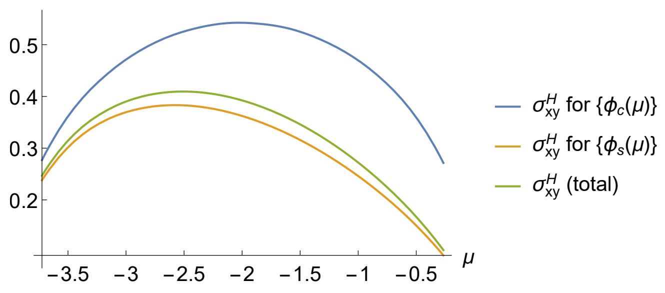
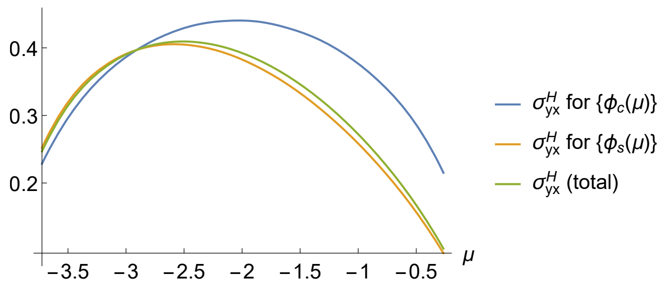


Figure 9: The curvature of the Fermi surface for $\mu = -0.1$ in the tight-binding model, in agreement with Fig. 2.

One could be led to believe that the main contribution to σ^H comes from the curved parts of the Fermi surface, that is, where $m_{\beta\mu}^{-1}$ is large. This we will investigate by dividing the Fermi surface up into intervals of ϕs with eg. $\kappa(\mu,\phi) > \frac{1}{10}\kappa_{max}$, calling these $\{\phi_c(\mu)\}$, and intervals where $\kappa(\mu,\phi) < \frac{1}{10}\kappa_{max}$, which we will call $\{\phi_s(\mu)\}$. Calculating $\sigma_{yx}^H(\mu)$ and $\sigma_{xy}^H(\mu)$ from Eqs. 6.3 and 6.4 but only integrating over either $\{\phi_c(\mu)\}$ or $\{\phi_s(\mu)\}$ yields the contributions to the total $\sigma_{xy}^H(\mu)$ and $\sigma_{yx}^H(\mu)$ from the two components of the Fermi surface; the curved



(a)



(b)

Figure 10: The Hall conductivity components σ^H_{xy} (Fig. 10a) and σ^H_{yx} (Fig. 10b), normalized by the perimeter $L(\mu)$ of the Fermi surface, plotted as functions of the chemical potential μ (green graphs). The blue graphs are the fractions of σ^H, coming from only integrating over ϕs where $\kappa(\mu,\phi) > \frac{1}{10}\kappa_{max}$ and then normalizing by the arch length $L_c(\mu)$. The yellow graphs are similarly the fractions of σ^H, coming from only integrating over ϕs where $\kappa(\mu,\phi) < \frac{1}{10}\kappa_{max}$ and are normalized as well by the arch length $L_s(\mu)$.

parts and the straight parts respectively. If these are furthermore normalized with respect to the arch lengths of the Fermi surface that correspond to the intervals $\{\phi_c(\mu)\}$ and $\{\phi_s(\mu)\}$: $L_{c,s}(\mu) = \int_{[\phi_{c,s}]} \mathrm{d}\phi \sqrt{k^2(\mu,\phi) + \left(\frac{\mathrm{d}k}{\mathrm{d}\phi}\right)^2}$, we can compare them with the total Hall conductivity, normalized by the total perimeter of the Fermi surface. This is shown in Figs. 10a and 10b for the xy and yx-components respectively. The total conductivity σ^H_{xy} and σ^H_{yx} can be regarded as a mean value from which the curved and straight parts deviate. One can see that for the xy-component, the curved parts of the Fermi surface contribute more than this average value whereas the straight parts contribute less. Regarding the yx-component, it has the same tendency but with a crossing of the graphs around $\mu = -3$. It is difficult to conclude anything certain from this about whether curved parts of the Fermi surface should contribute more than the straight parts to the Hall conductivity.

