CHAPTER 4

BOLTZMANN EQUATION FOR TRANSPORT

4.1 MOTION OF AN ELECTRON IN AN ENERGY BAND

4.1.1 Semiclassical equation of motion

We consider an electron subjected to slowly varying external fields.

Within a single isolated energy band n, the electron can be represented by a wave packet of Bloch states, narrowly distributed around a central wave vector $\mathbf{k}_c$.

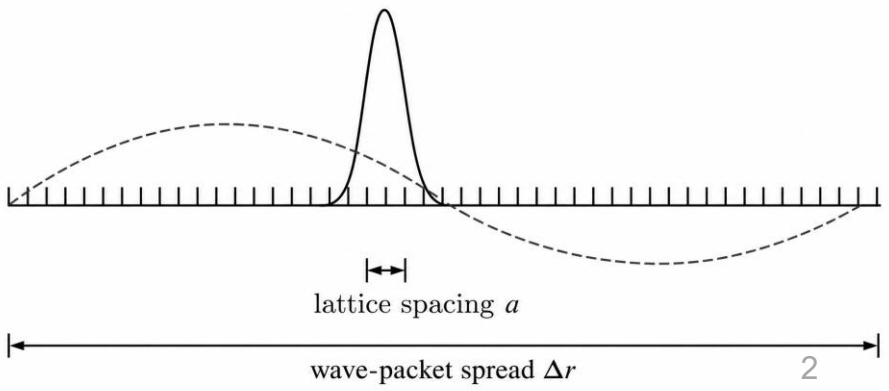
The width Δk of the packet in reciprocal space must be small compared with the size of the Brillouin zone

$$\Delta k \ll \frac{1}{a},$$ where a is the lattice constant.

Consequently, its spatial extent satisfies $$\Delta r \sim \frac{1}{\Delta k} \gg a,$$

Because the band energy $\varepsilon_n(\mathbf{k})$ varies smoothly over the narrow range Δk, the wave packet can be assigned the energy $\varepsilon_n(\mathbf{k}_c)$.

The semiclassical approximation is valid when the external fields vary negligibly over the spatial extent Δr of the packet. The electron state can be described by the position $\mathbf{r}_c$ and wave vector $\mathbf{k}_c$ of the packet centre.



4.1 MOTION OF AN ELECTRON IN AN ENERGY BAND

4.1.1 Semiclassical equation of motion

Slowly varying external fields act on the centre of a Bloch wave packet through classical forces.

The description is called semiclassical because the electronic states and the band dispersion $\varepsilon(\mathbf{k})$ are determined quantum mechanically, whereas the motion of the wave-packet centre is described by classical dynamical variables.

As in wave optics, the centre of a wave packet moves with the group velocity. In one dimension,

$$v_g = \frac{d\omega}{dk}.$$

Since the energy of a Bloch state is related to its angular frequency by $\varepsilon(k) = \hbar\omega(k)$,

the group velocity becomes

$$v(k) = \frac{1}{\hbar}\frac{d\varepsilon(k)}{dk}.$$

More generally, in three dimensions,

$$\mathbf{v}(\mathbf{k}) = \frac{1}{\hbar}\boldsymbol{\nabla}_{\mathbf{k}}\varepsilon(\mathbf{k}).$$

Thus, the band dispersion determines the velocity associated with each wave vector $\mathbf{k}$.

4.1 MOTION OF AN ELECTRON IN AN ENERGY BAND

4.1.1 Semiclassical equation of motion

For an electron wave packet in a band $\varepsilon(\mathbf{k})$, the group velocity is determined by its central wave vector $\mathbf{k}$.

$$\mathbf{v}(\mathbf{k}) = \frac{1}{\hbar}\nabla_{\mathbf{k}}\varepsilon(\mathbf{k})$$

In the absence of external fields, $\mathbf{k}$ remains constant; consequently, the wave-packet $\mathbf{v}(\mathbf{k})$ is also constant.

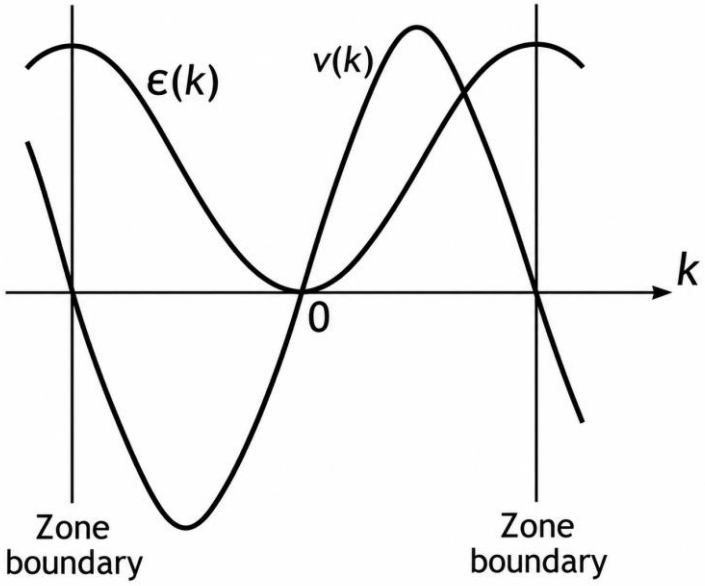
The effects of the periodic crystal potential are already contained in the Bloch states and in the band dispersion $\varepsilon(\mathbf{k})$. They must therefore not be regarded as an additional external force acting on the electron.

