An Introduction to the Electric Conduction in Crystals

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1 Velocity of band electrons and current density

The electronic states of crystals are described by the band structure $E_n(\mathbf{k})$, where n is the discrete band index and $\mathbf{k}$ the continuous Bloch vector restricted to the first Brillouin zone.[2] In a single-particle description these energies $E_n(\mathbf{k})$ are the eigenvalues of the crystal Hamiltonian

$$\hat{H}(\mathbf{r})\Psi_{n\mathbf{k}}(\mathbf{r}) = E_n(\mathbf{k})\Psi_{n\mathbf{k}}(\mathbf{r}) \tag{1}$$

Being stationary states, the time and space dependence of the Bloch functions $\Psi_{n\mathbf{k}}(\mathbf{r},t)$ is just given by

$$\Psi_{n\mathbf{k}}(\mathbf{r},t) = \mathrm{e}^{\mathrm{i}(\mathbf{k}\cdot\mathbf{r}-\omega_n(\mathbf{k})t)}u_{n\mathbf{k}}(\mathbf{r}) \quad \text{with} \quad \omega_n(\mathbf{k}) = \frac{1}{\hbar}E_n(\mathbf{k}) \tag{2}$$

where $u_{n\mathbf{k}}(\mathbf{r}+\mathbf{R}) = u_{n\mathbf{k}}(\mathbf{r})$ is a lattice-periodic function. The plane waves $\mathrm{e}^{\mathrm{i}(\mathbf{k}\cdot\mathbf{r}-\omega_n(\mathbf{k})t)}$ provide a constant probability density over the entire crystal. Localized states (with an extension still much larger than the unit cell) can be described by wave packets containing $\mathbf{k}$-values from a small interval around $\mathbf{k}_0$ and a fixed band. Then this wave packet moves with the group velocity[3] $\mathbf{v}_n(\mathbf{k}_0) = \frac{\partial\omega_n(\mathbf{k})}{\partial\mathbf{k}}_{|\mathbf{k}=\mathbf{k}_0}$. Thus we find:

Bloch states with Bloch vector $\mathbf{k}_0$ in band n provide moving electrons with velocity

$$\mathbf{v}_n(\mathbf{k}_0) = \frac{1}{\hbar}\frac{\partial E_n(\mathbf{k})}{\partial\mathbf{k}}_{|\mathbf{k}=\mathbf{k}_0} \tag{3}$$

This velocity is also called the band velocity of the electron. Alternatively, this relation can be proven by considering the current density carried by the Bloch state, see e.g. Appendix E of [1].

The current density carried by a band n is obtained by summing over all Bloch vectors within the first Brillouin zone (we assume a finite crystal with volume V to simplify the counting)

$$\mathbf{j}_n = \frac{-2(\text{for spin})e}{V}\sum_{\mathbf{k}} f_n(\mathbf{k})\mathbf{v}_n(\mathbf{k})$$

where $f_n(\mathbf{k}) \in [0,1]$ denotes the occupation of the Bloch state. Now the spacing between the allowed $\mathbf{k}$-values is $\Delta k^3 = (2\pi)^3/V$, so that we can replace the sum by an integral $\sum_{\mathbf{k}} \to \frac{V}{(2\pi)^3}\int \mathrm{d}^3k$ (called continuum limit) and obtain

$$\mathbf{j}_n = \frac{-2(\text{for spin})e}{(2\pi)^3}\int_{\text{first Brillouin zone}} \mathrm{d}^3k\, f_n(\mathbf{k})\mathbf{v}_n(\mathbf{k}) \tag{4}$$

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[2] See notes `http://www.teorfys.lu.se/staff/Andreas.Wacker/Scripts/bandstructure_intro.pdf`

[3] See notes `http://www.teorfys.lu.se/staff/Andreas.Wacker/Scripts/wavepacket.pdf`

In the following we frequently drop the subscript of the integral and tacitly assume that the k-integral always covers the first Brillouin zone.