E A solution to the Boltzmann equation with $\gamma = 0$

Here we do the calculations equivalent to the ones in Secs. 7.1 and 7.2, only with $\gamma = 0$. This means $k_1'(\varepsilon_F) = 0$ and so:

$$\frac{k_x}{k} = \frac{\partial k}{\partial \varepsilon}\frac{\partial \varepsilon}{\partial k_x} + \frac{\partial k}{\partial \phi}\frac{\partial \phi}{\partial k_x} = \frac{\partial k_0}{\partial \varepsilon}\frac{\partial \varepsilon}{\partial k_x} + k_0 4\beta \sin(4\phi)\frac{k_y}{k^2} \implies$$

$$\frac{\partial\varepsilon}{\partial k_x}\Big|_{\varepsilon_F} = \frac{1}{k_0'}\big(1 - 4\beta\tan(\phi)\sin(4\phi)\big)\cos(\phi), \tag{E.1}$$

and:

$$\frac{\partial\varepsilon}{\partial k_y}\Big|_{\varepsilon_F} = \frac{1}{k_0'}\big(1 + 4\beta\cot(\phi)\sin(4\phi)\big)\sin(\phi). \tag{E.2}$$

These can of course be written as Fourier series:

$$\frac{\partial\varepsilon}{\partial k_x}\Big|_{\varepsilon_F} = \sum_n \lambda_n \mathrm{e}^{in\phi}, \qquad \lambda_1 = \lambda_{-1} = \frac{1}{2k_0'},\ \lambda_3 = \lambda_{-3} = -\lambda_5 = -\lambda_{-5} = \frac{-\beta}{k_0'}.$$

$$\frac{\partial\varepsilon}{\partial k_y}\Big|_{\varepsilon_F} = \sum_n \xi_n \mathrm{e}^{in\phi}, \qquad \xi_1 = -\xi_{-1} = \frac{-i}{2k_0'},\ \xi_3 = -\xi_{-3} = \xi_5 = -\xi_{-5} = \frac{-i\beta}{k_0'}.$$

Eqs. E.1 and E.2 leads to:

$$\begin{aligned}\mathbf{v}\cdot\mathbf{k} &= v_x k_x + v_y k_y \\ &= \frac{1}{\hbar}\Big[\frac{k}{k_0'}(1 - 4\beta\tan(\phi)\sin(4\phi))\cos^2(\phi) + \frac{k}{k_0'}(1 + 4\beta\cot(\phi)\sin(4\phi))\sin^2(\phi)\Big] \\ &= \frac{1}{\hbar}\frac{k}{k_0'} \implies \end{aligned} \tag{E.3}$$

$$\frac{\mathrm{d}\tilde{\phi}}{\mathrm{d}\phi} = \frac{\hbar}{\hbar^2 k_0' k_0}\frac{k^2\hbar k_0'}{k} = \frac{k}{k_0} = 1 + \beta\cos(4\phi). \tag{E.4}$$

This means we will get other coefficients l_k ($l_0 = \frac{1}{\tau}$, $l_4 = l_{-4} = \frac{\beta}{2\tau}$) than with $\gamma \neq 0$, but otherwise the calculations follow just the same pattern as in Secs. 7.1 and 7.2, resulting in the conductivities:

$$\sigma_{xx}(\beta) = \sigma_{yy}(\beta) = \frac{e^3 B}{\pi\hbar^4\omega_c}\frac{\tau}{2k_0'^2}\Big[\frac{1}{1+(\omega_c\tau)^2} + \frac{16 + 319(\omega_c\tau)^2 + 675(\omega_c\tau)^4}{2(1+(\omega_c\tau)^2)(1+9(\omega_c\tau)^2)(1+25(\omega_c\tau)^2)}\beta^2\Big].$$

$$\sigma_{yx}(\beta) = -\sigma_{xy}(\beta) = \frac{e^3 B}{\pi\hbar^4\omega_c}\frac{\tau}{2k_0'^2}\Big[\frac{(\omega_c\tau)}{1+(\omega_c\tau)^2} + \frac{16(\omega_c\tau) - 131(\omega_c\tau)^3 + 225(\omega_c\tau)^5}{2(1+(\omega_c\tau)^2)(1+9(\omega_c\tau)^2)(1+25(\omega_c\tau)^2)}\beta^2\Big].$$