In the one-dimensional case, $v(k) = 0$ at the extrema of $\varepsilon(k)$, where

$$\frac{d\varepsilon(k)}{dk} = 0.$$

In particular, for the lowest band, these extrema occur at the centre of the Brillouin zone and at its boundaries.

Therefore, ther group velocity vanishes at the extrema of the energy band, both at the zone centre and at the zone boundaries.



4.1 MOTION OF AN ELECTRON IN AN ENERGY BAND

4.1.1 Semiclassical equation of motion

We now consider the effect of an external force on an electron wave packet.

Let us first restrict the discussion to one dimension. We assume that the force is sufficiently weak and slowly varying that the wave packet remains within the same energy band; interband transitions are therefore neglected.

During the time interval dt, the work done by an external force F is:

$$dW = F\, v(k)\, dt.$$

This work changes the energy of the wave packet:

$$d\varepsilon = \frac{d\varepsilon(k)}{dk}\, dk.$$

Using the group-velocity relation, we obtain:

$$v(k) = \frac{1}{\hbar}\frac{d\varepsilon(k)}{dk}$$

$$d\varepsilon = \hbar v(k)\, dk.$$

Equating the work done by the force to the change in band energy gives

$$F\, v(k)\, dt = \hbar v(k)\, dk.$$

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4.1.1 Semiclassical equation of motion

$$F\,v(k)\,dt = \hbar v(k)\,dk$$

Therefore,

$$F = \hbar \frac{dk}{dt}.$$

In three dimensions, the semiclassical equation of motion becomes:

$$\hbar \frac{d\mathbf{k}}{dt} = \mathbf{F}.$$

An external force therefore changes the wave vector $\mathbf{k}$ of the Bloch wave packet in the same formal way as it changes the momentum of a free particle.

However, $\hbar\mathbf{k}$ is the **crystal momentum** (or quasimomentum) of the Bloch electron. It is not, in general, equal to the mechanical momentum of the electron.

Differentiating the velocity with respect to time gives the electron acceleration:

$$v(k) = \frac{1}{\hbar}\frac{d\varepsilon(k)}{dk}$$

$$a = \frac{dv}{dt} = \frac{1}{\hbar}\frac{d^2\varepsilon(k)}{dk^2}\frac{dk}{dt}.$$

4.1 MOTION OF AN ELECTRON IN AN ENERGY BAND

4.1.2 Dynamic effective mass

$$F = \hbar \frac{dk}{dt} \qquad a = \frac{1}{\hbar} \frac{d^2\varepsilon(k)}{dk^2} \frac{dk}{dt}$$

Using the expression obtained for the acceleration, we find

$$a = \frac{1}{\hbar^2} \frac{d^2\varepsilon(k)}{dk^2} F.$$

This motivates the definition of the effective mass:

$$\frac{1}{m^*(k)} \equiv \frac{1}{\hbar^2} \frac{d^2\varepsilon(k)}{dk^2}.$$

The equation of motion can therefore be written in the Newton-like form:

$$F = m^*(k)\, a.$$

The effective mass is determined by the local curvature of the energy band and may depend on k. In particular, its sign follows the sign of $d^2\varepsilon/dk^2$.

4.1 MOTION OF AN ELECTRON IN AN ENERGY BAND

4.1.2 Dynamic effective mass

$$\frac{1}{m^*(k)} \equiv \frac{1}{\hbar^2}\frac{d^2\varepsilon(k)}{dk^2}$$

In three dimensions, the effective mass is generally a 3×3 tensor.

The inverse effective-mass tensor is defined by

$$[\mathbf{M}^{*-1}(\mathbf{k})]_{ij} \equiv \frac{1}{\hbar^2}\frac{\partial^2 \varepsilon(\mathbf{k})}{\partial k_i \, \partial k_j}.$$

The acceleration of the wave packet is therefore.

$$a_i = \sum_j [\mathbf{M}^{*-1}(\mathbf{k})]_{ij} F_j.$$

Equivalently,

$$\mathbf{a} = \mathbf{M}^{*-1}(\mathbf{k}) \cdot \mathbf{F}.$$

For an anisotropic band, the acceleration $\mathbf{a}$ need not be parallel to the applied force $\mathbf{F}$.

The effect of the periodic crystal lattice is already contained in the dispersion relation $\varepsilon(\mathbf{k})$, and therefore in the effective-mass tensor. For an isotropic parabolic band, the tensor reduces to the scalar effective mass introduced in the one-dimensional case.

4.1 MOTION OF AN ELECTRON IN AN ENERGY BAND

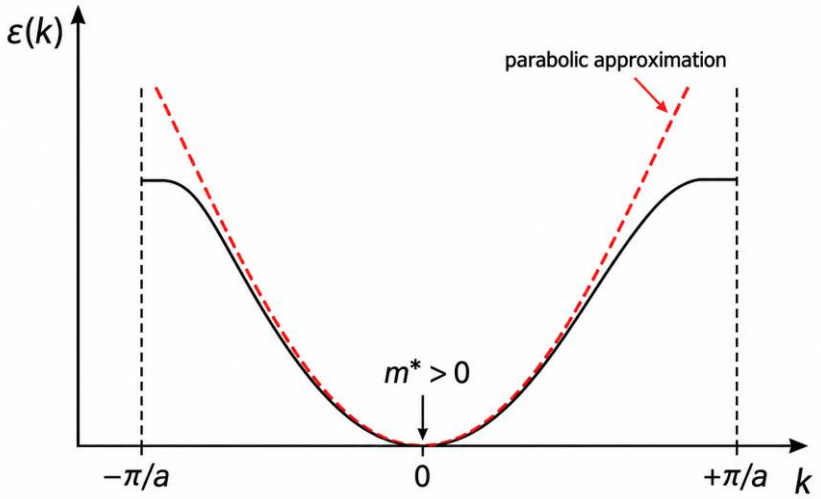
4.1.3 Parabolic approximation

Near a band minimum at k_0, the energy dispersion can be expanded in powers of $k - k_0$. Since the group velocity vanishes at the minimum,