Any band structure has the symmetry[4] $E_n(-\mathbf{k}) = E_n(\mathbf{k})$, which provides $\mathbf{v}_n(-\mathbf{k}) = -\mathbf{v}_n(\mathbf{k})$. In thermal equilibrium the occupation of the Bloch states is given by the Fermi distribution

$$f_n^0(\mathbf{k}) = \frac{1}{e^{E_n(\mathbf{k})/k_BT}+1} \tag{5}$$

and thus $f_n^0(-\mathbf{k}) = f_n^0(\mathbf{k})$. Therefore the velocities of the states with $-\mathbf{k}$ and $\mathbf{k}$ compensate each other so that total current vanishes in thermal equilibrium. This obviously also holds for a completely filled band with $f_n(\mathbf{k}) \equiv 1$. Thus we find

Only partially filled bands, where the electron distribution is not in equilibrium, contribute to the electric current.

2 Kinetics in an electric field

If a force $\mathbf{F}$ is acting on a moving particle with velocity $\mathbf{v}$ the power $P = \mathbf{F}\cdot\mathbf{v}$ is the energy transferred to the particle per time. For electrons in a crystal this change in energy, means that another state in the band structure with a different energy has to be taken. As the band structure is continuous in the Bloch vector, this means, that the change in energy is associated with a change in Bloch vector. For a localized wave packet around $\mathbf{k}_0$ this means

$$\mathbf{v}_n(\mathbf{k}_0)\cdot\mathbf{F} = P = \frac{\mathrm{d}E_n(\mathbf{k}_0)}{\mathrm{d}t} = \frac{\partial E_n(\mathbf{k})}{\partial \mathbf{k}}_{|\mathbf{k}=\mathbf{k}_0}\cdot\dot{\mathbf{k}}_0 = \mathbf{v}_n(\mathbf{k}_0)\cdot\hbar\dot{\mathbf{k}}_0$$

where Eq. (3) was used. This equation is satisfied if $\hbar\dot{\mathbf{k}}_0 = \mathbf{F}$ holds (note that this is only necessary to hold in the direction of $\mathbf{v}_n(\mathbf{k}_0)$, a full proof goes far beyond these notes). The force on electrons results from electric ($\boldsymbol{\mathcal{E}}$) and magnetic ($\mathbf{B}$) fields as given by the Lorentz force $\mathbf{F} = -e(\boldsymbol{\mathcal{E}} + \mathbf{v}\times\mathbf{B})$ providing

In the presence of electric and magnetic fields the Bloch vector $\mathbf{k}$ of a Bloch state changes according to

$$\hbar\dot{\mathbf{k}} = -e\left[\boldsymbol{\mathcal{E}} + \mathbf{v}_n(\mathbf{k})\times\mathbf{B}\right] \tag{6}$$

The electric and magnetic fields break the translational invariance of the Hamiltonian. Thus the Bloch states are no longer eigenstates but change in time according to Eq. (6). (This is also the basis of a proof for the case of the electric field given in Appendix E of [2].) At the same time the band index is conserved unless the fields are strong.[5] Note that the proof of Eq. (6) for the magnetic field is far from trivial and its validity is debated.

For free particles the de Broglie relation ($p = h/\lambda$) reads $\mathbf{p} = \hbar\mathbf{k}$ in vector notation. Thus Newton's law $\dot{\mathbf{p}} = \mathbf{F}$ directly transfers to $\hbar\dot{\mathbf{k}} = \mathbf{F}$ in full analogy for the situation of electrons in crystals discussed above. Therefore the quantity $\hbar\mathbf{k}$ is often called *quasi-momentum* for Bloch electrons.