Simplifying with $\alpha = \omega_c\tau$ and:

$$\sigma_0 = \frac{e^3 B}{\pi\hbar^4\omega_c}\frac{\tau}{2k_0'^2},$$

we can also write this in the form of Smith & Højgaard [3, p. 133]:

$$\sigma_{xx}(\beta) = \sigma_{yy}(\beta) = \sigma_0\Big[\frac{1}{1+\alpha^2}\Big(1 + \frac{31}{32}\beta^2\Big) + \frac{225}{64}\Big(\frac{1}{1+9\alpha^2} + \frac{1}{1+25\alpha^2}\Big)\beta^2\Big]. \tag{E.5}$$

$$\sigma_{yx}(\beta) = -\sigma_{xy}(\beta) = \sigma_0\Big[\frac{\alpha}{1+\alpha^2}\Big(1 + \frac{31}{32}\beta^2\Big) + \frac{225}{64}\Big(\frac{-3\alpha}{1+9\alpha^2} + \frac{5\alpha}{1+25\alpha^2}\Big)\beta^2\Big]. \tag{E.6}$$

The full solution to $\sigma_{\mu\nu}$ contains higher orders of β and is plotted in Fig. 11. The value of β seems to have a larger effect on the longitudinal than on the transverse conductivity, which is surprising as $\sigma_{yx}(\beta)$ exactly describes the electron transport on the Fermi surface which is modulated by the very same β.

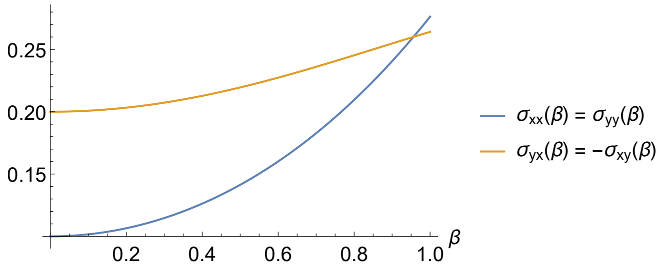


Figure 11: Graph showing the longitudinal and transverse conductivity of the Fermi surface $k_0(\varepsilon_F)(1+\beta\cos(4\phi))$ for $\beta \in [0,1]$.

Now, we want to see what happens to Eqs. E.5 and E.6 in the limits of either low or high $\mathbf{B}$, starting with the high-field limit, $\omega_c\tau = \alpha \to \infty$. Then the Hall conductivity in Eq. E.6 becomes:

$$\begin{aligned}
\sigma_{yx} &= \frac{n_0 e^2\tau}{m_0}\Big[\dots\Big] = \frac{n_0 e\omega_c\tau}{B}\Big[\dots\Big] \\
&= \frac{n_0 e}{B}\Big[\frac{1}{1/\alpha^2+1}\Big(1+\frac{31}{32}\beta^2\Big) - \frac{3}{1/\alpha^2+9}\frac{225\beta^2}{64} + \frac{5}{1/\alpha^2+25}\frac{225\beta^2}{64}\Big] \\
&\simeq \frac{n_0 e}{B}\Big[\Big(1-\frac{1}{\alpha^2}\Big)\Big(1+\frac{31}{32}\beta^2\Big) - \frac{1}{3}\Big(1-\frac{1}{(3\alpha)^2}\Big)\frac{225\beta^2}{64} + \frac{1}{5}\Big(1-\frac{1}{(5\alpha)^2}\Big)\frac{225\beta^2}{64}\Big] \\
&\simeq \frac{n_0 e}{B}\Big[1+\beta^2\Big(\frac{31}{32}-\frac{225}{3\cdot 64}+\frac{225}{5\cdot 64}\Big)\Big] = \frac{n_0 e}{B}(1+\beta^2/2) = \frac{ne}{B},
\end{aligned} \tag{E.7}$$

which is just what we got in the high-field limit in Sec. 3.3 within the free electron model. In the low-field limit, $\omega_c\tau = \alpha \to 0$:

$$\begin{aligned}
\sigma_{yx} &\simeq \sigma_0\Big[\alpha(1-\alpha^2)\Big(1+\frac{31}{32}\beta^2\Big) - 3\alpha(1-(3\alpha)^2)\frac{225\beta^2}{64} + 5\alpha(1-(5\alpha)^2)\frac{225\beta^2}{64}\Big] \\
&\simeq \sigma_0\alpha\Big[1+\beta^2\Big(\frac{31}{32}-\frac{3\cdot 225}{64}+\frac{5\cdot 225}{64}\Big)\Big] = \sigma_0\alpha(1+8\beta^2).
\end{aligned}$$

The zero-field conductivity, one gets from Eq. E.5 to be: $\sigma_{xx} = \sigma_{yy} = \sigma_0\Big[1+\beta^2\Big(\frac{31}{32}+2\frac{225}{64}\Big)\Big] = \sigma_0(1+8\beta^2)$.

F High-field expansion

This section is a review of the high-field expansion in Smith & Højgaard pages 127 to 130 [3].

In high $\mathbf{B}$-fields, the orbit period T will be much shorter than the collision time τ and so the electron can, with high probability, orbit all the way around the Fermi surface without being scattered by impurities, phonons, or other electrons. [7] Hence, one would think that the conductivity in high magnetic fields should reveal something about the shape of the Fermi surface. Starting from the Boltzmann equation in the form of Eq. 7.3, but without the RTA,

[7] It is assumed that the Fermi surface is only inside the first Brillouin zone, that is, $-\pi/a < k_F^x, k_F^y > \pi/a$, with a being the lattice constant.

and introducing the operator H and the vector $\boldsymbol{\psi}$, we have:

$$-e\mathbf{E}\cdot\mathbf{v}\frac{\partial f_0}{\partial\varepsilon}+\frac{\partial g}{\partial\tilde{t}}=\Big(\frac{\partial f}{\partial t}\Big)_{coll}, \qquad \Big(\frac{\partial f}{\partial t}\Big)_{coll}\equiv -Hg, \qquad g=e\mathbf{E}\cdot\boldsymbol{\psi}\frac{\partial f_0}{\partial\varepsilon}.$$

$$\begin{aligned}
-e\mathbf{E}\cdot\mathbf{v}\frac{\partial f_0}{\partial\varepsilon}+\frac{\partial g}{\partial\tilde{t}}&=-Hg \implies\\
-e\mathbf{E}\cdot\mathbf{v}\frac{\partial f_0}{\partial\varepsilon}+e\mathbf{E}\cdot\frac{\partial\boldsymbol{\psi}}{\partial\tilde{t}}\frac{\partial f_0}{\partial\varepsilon}&=-He\mathbf{E}\cdot\boldsymbol{\psi}\frac{\partial f_0}{\partial\varepsilon} \implies\\
-\mathbf{E}\cdot\mathbf{v}+\mathbf{E}\cdot\frac{\partial\boldsymbol{\psi}}{\partial\tilde{t}}&=-H\mathbf{E}\cdot\boldsymbol{\psi} \implies\\
\frac{\partial\boldsymbol{\psi}}{\partial\tilde{t}}+H\boldsymbol{\psi}&=\mathbf{v}.
\end{aligned} \tag{F.1}$$

In the last line, we have taken the scalar product with $\mathbf{E}$ from the left and used that $\mathbf{E}$ is independent of the collision integral. The conductivity tensor then becomes (from Eq. 7.4):

$$\sigma_{ij}=\frac{e^3B}{2\pi^2\hbar^2}\int \mathrm{d}\varepsilon\Big(-\frac{\partial f_0}{\partial\varepsilon}\Big)\int \mathrm{d}\tilde{t}\, v_i\psi_j=\frac{e^3B}{2\pi^2\hbar^2}\int_0^{T_F}\mathrm{d}\tilde{t}\, v_i\psi_j,$$