$$\left.\frac{d\varepsilon_n}{dk}\right|_{k_0} = 0,$$

the leading variation of the energy is quadratic:

$$\varepsilon_n(k) \simeq \varepsilon_n(k_0) + \frac{\hbar^2}{2m^*}(k - k_0)^2.$$



The effective mass is determined by the local curvature of the band:

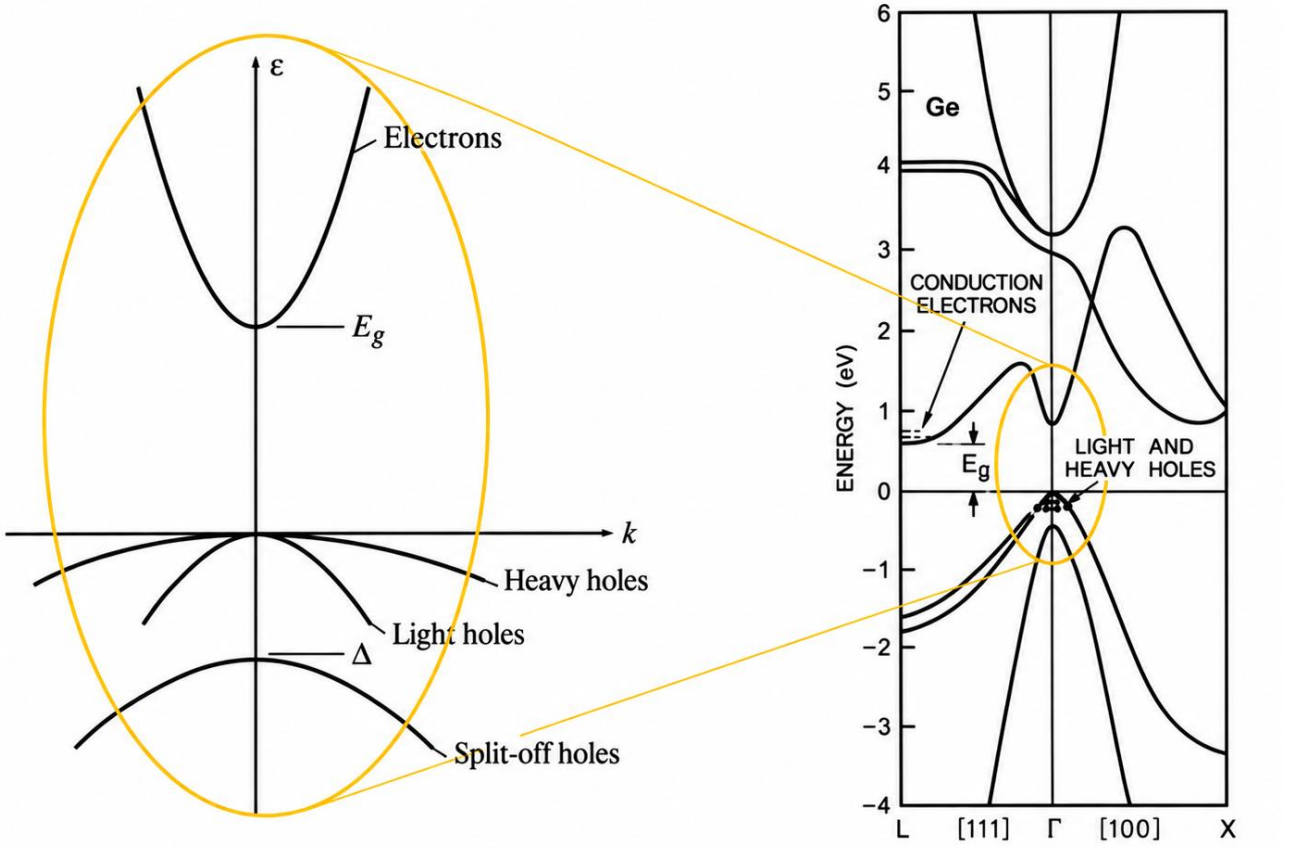
$$\frac{1}{m^*} = \frac{1}{\hbar^2}\left.\frac{d^2\varepsilon_n(k)}{dk^2}\right|_{k_0}.$$

Thus, close to a conduction-band minimum, an electron behaves as a free particle with mass m^*, rather than with the bare electron mass.

4.1 MOTION OF AN ELECTRON IN AN ENERGY BAND

4.1.3 Parabolic approximation

The enlargement around Γ (for Ge in the Figure, as an example) highlights the nearly parabolic conduction-band minimum, where the effective-mass approximation provides an accurate description of electron dynamics.