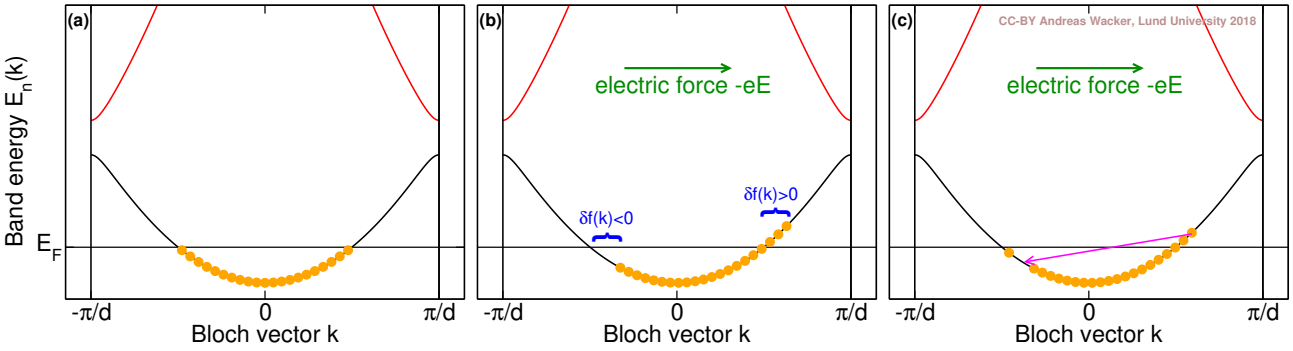

Figure 1: Occupation of Bloch states in equilibrium (a) and after a short pulse with a negative electric field. (c) sketches a stationary state, where scattering processes (as indicated by the magenta arrow) compensate the acceleration by a constant field. See also the animation www.teorfys.lu.se/staff/Andreas.Wacker/Scripts/current-by-field-and-scattering.gif.

3 Qualitative description of current in one dimension

Figure 1(a) shows the occupation of Bloch states in a one-dimensional structure, where two bands ($n = 1, 2$) are shown. In thermal equilibrium (here we assume $T \approx 0$) the lowest energy states are occupied up to the Fermi level E_F, as described by the distribution function $f_0(k) = \Theta(E_F - E(k))$ with the Heaviside function $\Theta(x) = 1$ for $x > 0$ and $\Theta(x) = 0$ for $x < 0$. As discussed above, no net current is flowing, as the right moving states with $v_1(k) > 0$ for $k > 0$ are fully compensated by left moving states with $v_1(k) < 0$ for $k < 0$. After a short pules with electric field $\mathcal{E}_0$ and time Δt, all k states are shifted by $\Delta k = \mathcal{E}_0 \Delta t/\hbar$ according to Eq. (6), as illustrated in Fig. 1(b) for a negative $\mathcal{E}_0$. This provides a new distribution function $f(k) = f_0(k) + \delta f(k)$, where $\delta f(k)$ is positive for $k_F < k < k_F + \Delta k$ and negative for $-k_F < k < -k_F + \Delta k$. The corresponding electrical current from Eq. (4)

$$j_1 = \frac{-2(\text{for spin})e}{2\pi} \int \mathrm{d}k\, \delta f(k) v_1(k)$$

is negative and thus points along the field.

The Bloch states are eigenstates of the perfect crystal and thus the electrons would remain in such a state forever. Additional external electric and magnetic fields provide the dynamics (6), transferring Bloch states into different ones in a well-defined manner. However, deviations from the exact lattice periodicity due to lattice vibrations or lattice defects provide transitions between different Bloch states by so called scattering processes. Typically, the energy of the electrons is decreased during scattering, where the excess energy is transferred to a thermal reservoir (such as the lattice vibrations). Such processes will eventually restore the equilibrium distribution $f_0(k)$, as demanded by thermodynamics. For a constant electric field the interplay between scattering and increasing k-values due to the field establishes a steady state as depicted in Fig. 1(c). This results in a constant current for a constant electric field and establishes the physical origin of the electric conductivity.

[4]This is called Kramer's degeneracy and is a consequence of the Hermiticity of the Hamiltonian. If the band structure is spin dependent, one has to flip the spin together with the direction of $\mathbf{k}$.