T_F marking that the integral is to be calculated at the Fermi energy (not to be confused with the Fermi temperature). In the high field limit, the dominating term on the LHS of Eq. F.1 is $\frac{\partial\boldsymbol{\psi}}{\partial\tilde{t}}$ since $\tilde{t}$ expresses the motion of the electron around the Fermi surface due to the magnetic field, while H is a formulation of the scattering. We make an expansion of $\boldsymbol{\psi}$ in the variable B^{-1}: $\boldsymbol{\psi}=\boldsymbol{\psi}^{(0)}+\boldsymbol{\psi}^{(1)}+\ldots$, where (i) denotes the power of B^{-1}. Putting this expansion into Eq. F.1 yields:

$$\frac{\partial}{\partial\tilde{t}}(\boldsymbol{\psi}^{(0)}+\boldsymbol{\psi}^{(1)}+\ldots)+H(\boldsymbol{\psi}^{(0)}+\boldsymbol{\psi}^{(1)}+\ldots)=\mathbf{v} \tag{F.2}$$

We separate Eq. F.2 into terms with equal powers of B:

$$\begin{aligned}
\frac{\partial}{\partial\tilde{t}}\boldsymbol{\psi}^{(0)}&=0 & \boldsymbol{\psi}^{(0)}&=\mathbf{C}^{(0)}\\
\frac{\partial}{\partial\tilde{t}}\boldsymbol{\psi}^{(1)}&=\mathbf{v}-H\boldsymbol{\psi}^{(0)} & \boldsymbol{\psi}^{(1)}&=\mathbf{C}^{(1)}+\int_0^{\tilde{t}}\mathrm{d}\tilde{t}_1\,(\mathbf{v}-H\mathbf{C}^{(0)})\\
\frac{\partial}{\partial\tilde{t}}\boldsymbol{\psi}^{(2)}&=-H\boldsymbol{\psi}^{(1)} & \boldsymbol{\psi}^{(2)}&=\mathbf{C}^{(2)}-\int_0^{\tilde{t}}\mathrm{d}\tilde{t}_1\,H\boldsymbol{\psi}^{(1)}\\
&\vdots & &\vdots
\end{aligned}$$

Here the left column is the differential form and the right one the integral form with the $\mathbf{C}^{(i)}$-vectors containing the integration constants. It is worth noticing that for the closed orbits, the partial derivatives average to zero due to the condition of periodicity:

$$\Big\langle\frac{\partial\boldsymbol{\psi}}{\partial\tilde{t}}\Big\rangle=\frac{1}{T}\int_0^T\mathrm{d}\tilde{t}\,\frac{\partial\boldsymbol{\psi}}{\partial\tilde{t}}=\frac{1}{T}(\boldsymbol{\psi}(T)-\boldsymbol{\psi}(0))=0 \implies$$

$$\begin{aligned}
\langle\mathbf{v}\rangle&=\langle H\mathbf{C}^{(0)}\rangle\\
\langle\mathbf{0}\rangle&=\langle H\boldsymbol{\psi}^{(1)}\rangle\\
&\vdots
\end{aligned}$$

Restraining ourselves to consider only closed orbits, and using Eq. 7.1 for expressing the velocity components, we have:

$$\langle v_x \rangle = \frac{1}{T}\int_0^T \mathrm{d}\tilde{t}\,\frac{\hbar}{eB}\frac{\mathrm{d}k_y}{\mathrm{d}\tilde{t}} = \frac{\hbar}{eB}\frac{1}{T}(k_y(T) - k_y(0)) = 0, \quad \langle v_y \rangle = 0$$
$$\implies \quad C_x^{(0)} = C_y^{(0)} \quad \implies \tag{F.3}$$

$$\begin{aligned}
&\boldsymbol{\psi}^{(0)} = \mathbf{0},\\
&\psi_x^{(1)} = C_x^{(1)} + \int_0^{\tilde{t}} \mathrm{d}\tilde{t}_1\,\frac{\hbar}{eB}\frac{\mathrm{d}k_y}{\mathrm{d}\tilde{t}_1} = C_x^{(1)} + \frac{\hbar}{eB}k_y(\tilde{t}),\\
&\psi_y^{(1)} = C_y^{(1)} - \frac{\hbar}{eB}k_x(\tilde{t}).
\end{aligned}$$