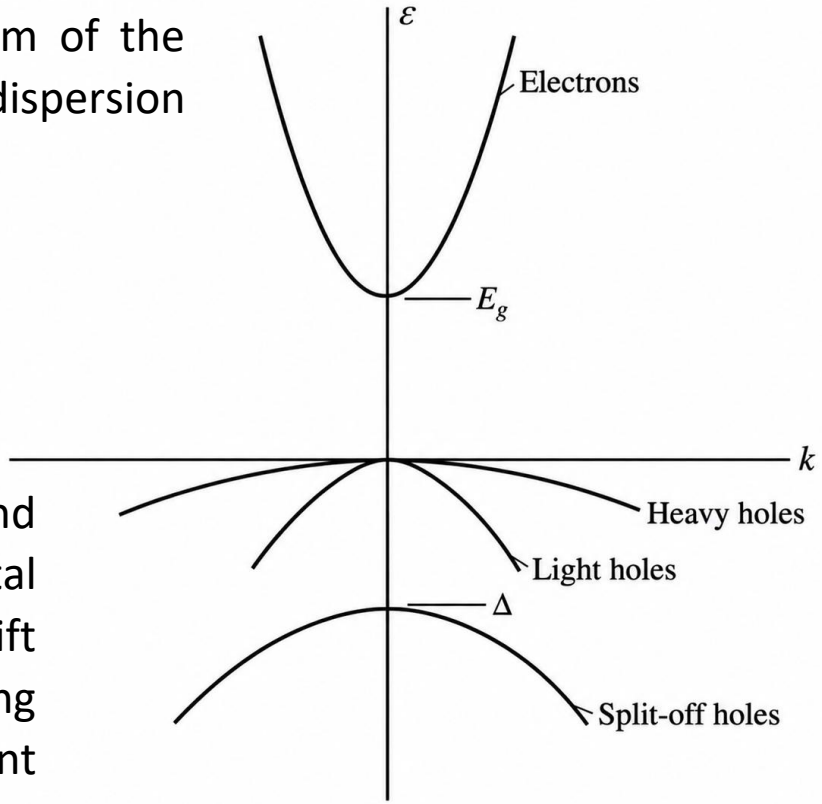
4.1 MOTION OF AN ELECTRON IN AN ENERGY BAND

4.1.3 Parabolic approximation

Let $\mathbf{k}_0$ denote the wave vector at the minimum of the conduction band. Close to this minimum, the dispersion relation can be approximated by

$$\varepsilon_c(\mathbf{k}) \simeq E_c + \frac{\hbar^2}{2m_e^*}|\mathbf{k} - \mathbf{k}_0|^2.$$

Here, $m_e^* > 0$ is the electron effective mass at the conduction-band edge.



The valence band splits into light- and heavy-hole branches because the crystal potential and spin–orbit interaction lift the degeneracy of the underlying electronic states, giving them different band curvatures and therefore different effective masses.

If the energy is measured from the maximum of the valence band, then $E_c = E_g$.

4.2 ELECTRONIC DISTRIBUTION FUNCTION

The Boltzmann transport equation provides a semiclassical description of charge transport based on the single-particle distribution function of Bloch electrons.

This formalism makes it possible to describe the response of electrons in a crystal to an electric field $\mathbf{E}$, a magnetic field $\mathbf{B}$, and a temperature gradient ∇T.

In addition to the single-electron approximation, the main assumptions are:

- Scattering events are random and can be described by transition probabilities.
- Successive scattering events are uncorrelated.
- The departure of the electron distribution from equilibrium is sufficiently small that it does not significantly modify the scattering probabilities.

These assumptions are generally appropriate in the linear-response regime, for weak external fields and well-defined electronic quasiparticles.

The strength of the Boltzmann approach lies in its ability to describe a broad range of transport phenomena in physical terms while incorporating realistic material parameters.

Transport phenomena are described in terms of the electron distribution function $f(\mathbf{k}, \mathbf{r}, t)$, defined through

$$dN = \frac{2}{(2\pi)^3} f(\mathbf{k}, \mathbf{r}, t)\, d^3k\, d^3r.$$

Here, dN is the number of electrons contained in the infinitesimal phase-space element $d^3k\, d^3r$, centred at $(\mathbf{r}, \mathbf{k})$. The factor 2 accounts for spin degeneracy.

4.2 ELECTRONIC DISTRIBUTION FUNCTION

At thermal equilibrium, in a spatially uniform crystal, the distribution function is independent of position and time and coincides with the Fermi–Dirac distribution:

$$dN = \frac{2}{(2\pi)^3} f(\mathbf{k}, \mathbf{r}, t)\, d^3k\, d^3r$$

$$f^0(\mathbf{k}) = \frac{1}{\exp\left[\dfrac{\varepsilon_{\mathbf{k}} - \mu}{k_B T}\right] + 1}.$$

This function gives the probability that the one-electron state of energy $\varepsilon_{\mathbf{k}}$ is occupied at temperature T and chemical potential μ.

The aim of transport theory is to determine the non-equilibrium distribution function $f(\mathbf{k}, \mathbf{r}, t)$ in the presence of external electric and magnetic fields, temperature gradients, and scattering processes. Once f is known, the macroscopic transport properties can be calculated.

Why is this a semiclassical approximation?

The distribution function $f(\mathbf{k}, \mathbf{r}, t)$ is expressed in terms of both position and wave vector. This does not imply that an electron has simultaneously well-defined $\mathbf{r}$ and $\mathbf{k}$. Rather, these quantities label the centre of an electronic wave packet.

The distribution function is meaningful only after a suitable coarse graining in phase space. The spatial region $\Delta^3 r$ must be large enough to contain many electrons, $n\,\Delta^3 r \gg 1$, where n is the electron density.