[5]Zener tunneling is a typical example where the electrons are transferred from the valence to the conduction band at a high electric field

4 Effective mass

The acceleration of Bloch electrons in x direction is given by

$$\dot{v}_x = \frac{\mathrm{d}}{\mathrm{d}t}\frac{1}{\hbar}\frac{\partial E_n(\mathbf{k})}{\partial k_x} = \frac{1}{\hbar}\sum_{j=x,y,z}\frac{\partial^2 E_n(\mathbf{k})}{\partial k_x \partial k_i}\dot{k}_j = \frac{1}{\hbar^2}\sum_{j=x,y,z}\frac{\partial^2 E_n(\mathbf{k})}{\partial k_x \partial k_j}(-e)\left[\boldsymbol{\mathcal{E}} + \mathbf{v}_n(\mathbf{k})\times\mathbf{B}\right]_j$$

where Eqs. (3,6) were used. The accelerations in y and z direction are analogously. In classical physics the ratio between force and acceleration is the mass m of the particle. In our case the acceleration is not necessarily parallel to the force and thus the mass has to be replaced by a matrix $\mathcal{M}$.

The effective mass of a Bloch electron is given by the matrix $\mathcal{M}_n(\mathbf{k})$ where the elements of the inverse matrix are given

$$\left[\mathcal{M}_n^{-1}(\mathbf{k})\right]_{ij} = \frac{1}{\hbar^2}\frac{\partial^2 E_n(\mathbf{k})}{\partial k_i \partial k_j} \tag{7}$$

which provides the acceleration

$$\dot{\mathbf{v}}_n(\mathbf{k}) = -e\mathcal{M}_n^{-1}(\mathbf{k})\cdot\left[\boldsymbol{\mathcal{E}} + \mathbf{v}_n(\mathbf{k})\times\mathbf{B}\right] \tag{8}$$

For free electrons with $E_n(\mathbf{k}) = \hbar^2\mathbf{k}^2/2m$ we find $\mathcal{M}_{ij}^{-1} = \delta_{ij}/m$ or $\mathcal{M} = m\mathcal{I}$, where $\mathcal{I}$ is the unit matrix.

For one-dimensional structures with period d, the Brillouin zone extends from $-\pi/d$ to π/d. Then we find

$$\int_{-\pi/d}^{\pi/d}\mathrm{d}k\frac{1}{m_n(k)} = \frac{1}{\hbar^2}\left(\frac{\partial E_n(\pi/d)}{\partial k} - \frac{\partial E_n(-\pi/d)}{\partial k}\right)$$

As the Bloch vectors k and $k + 2\pi/d$ are equivalent, we have $E_n(k + 2\pi/d) = E_n(k)$ and correspondingly, both terms in the bracket cancel each other. Similarly one can show in three dimensions (using the technique discussed in appendix J of [1])

$$\int_{\text{first Brillouin zone}}\mathrm{d}^3k\left[\mathcal{M}_n(\mathbf{k})\right]^{-1} = 0 \tag{9}$$

and the average (inverse) mass in a band is zero. This will be used to study the conduction properties of solids in the subsequent section.

5 Quantifying the conductivity of crystals

If an electric field is applied to a crystal, the Bloch vector changes according to Eq. (6) and the carriers accelerate according to Eq. (8). Summing over an entire band, we obtain the total acceleration in band n.

$$n_n\langle\dot{\mathbf{v}}\rangle = \frac{2(\text{for spin})}{V}\sum_{\mathbf{k}} f_{n\mathbf{k}}\mathcal{M}_n^{-1}(\mathbf{k})(-e\boldsymbol{\mathcal{E}}) = \frac{2}{(2\pi)^3}\int\mathrm{d}^3k\, f_n(\mathbf{k})\mathcal{M}_n^{-1}(\mathbf{k})(-e\boldsymbol{\mathcal{E}}) \tag{10}$$

where $n_n = \frac{2}{V}\sum_{\mathbf{k}} f_n(\mathbf{k})$ is the electron density in the band n. (Here we used the continuum limit in the second part.)