Here we have chosen our coordinate system such that $k_x(0) = k_y(0) = 0$. Since $\boldsymbol{\psi}^{(0)} = \mathbf{0}$, the conductivity tensor will be an integral over terms with B^{-1} or lower powers. Taking first a look at the diagonal terms, generated by $\boldsymbol{\psi}^{(1)}$:

$$\sigma_{xx}^{(1)} = \frac{e^3 B}{2\pi^2\hbar^2}\int_0^{T_F} \mathrm{d}\tilde{t}\,\frac{\hbar}{eB}\frac{\mathrm{d}k_y}{\mathrm{d}\tilde{t}}\Big(C_x^{(1)} + \frac{\hbar}{eB}k_y\Big).$$

Since:

$$\begin{aligned}
\int_0^T \mathrm{d}\tilde{t}\,\frac{\mathrm{d}k_y}{\mathrm{d}\tilde{t}} &= k_y(T) - k_y(0) = 0\,,\\
\int_0^T \mathrm{d}\tilde{t}\,\frac{\mathrm{d}k_y}{\mathrm{d}\tilde{t}}k_y &= \int_{k_y(0)}^{k_y(T)} \mathrm{d}k_y\,k_y = 0\,,
\end{aligned}$$

we get $\sigma_{xx}^{(1)} = 0$ which means the dominating part of σ_{xx} will be of order B^{-2} and likewise for σ_{yy}.

The off-diagonal elements, generated by $\boldsymbol{\psi}^{(1)}$, are:

$$\begin{aligned}
\sigma_{xy}^{(1)} &= \frac{e^3 B}{2\pi^2\hbar^2}\int_0^{T_F} \mathrm{d}\tilde{t}\,v_x\psi_y^{(1)} = \frac{e^3 B}{2\pi^2\hbar^2}\int_0^{T_F} \mathrm{d}\tilde{t}\,\frac{\hbar}{eB}\frac{\mathrm{d}k_y}{\mathrm{d}\tilde{t}}\Big(C_y^{(1)} - \frac{\hbar}{eB}k_x\Big)\\
&= \frac{-e}{2\pi^2 B}\int_0^{T_F} \mathrm{d}\tilde{t}\,\frac{\mathrm{d}k_y}{\mathrm{d}\tilde{t}}k_x = \frac{-e}{2\pi^2 B}\int_{k_y(0)}^{k_y(T)} \mathrm{d}k_y\,k_x\\
&= \frac{-e}{2\pi^2 B}A_e.
\end{aligned}$$

Here, we have again used the periodicity of k_x and k_y in $\tilde{t}$ to see that the $C_y^{(1)}$-term disappears. The A_e in the last line denotes the area of the Fermi surface (which can be parametrized by $k_x(k_y)$), in the case where the perimeter encloses states with energies lower than ε_F. This leads to electron-like orbits. As the electron number density is $n = \frac{A_e}{2\pi^2}$, we get for the conductivity:

$$\sigma_{xy}^{(1)} = \frac{-en}{B},$$

which is exactly what we got in Sec. 3.3.

G The method of Smith & Højgaard for an arbitrary Fermi surface

Say we were given an arbitrary function $k(\varepsilon, \phi)$ which describes the contours of constant energy for some material. Is it then possible, by the method of Smith & Højgaard [3] to solve the Boltzmann equation for the difference in the distribution function from equilibrium, $g = f - f_0$? Proceeding like in Sec. 7, we still have the modified Boltzmann equation:

$$\Big(\omega_c \frac{\partial}{\partial \tilde{\phi}} + \frac{1}{\tau}\Big) g = e\mathbf{E} \cdot \mathbf{v} \frac{\partial f_0}{\partial \varepsilon}, \tag{G.1}$$

and the expression for the cyclotron mass at the Fermi energy:

$$m_0 = \frac{\hbar^2}{2\pi} \frac{\partial A}{\partial \varepsilon}\Big|_{\varepsilon_F} = \frac{\hbar^2}{2\pi} \frac{\partial}{\partial \varepsilon} \Big(\int_0^{2\pi} \mathrm{d}\phi \int_0^{k_F} \mathrm{d}k\, k(\varepsilon, \phi) \Big)\Big|_{\varepsilon_F}.$$