4.2 ELECTRONIC DISTRIBUTION FUNCTION

At the same time, the spatial region must remain small on the scale over which the macroscopic properties of the system vary appreciably. If an external perturbation varies over a characteristic length scale λ, we require $|\Delta\mathbf{r}| \ll \lambda$.

Finally, the phase-space cell must be consistent with the uncertainty principle. For each Cartesian direction,

$$\Delta k_i \, \Delta r_i \gtrsim \frac{1}{2},$$

since $\mathbf{p} = \hbar\mathbf{k}$.

In practice, the phase-space cell is chosen sufficiently large to contain many quantum states, while remaining small compared with the length and wave-vector scales over which f varies.

A system initially at thermal equilibrium can be driven out of equilibrium by external fields. Its distribution function can then evolve in time because of two distinct mechanisms:

- drift in phase space, caused by external forces;
- scattering processes, caused by collisions.

Within the Boltzmann approximation, the contributions of drift and collisions to the time variation of the distribution function are treated separately.

4.2 ELECTRONIC DISTRIBUTION FUNCTION

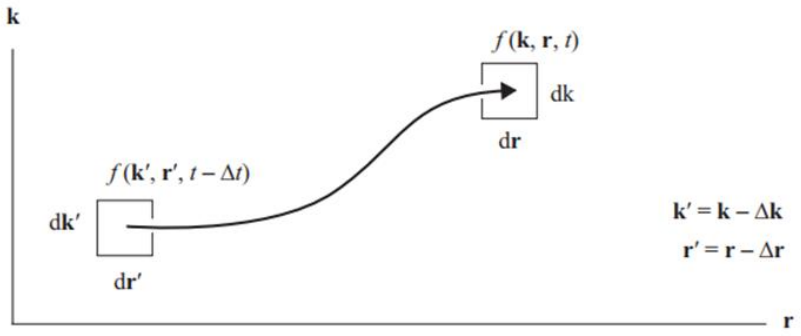
4.2.1 Equation of motion

Therefore:

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

The drift term can be evaluated by following the semiclassical evolution of an electron wave packet in phase space, i.e. by determining the time evolution of $\mathbf{r}$ and $\mathbf{k}$.

To evaluate the drift term, let us consider an infinitesimal phase-space volume element $d^3k'\,d^3r'$, centred at $(\mathbf{k}',\mathbf{r}')$ at time $t-\Delta t$.



During the time interval Δt, this element evolves into the phase-space volume element $d^3k\,d^3r$, centred at $(\mathbf{k},\mathbf{r})$ at time t, where

$$\mathbf{k} = \mathbf{k}' + \Delta\mathbf{k}, \qquad \mathbf{r} = \mathbf{r}' + \Delta\mathbf{r}.$$

In the absence of collisions, the number of electrons contained in the phase-space element is conserved during the drift motion. Therefore,

$$f(\mathbf{k},\mathbf{r},t)\,d^3k\,d^3r = f(\mathbf{k}',\mathbf{r}',t-\Delta t)\,d^3k'\,d^3r'.$$

4.2 ELECTRONIC DISTRIBUTION FUNCTION

4.2.1 Equation of motion

For a sufficiently short time interval Δt, the changes $\Delta\mathbf{r}$ and $\Delta\mathbf{k}$ are infinitesimal. We may therefore expand the distribution function to first order:

$$f(\mathbf{k}', \mathbf{r}', t - \Delta t) = f(\mathbf{k} - \Delta\mathbf{k}, \mathbf{r} - \Delta\mathbf{r}, t - \Delta t)$$
$$\simeq f(\mathbf{k}, \mathbf{r}, t) - \nabla_{\mathbf{k}} f(\mathbf{k}, \mathbf{r}, t) \cdot \Delta\mathbf{k} - \nabla_{\mathbf{r}} f(\mathbf{k}, \mathbf{r}, t) \cdot \Delta\mathbf{r} - \frac{\partial f}{\partial t}\Delta t.$$

For collision-less Hamiltonian motion, Liouville's theorem states that the volume of a phase-space element is conserved:

$$d^3k'\, d^3r' = d^3k\, d^3r.$$

Liouville's theorem: under collisionless Hamiltonian evolution, the volume of an infinitesimal phase-space element is conserved.

Substituting this result and the first-order expansion, we obtain

$$f(\mathbf{k}, \mathbf{r}, t)\, d^3k\, d^3r = f(\mathbf{k}', \mathbf{r}', t - \Delta t)\, d^3k'\, d^3r'$$

$$f(\mathbf{k}, \mathbf{r}, t) = f(\mathbf{k}, \mathbf{r}, t) - \nabla_{\mathbf{k}} f(\mathbf{k}, \mathbf{r}, t) \cdot \Delta\mathbf{k} - \nabla_{\mathbf{r}} f(\mathbf{k}, \mathbf{r}, t) \cdot \Delta\mathbf{r} - \frac{\partial f}{\partial t}\Delta t.$$

from which:

$$\frac{\partial f}{\partial t}\Delta t = -\nabla_{\mathbf{k}} f \cdot \Delta\mathbf{k} - \nabla_{\mathbf{r}} f \cdot \Delta\mathbf{r}.$$

4.2 ELECTRONIC DISTRIBUTION FUNCTION

4.2.1 Equation of motion

Dividing by Δt, we identify the drift contribution to the time variation of the distribution function:

$$\frac{\partial f}{\partial t}\Delta t = -\nabla_{\mathbf{k}} f \cdot \Delta\mathbf{k} - \nabla_{\mathbf{r}} f \cdot \Delta\mathbf{r}$$

$$\left(\frac{\partial f}{\partial t}\right)_{\text{drift}} = -\nabla_{\mathbf{k}} f \cdot \dot{\mathbf{k}} - \nabla_{\mathbf{r}} f \cdot \dot{\mathbf{r}}.$$

For an electron in a Bloch band, the semiclassical equations of motion are:

$$\hbar\dot{\mathbf{k}} = -e\left(\mathbf{E} + \frac{1}{c}\mathbf{v} \times \mathbf{B}\right), \qquad \dot{\mathbf{r}} = \mathbf{v}.$$

where $\mathbf{E}$ and $\mathbf{B}$ are externally applied electric and magnetic fields, respectively.