For a full band, we have $f_n(\mathbf{k}) = 1$ for all $\mathbf{k}$ and thus Eq. (9) provides a zero net acceleration. Thus the average velocity remains zero and there is no current flowing in the presence of an

electric field. For an empty band there is obviously neither any contribution to the electrical current. Again we find, that only partially filled bands contribute to the electric conduction for moderate fields. (For very high fields transitions to higher bands provide a breakdown)

Due to the Pauli principle each level can be occupied by a single electron (or two in the common case of spin degeneracy). Then the energetically lowest state is obtained by subsequently occupying the levels with increasing energy until the number of electrons matches the ionic charges to guarantee charge neutrality. The energy of the uppermost occupied level is called the Fermi level E_F. Thus for zero temperature the occupation probability becomes $f_n(\mathbf{k}) = \Theta(E_F - E_n(k))$. If the Fermi level is located within an energy gap (of width E_g) in the bandstructure all bands are either entirely filled or empty and the conductance vanishes in an ideal case. As thermal excitations always provide a few carriers in the empty bands, there is some residual conductivity for *semiconductors*, unless $E_g \gg k_B T$, which is the case for *insulators*. The differentiation between semiconductors and insulators is however not sharp. On the other hand, a much higher conductance is found for *metals*, where the Fermi level is within the conduction band.

The lack of exact periodicity of a real crystal provides scattering between the Bloch states, which effectively randomizes the motion of electrons and leads eventually to a relaxation of the electron distribution function $f_n(\mathbf{k})$ towards the equilibrium $f_n^0(\mathbf{k})$. In particular this acts as a kind of friction to the mean electron velocity

$$\left.\frac{\mathrm{d}\langle\mathbf{v}\rangle}{\mathrm{d}t}\right|_{\text{scatt}} = -\frac{\langle\mathbf{v}\rangle}{\tau} \tag{11}$$

where the (momentum) scattering time τ relates to the microscopic transition rate between the Bloch states. As a consequence the total change in average velocity is $\mathrm{d}\langle\mathbf{v}\rangle/\mathrm{d}t = \langle\dot{\mathbf{v}}\rangle + \left.\frac{\mathrm{d}\langle\mathbf{v}\rangle}{\mathrm{d}t}\right|_{\text{scatt}}$ as given by Eqs. (10,11). In a stationary state, $\langle\mathbf{v}\rangle$ is constant and thus satisfies

$$n_n\langle\mathbf{v}\rangle_{\text{stationary}} = \frac{2\tau}{(2\pi)^3}\int \mathrm{d}^3k\, f_n(\mathbf{k})\mathcal{M}_n^{-1}(\mathbf{k})\cdot(-e\boldsymbol{\mathcal{E}}) \tag{12}$$

For weak fields, the occupation function $f_{n\mathbf{k}}$ can be approximated by the thermal distribution $f^0_{n\mathbf{k}}$ and we obtain the current density $\mathbf{j}_n = -en_n\langle\mathbf{v}\rangle_{\text{stationary}}$ of the band n

$$\mathbf{j}_n = \frac{2e^2\tau}{(2\pi)^3}\int \mathrm{d}^3k\, f_n^0(\mathbf{k})\mathcal{M}_n^{-1}(\mathbf{k})\cdot\boldsymbol{\mathcal{E}} \tag{13}$$

Summing over all partically occupied bands, this provides us with a linear relation $\mathbf{j} = \underline{\underline{\sigma}}\cdot\boldsymbol{\mathcal{E}}$, where the matrix of the *conductivity* $\underline{\underline{\sigma}}$ is obtained by summing over all relevant (i.e. partially occupied) bands. Multiplying by geometrical factors, this provide Ohm's law $I = U/R$ for a finite piece of material. Eq. (13) can be simplified for special cases as discussed in the following subsections:

5.1 Simple metals with free electron behavior

In a free electron model, which is good for many metals, we simply get $E_n(\mathbf{k}) \approx \hbar^2k^2/2m_e$. In this case the inverse mass is constant and Eq. (13) provides the

Electric conductivity of simple metals $\quad \sigma = \dfrac{n_c e^2\tau}{m_e}$

Assuming that the electron density matches the atomic density of about $(3\text{Å})^{-3} \approx 4\times10^{22}/\text{cm}^3$ and $\tau \sim 10$ fs we obtain $\sigma \sim 10^7$ A/Vm. This matches measured conductivities of iron and platinum at room temperature. The conductivities of copper and silver are six times larger corresponding to longer scattering times.