The expressions for the velocity components v_x,v_y at the Fermi energy are:

$$\begin{aligned} \frac{\partial \varepsilon}{\partial k_x}\Big|_{\varepsilon_F} &= \frac{1}{k'(\varepsilon, \phi)|_{\varepsilon_F}} \Big(\cos(\phi) + \frac{\sin(\phi)}{k(\varepsilon, \phi)|_{\varepsilon_F}} \frac{\partial k}{\partial \phi}\Big|_{\varepsilon_F} \Big) \\ \frac{\partial \varepsilon}{\partial k_y}\Big|_{\varepsilon_F} &= \frac{1}{k'(\varepsilon, \phi)|_{\varepsilon_F}} \Big(\sin(\phi) - \frac{\cos(\phi)}{k(\varepsilon, \phi)|_{\varepsilon_F}} \frac{\partial k}{\partial \phi}\Big|_{\varepsilon_F} \Big). \end{aligned}$$

Hence:

$$\mathbf{v} \cdot \mathbf{k} = \frac{k|_{\varepsilon_F}}{\hbar k'|_{\varepsilon_F}} \Big(\Big(1 + \frac{\tan(\phi)}{k|_{\varepsilon_F}} \frac{\partial k}{\partial \phi}\Big|_{\varepsilon_F}\Big) \cos^2(\phi) + \Big(1 - \frac{\cot(\phi)}{k|_{\varepsilon_F}} \frac{\partial k}{\partial \phi}\Big|_{\varepsilon_F}\Big) \sin^2(\phi) \Big) = \frac{k|_{\varepsilon_F}}{\hbar k'|_{\varepsilon_F}}.$$

Since we still have $\frac{\mathrm{d}\tilde{\phi}}{\mathrm{d}\phi} = \frac{\hbar}{m_0} \frac{k^2}{\mathbf{v} \cdot \mathbf{k}}$, this becomes:

$$\frac{\mathrm{d}\tilde{\phi}}{\mathrm{d}\phi} = \frac{\hbar}{m_0} \frac{k^2 \hbar k'}{k}\Big|_{\varepsilon_F} = \frac{2\pi k k'|_{\varepsilon_F}}{\frac{\partial}{\partial \varepsilon} \Big(\int_0^{2\pi} \mathrm{d}\phi \int_0^{k_F} \mathrm{d}k\, k(\varepsilon, \phi) \Big)\Big|_{\varepsilon_F}}.$$

If we can write the reciprocal of this, $\frac{\mathrm{d}\phi}{\mathrm{d}\tilde{\phi}}$, as a Fourier series, so that Eq. G.1 can be expressed as:

$$\Big(\omega_c \frac{\partial}{\partial \phi} + \sum_k l_k \mathrm{e}^{ik\phi}\Big) \sum_n g_n \mathrm{e}^{in\phi} = \tilde{E} \sum_m r_m^{(\nu)} \mathrm{e}^{im\phi},$$

with

$$\sum_k l_k \mathrm{e}^{ik\phi} = \frac{1}{\tau} \left(\frac{\frac{\partial}{\partial \varepsilon} \Big(\int_0^{2\pi} \mathrm{d}\phi \int_0^{k_F} \mathrm{d}k\, k(\varepsilon, \phi) \Big)\Big|_{\varepsilon_F}}{2\pi k k'|_{\varepsilon_F}} \right),$$

and

$$\tilde{E} \sum_m r_m^{(\nu)} = \frac{eE}{\hbar} \frac{\partial f_0}{\partial \varepsilon} \left(\frac{\frac{\partial}{\partial \varepsilon} \Big(\int_0^{2\pi} \mathrm{d}\phi \int_0^{k_F} \mathrm{d}k\, k(\varepsilon, \phi) \Big)\Big|_{\varepsilon_F}}{2\pi k k'|_{\varepsilon_F}} \right) \sum_{m'} \zeta_{m'} \mathrm{e}^{im'\phi}.$$

Then it is possible to solve for g as a Fourier series and to find $\sigma_{\mu\nu}$ like in Sec. 7.2.