Substituting them in the previous expression, we obtain:

$$\left(\frac{\partial f}{\partial t}\right)_{\text{drift}} = \frac{e}{\hbar}\left(\mathbf{E} + \frac{1}{c}\mathbf{v} \times \mathbf{B}\right) \cdot \nabla_{\mathbf{k}} f - \mathbf{v} \cdot \nabla_{\mathbf{r}} f.$$

The first term describes the change in the distribution function caused by the acceleration of electrons in $\mathbf{k}$-space under the action of the electromagnetic fields. The second term describes the drift of electrons in real space with group velocity $\mathbf{v}$.

4.2 ELECTRONIC DISTRIBUTION FUNCTION

4.2.1 Equation of motion

The collision term $\left(\frac{\partial f}{\partial t}\right)_{coll}$ describes the variation of $f(\mathbf{k}, \mathbf{r}, t)$ caused by scattering processes.

$$\frac{\partial f(\mathbf{k}, \mathbf{r}, t)}{\partial t} = \left(\frac{\partial f}{\partial t}\right)_{\text{drift}} + \left(\frac{\partial f}{\partial t}\right)_{\text{coll}}$$

Let $W_{\mathbf{k}' \to \mathbf{k}}$ denote the transition probability per unit time for an electron to scatter from state $\mathbf{k}'$ into state $\mathbf{k}$. The collision term is the difference between the scattering-in and scattering-out contributions:

$$\left(\frac{\partial f_{\mathbf{k}}}{\partial t}\right)_{\text{coll}} = \sum_{\mathbf{k}'} [\, W_{\mathbf{k}' \to \mathbf{k}} f_{\mathbf{k}'}(1 - f_{\mathbf{k}}) - W_{\mathbf{k} \to \mathbf{k}'} f_{\mathbf{k}}(1 - f_{\mathbf{k}'})$$

where $f_{\mathbf{k}} \equiv f(\mathbf{k}, \mathbf{r}, t)$, $\quad f_{\mathbf{k}'} \equiv f(\mathbf{k}', \mathbf{r}, t)$.

For elastic scattering by non-magnetic centres, in the absence of a magnetic-field effect on the scattering rates, microscopic reversibility gives

$$W_{\mathbf{k}' \to \mathbf{k}} = W_{\mathbf{k} \to \mathbf{k}'}.$$

If the scattering centres are uniformly distributed, the transition probability is independent of position. The collision term then becomes

$$\left(\frac{\partial f_{\mathbf{k}}}{\partial t}\right)_{\text{coll}} = \sum_{\mathbf{k}'} W_{\mathbf{k}' \to \mathbf{k}} (f_{\mathbf{k}'} - f_{\mathbf{k}}),$$

4.2 ELECTRONIC DISTRIBUTION FUNCTION

4.2.1 Equation of motion

$$\frac{\partial f(\vec{k},\vec{r},t)}{\partial t} = \left(\frac{\partial f}{\partial t}\right)_{drift} + \left(\frac{\partial f}{\partial t}\right)_{coll}$$

$$\left(\frac{\partial f_{\mathbf{k}}}{\partial t}\right)_{\text{coll}} = \sum_{\mathbf{k}'} W_{\mathbf{k}'\to\mathbf{k}}\,(f_{\mathbf{k}'} - f_{\mathbf{k}}),$$

$$\left(\frac{\partial f}{\partial t}\right)_{\text{drift}} = \frac{e}{\hbar}\left(\mathbf{E} + \frac{1}{c}\mathbf{v}\times\mathbf{B}\right)\cdot\nabla_{\mathbf{k}} f - \mathbf{v}\cdot\nabla_{\mathbf{r}} f$$

In the continuous limit, the summation over $\mathbf{k}'$ can be replaced by an integral over $\mathbf{k}'$, using a measure consistent with the normalization adopted for the transition probability $\boldsymbol{W}$.

The Boltzmann transport equation can therefore be written as:

$$\frac{\partial f}{\partial t} + \mathbf{v}\cdot\nabla_{\mathbf{r}} f - \frac{e}{\hbar}\left(\mathbf{E} + \frac{1}{c}\mathbf{v}\times\mathbf{B}\right)\cdot\nabla_{\mathbf{k}} f = \left(\frac{\partial f}{\partial t}\right)_{\text{coll}}.$$

Equivalently, keeping the drift terms on the right-hand side,

$$\frac{\partial f}{\partial t} = \frac{e}{\hbar}\left(\mathbf{E} + \frac{1}{c}\mathbf{v}\times\mathbf{B}\right)\cdot\nabla_{\mathbf{k}} f - \mathbf{v}\cdot\nabla_{\mathbf{r}} f + \int d^3k'\, W_{\mathbf{k}'\to\mathbf{k}}(f_{\mathbf{k}'} - f_{\mathbf{k}})$$

4.2 ELECTRONIC DISTRIBUTION FUNCTION

4.2.1 Equation of motion

$$\frac{\partial f}{\partial t} = \frac{e}{\hbar}\left(\mathbf{E} + \frac{1}{c}\mathbf{v}\times\mathbf{B}\right)\cdot\nabla_{\mathbf{k}} f - \mathbf{v}\cdot\nabla_{\mathbf{r}} f + \int d^3k'\, W_{\mathbf{k}'\to\mathbf{k}}(f_{\mathbf{k}'} - f_{\mathbf{k}})$$

The Boltzmann transport equation is an integro-differential equation and, in general, it is difficult to solve.