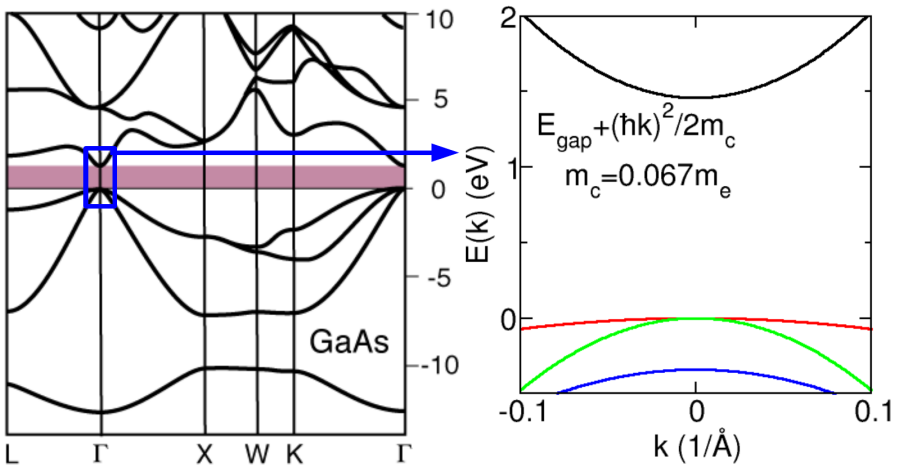

Figure 2: Band structure close the minimum of the conduction and maximum of the valence band of GaAs. [Left panel adapted from M. Rohlfing *et al.*, Phys. Rev. B **48**, 17791 (1993)].

5.2 Semiconductors with some electrons in the conduction band

An ideal semiconductor has no electrons in the lowest empty band above E_F called *conduction band*. However due to thermal excitations, doping, irradiation, or charges electrically induced at interfaces there may be a few electrons with density n_c in the conduction band. Typical values for n_c vary between $10^{15}/\mathrm{cm}^3$ and $10^{19}/\mathrm{cm}^3$ which is several orders of magnitudes lower than in metals. Thus only the energetically lowest states of the conduction band close to its minimum are occupied. Close to its minimum the conduction band energies $E_c(\mathbf{k})$ are quadratic in $\mathbf{k}$, see Fig. 2. If the minimum is at the Γ point, which is the case for several III/V semiconductors such as GaAs[6], we may write

$$E_c(\mathbf{k}) \approx E_c + \frac{\hbar^2\mathbf{k}^2}{2m_c}$$

where the effective mass of the conduction band m_c is a parameter obtained from the second derivative of the band structure, i.e. $\mathcal{M}_c(\mathbf{k}=0) = m_c\mathcal{I}$. Typical values are of the order of $0.1m_e$. Similar to the case of metals we thus find $\sigma = \frac{n_c e^2\tau}{m_c}$, where now the effective mass replaces the electron mass. As the electron density can change over a larger range, one typically defines the

Mobility of electrons in the conduction band in a semiconductor

$$\mu_e = \frac{e\tau}{m_c} \quad \text{satisfying} \quad \langle\mathbf{v}\rangle = -\mu_e\boldsymbol{\mathcal{E}}$$

where the sign results from the electron charge. Typical values for the electron mobility in semiconductors are between $10^3\mathrm{cm}^2/\mathrm{Vs}$ and $10^4\mathrm{cm}^2/\mathrm{Vs}$ at room temperature corresponding to $\tau \sim 0.3$ ps. Much larger scattering times and mobilities can be obtained in clean samples at low temperatures.

[6]Things are more complicated in silicon, where there are several equivalent minima at finite $\mathbf{k}$ which all have an anisotropic mass tensor. However one can define the conductivity effective mass, so that the result looks alike.

5.3 Semiconductors with some holes in the valence band

The energetically lowest state of an ideal semiconductor is achieved if all states of the *valence band* (the uppermost filled band) are occupied. However due to thermal excitations, doping, irradiation, or charges electrically induced at interfaces there may be a few electrons missing. Writing the occupation probability of the valence band as $f_v(\mathbf{k}) = 1 - f_h(-\mathbf{k})$, we can interpret $f_h(\mathbf{k})$ as the probability to find a missing electron, called *hole*, at $-\mathbf{k}$.[7] The density of holes n_h typically varies between $10^{15}/\mathrm{cm}^3$ and $10^{19}/\mathrm{cm}^3$, which is several orders of magnitudes lower than the total number of states in the valence band. Thus only the energetically highest states of the valence band, close to its maximum are emptied. Close to its maximum the valence band energies $E_v(\mathbf{k})$ are quadratic in $\mathbf{k}$, see Fig. 2. If the maximum is at the Γ point, which is the case for all commonly used semiconductors[8], we may write

$$E_v(\mathbf{k}) \approx E_v - \frac{\hbar^2\mathbf{k}^2}{2m_h}$$

where the *hole mass* m_h of the conduction band is a parameter obtained from the second derivative of the band structure, i.e. $\mathcal{M}_v(\mathbf{k}=0) = -m_h\mathcal{I}$. Note that $\mathcal{M}_v(\mathbf{k}=0)$ is negative as we are at a maximum of the band, while we define m_h to be positive. Now Eq. (13) becomes

$$\begin{aligned}\mathbf{j} =& \frac{e^2\tau}{(2\pi)^3}\int \mathrm{d}^3k\, \left[1 - f_h^0(-\mathbf{k})\right] \mathcal{M}_v^{-1}(\mathbf{k})\boldsymbol{\mathcal{E}} \\ \approx& \frac{e^2\tau}{(2\pi)^3}\int \mathrm{d}^3k\, f_h^0(-\mathbf{k})\frac{1}{m_h}\boldsymbol{\mathcal{E}} = n_h\frac{e^2\tau}{m_h}\boldsymbol{\mathcal{E}}\end{aligned}$$

where Eq. (9) was used and the approximation $\mathcal{M}_v(\mathbf{k}) \approx -m_h\mathcal{I}$ was applied as $f_h(\mathbf{k})$ is vanishing unless close to the maximum of the valence band. This provides the conductivity $\sigma = \frac{n_h e^2\tau}{m_h}$. Note that instead of the electron density, the hole density determines the contribution to the conductance from the valence band. Thus one may say that the current is carried by holes with a positive charge e and an average velocity $\mu_h\boldsymbol{\mathcal{E}}$ where the hole mobility is given by $\mu_h = e\tau/m_h$ in full analogy to the situation in the conduction band.

6 Hall effect

Let us have a closer look at the acceleration due to the magnetic term of (6). For this case the acceleration provides analogously to Eq. (10)

$$n_n\langle\dot{\mathbf{v}}\rangle_{|\mathrm{mag}} = \frac{-2e}{(2\pi)^3}\int \mathrm{d}^3k\, f_n(\mathbf{k})\mathcal{M}_n^{-1}(\mathbf{k})\cdot[\mathbf{v}_n(\mathbf{k})\times\mathbf{B}]$$

Writing $f_n(\mathbf{k}) = f_n^0(\mathbf{k}) + \delta f_n(\mathbf{k})$ we find that $f_n^0(\mathbf{k})$ does to contribute to $\langle\dot{\mathbf{v}}\rangle_{|\mathrm{mag}}$ as the terms with $\pm\mathbf{k}$, which have the same energy and opposite velocity due to the Kramers degeneracy, cancel each other. Thus

$$n_n\langle\dot{\mathbf{v}}\rangle_{|\mathrm{mag}} = \frac{-2e}{(2\pi)^3}\int \mathrm{d}^3k\, \delta f_n(\mathbf{k})\mathcal{M}_n^{-1}(\mathbf{k})\cdot[\mathbf{v}_n(\mathbf{k})\times\mathbf{B}] \tag{14}$$

is only present for non-equilibrium distributions, such as for current flow as discussed in Sec. 3.