However, once the distribution function $f(\mathbf{k},\mathbf{r},t)$ is known, a wide range of transport properties can be calculated.

For example, the electronic current density is the local charge flux. For electrons, whose charge is $-e$, it is given by

$$\mathbf{j}(\mathbf{r},t) = -\frac{2e}{(2\pi)^3}\int_{\mathrm{BZ}} d^3k\, \mathbf{v}(\mathbf{k})\, f(\mathbf{k},\mathbf{r},t),$$

$$dN = \frac{2}{(2\pi)^3} f(\mathbf{k},\mathbf{r},t)\, d^3k\, d^3r$$

where the factor 2 accounts for spin degeneracy and

$$\mathbf{v}(\mathbf{k}) = \frac{1}{\hbar}\nabla_{\mathbf{k}}\varepsilon(\mathbf{k})$$ is the group velocity.

For a crystal with several energy bands, the distribution function, group velocity, and transition probability must carry a band index: $f_n(\mathbf{k},\mathbf{r},t)$, $\mathbf{v}_n(\mathbf{k}) = \frac{1}{\hbar}\nabla_{\mathbf{k}}\varepsilon_n(\mathbf{k})$, $W^{n'\to n}_{\mathbf{k}'\to\mathbf{k}}$.

4.2 ELECTRONIC DISTRIBUTION FUNCTION

4.2.2 Transport under steady-state conditions

In many transport experiments, the system is studied under steady-state conditions. In this case, the distribution function is time independent:

$$\frac{\partial f(\mathbf{k},\mathbf{r},t)}{\partial t} = 0.$$

$$\frac{\partial f(\vec{k},\vec{r},t)}{\partial t} = \left(\frac{\partial f}{\partial t}\right)_{drift} + \left(\frac{\partial f}{\partial t}\right)_{coll}$$

Therefore, the drift and collision contributions must balance:

$$0 = \left(\frac{\partial f}{\partial t}\right)_{\text{drift}} + \left(\frac{\partial f}{\partial t}\right)_{\text{coll}}.$$

The stationary Boltzmann equation can be written as:

$$\frac{\partial f}{\partial t} = \frac{e}{\hbar}\left(\mathbf{E} + \frac{1}{c}\mathbf{v}\times\mathbf{B}\right)\cdot\nabla_{\mathbf{k}} f - \mathbf{v}\cdot\nabla_{\mathbf{r}} f + \int d^3k'\, W_{\mathbf{k}'\to\mathbf{k}}(f_{\mathbf{k}'} - f_{\mathbf{k}})$$

$$\left[\mathbf{v}(\mathbf{k})\cdot\nabla_{\mathbf{r}} - \frac{e}{\hbar}\left(\mathbf{E} + \frac{1}{c}\mathbf{v}(\mathbf{k})\times\mathbf{B}\right)\cdot\nabla_{\mathbf{k}}\right] f(\mathbf{k},\mathbf{r}) = \left(\frac{\partial f}{\partial t}\right)_{\text{coll}}.$$

This equation must be solved to determine the nonequilibrium distribution function $f(\mathbf{k},\mathbf{r})$ in the steady-state transport regime. The crystal-specific quantities entering the equation are the band velocity $\mathbf{v}(\mathbf{k})$ and the scattering rates contained in the collision term.

4.2 ELECTRONIC DISTRIBUTION FUNCTION

4.2.2 Transport under steady-state conditions

Let us first consider the simplest case: a spatially homogeneous crystal, with a uniform statistical distribution of defects and impurities, at thermal equilibrium. In this case

$$\mathbf{E} = \mathbf{B} = 0, \qquad \nabla T = 0, \qquad \nabla_{\mathbf{r}} f^0 = 0.$$

The distribution function is then the equilibrium Fermi–Dirac distribution:

$$f(\mathbf{k}, \mathbf{r}) = f^0(\mathbf{k}) = \frac{1}{\exp\left[\dfrac{\varepsilon(\mathbf{k}) - \mu}{k_B T}\right] + 1}.$$

Since f^0 depends only on the energy, elastic scattering between states of equal energy gives:

$$\left(\frac{\partial f^0}{\partial t}\right)_{\text{coll}} = \int d^3 k' \, W_{\mathbf{k}' \to \mathbf{k}} [f^0(\mathbf{k}') - f^0(\mathbf{k})] = 0.$$

$$\left(\frac{\partial f}{\partial t}\right)_{coll} = \int d^3 k' \, W_{\mathbf{k}' \to \mathbf{k}} (f_{\mathbf{k}'} - f_{\mathbf{k}})$$

Thus, the equilibrium Fermi–Dirac distribution is a stationary solution of the Boltzmann equation.