[7] The change of sign in $-\mathbf{k}$ is not of relevance for our treatment here. It is needed for full consistency [2].

[8] The situation is actually more complicated due to the presence of three maxima at the Γ point.

If the effective mass is constant and isotropic $\mathcal{M}_n^{-1}(\mathbf{k}) \approx 1/m_{\text{relevant}}$ for the region with $\delta f(\mathbf{k}) \neq 0$ (e.g., this applies to all three cases discussed in Secs. 5.1,5.2,5.3) we find

$$n_n \langle \dot{\mathbf{v}} \rangle_{|\text{mag}} = \frac{1}{m_{\text{relevant}}} \mathbf{j} \times \mathbf{B} \tag{15}$$

where the current density is obtained from Eq. (4) taking into account that $f_n^0(\mathbf{k})$ provides a zero result. In the stationary state, this acceleration perpendicular to the main current flow is compensated by the Hall field $\boldsymbol{\mathcal{E}}_H$ yielding the acceleration from Eq. (10)

$$-n_n \langle \dot{\mathbf{v}} \rangle_{|\text{mag}} = n_n \langle \dot{\mathbf{v}} \rangle_{|\text{Hall}} = -\frac{2e}{(2\pi)^3} \int \mathrm{d}^3k \, f_n(\mathbf{k}) \mathcal{M}_n^{-1}(\mathbf{k}) \cdot \boldsymbol{\mathcal{E}}_H \approx -\frac{2e}{(2\pi)^3} \int \mathrm{d}^3k \, f_n^0(\mathbf{k}) \mathcal{M}_n^{-1}(\mathbf{k}) \cdot \boldsymbol{\mathcal{E}}_H$$

(If more than one band is partially occupied, we need to sum over the corresponding bands, which makes things more complicated.) In the three cases of Secs. 5.1,5.2,5.3), the right-hand side can be easily evaluated. We find for

simple metals: $-n_n \langle \dot{\mathbf{v}} \rangle_{|\text{mag}} \approx -e n_c \boldsymbol{\mathcal{E}}_H / m_e$. With $m_{\text{relevant}} = m_e$ in Eq. (15) this yields

$$\boldsymbol{\mathcal{E}}_H = R_H \mathbf{B} \times \mathbf{j} \quad \text{with } R_H = -\frac{1}{n_c e}$$

in agreement with the Drude model.

semiconductors with conduction electrons: $-n_n \langle \dot{\mathbf{v}} \rangle_{|\text{mag}} \approx -e n_c \boldsymbol{\mathcal{E}}_H / m_c$. With $m_{\text{relevant}} = m_c$ in Eq. (15) this yields again

$$\boldsymbol{\mathcal{E}}_H = R_H \mathbf{B} \times \mathbf{j} \quad \text{with } R_H = -\frac{1}{n_c e}$$

semiconductors with missing valence electrons/holes: $-n_n \langle \dot{\mathbf{v}} \rangle_{|\text{mag}} \approx -e n_h \boldsymbol{\mathcal{E}}_H / m_h$. With $m_{\text{relevant}} = -m_h$ in Eq. (15) this yields

$$\boldsymbol{\mathcal{E}}_H = R_H \mathbf{B} \times \mathbf{j} \quad \text{with } R_H = \frac{1}{n_h e}$$

which agrees with the concept of a flow of positively charged particles with density n_h.

Several metals have actually the Fermi level close to the top of a band, where the effective mass is negative. Albeit details are more complicated and typically several bands are partially occupied, this resembles the holes in semiconductors and allows for positive Hall coefficients as easily observed in Zinc, which also exhibits a strong anisotropy[3]. (Positive Hall coefficients appear in many other metals, such as Aluminium and Indium, see Table 4 of [2], albeit only at low magnetic fields [4].)

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