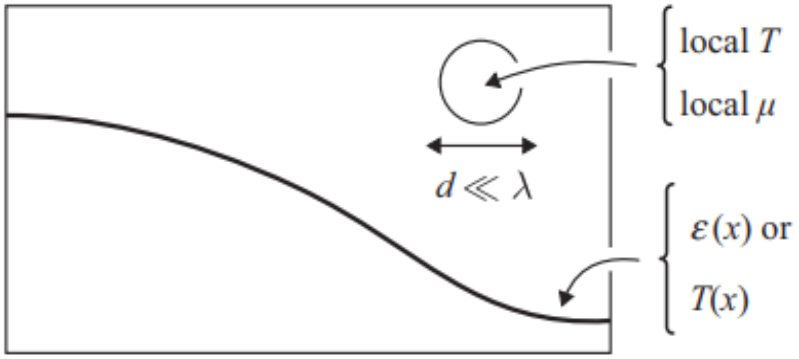
To describe a weakly non-uniform system, we introduce the concept of local equilibrium.

4.2 ELECTRONIC DISTRIBUTION FUNCTION

4.2.2 Transport under steady-state conditions

For perturbations that vary slowly over a characteristic length scale λ, it is meaningful to define a local temperature $T(\mathbf{r})$ and a local chemical potential $\mu(\mathbf{r})$. These quantities are defined within a region of size d such that

$$\ell \ll d \ll \lambda,$$



where ℓ is the electron mean free path. Thus, although T and μ may vary across the sample, they are approximately constant within each local region.

At position $\mathbf{r}$, the local-equilibrium distribution is

$$f^0(\mathbf{k},\mathbf{r}) = \frac{1}{\exp\left[\dfrac{\varepsilon(\mathbf{k}) - \mu(\mathbf{r})}{k_B T(\mathbf{r})}\right] + 1}.$$

The actual distribution function is written as

$$f(\mathbf{k},\mathbf{r}) = f^0(\mathbf{k},\mathbf{r}) + f^{(1)}(\mathbf{k},\mathbf{r}),$$

where $f^{(1)}$ is the small nonequilibrium correction induced by the external perturbations.

4.2 ELECTRONIC DISTRIBUTION FUNCTION

4.2.2 Transport under steady-state conditions

$$f(\mathbf{k},\mathbf{r}) = f^0(\mathbf{k},\mathbf{r}) + f^{(1)}(\mathbf{k},\mathbf{r})$$

In the linear-response regime: $\left|f^{(1)}\right| \ll f^0$

Here, f^0 is the local-equilibrium Fermi–Dirac distribution.

$$f^0(\mathbf{k},\mathbf{r}) = \frac{1}{\exp\left[\frac{\varepsilon_{\mathbf{k}} - \mu(\mathbf{r})}{k_B T(\mathbf{r})}\right] + 1}$$

Since f^0 is a local-equilibrium distribution, its collision integral vanishes:

$$\left(\frac{\partial f^0}{\partial t}\right)_{\text{coll}} = 0.$$

However, f^0 generally has a nonzero drift term when external fields or spatial gradients are present. This drift term acts as the driving term for the nonequilibrium correction $f^{(1)}$.

Let us substitute

$$f(\mathbf{k},\mathbf{r}) = f^0(\mathbf{k},\mathbf{r}) + f^{(1)}(\mathbf{k},\mathbf{r})$$

into the stationary Boltzmann equation:

$$\left[\mathbf{v}(\mathbf{k})\cdot\nabla_{\mathbf{r}} - \frac{e}{\hbar}\left(\mathbf{E} + \frac{1}{c}\mathbf{v}(\mathbf{k})\times\mathbf{B}\right)\cdot\nabla_{\mathbf{k}}\right] f(\mathbf{k},\mathbf{r}) = \left(\frac{\partial f^{(1)}}{\partial t}\right)_{\text{coll}}$$

4.2 ELECTRONIC DISTRIBUTION FUNCTION

5.2.2 Transport under steady-state conditions

$$\left[\mathbf{v}(\mathbf{k})\cdot\nabla_{\mathbf{r}}-\frac{e}{\hbar}\left(\mathbf{E}+\frac{1}{c}\mathbf{v}(\mathbf{k})\times\mathbf{B}\right)\cdot\nabla_{\mathbf{k}}\right]f(\mathbf{k},\mathbf{r})=\left(\frac{\partial f^{(1)}}{\partial t}\right)_{\text{coll}}$$

$$f(\mathbf{k},\mathbf{r})=f^{0}(\mathbf{k},\mathbf{r})+f^{(1)}(\mathbf{k},\mathbf{r})$$

$$\left(\frac{\partial f^{0}}{\partial t}\right)_{\text{coll}}=0$$

Expanding the drift operator, we obtain:

$$\mathbf{v}(\mathbf{k})\cdot\nabla_{\mathbf{r}}f^{0}+\mathbf{v}(\mathbf{k})\cdot\nabla_{\mathbf{r}}f^{(1)}-\frac{e}{\hbar}\left(\mathbf{E}+\frac{1}{c}\mathbf{v}(\mathbf{k})\times\mathbf{B}\right)\cdot\nabla_{\mathbf{k}}f^{0}-\frac{e}{\hbar}\left(\mathbf{E}+\frac{1}{c}\mathbf{v}(\mathbf{k})\times\mathbf{B}\right)\cdot\nabla_{\mathbf{k}}f^{(1)}=\left(\frac{\partial f^{(1)}}{\partial t}\right)_{\text{coll}}$$

To linearize this equation, we use the following two observations:

1. Since f^{0} depends on $\mathbf{k}$ only through the energy $\varepsilon_{\mathbf{k}}$,

$$\nabla_{\mathbf{k}}f^{0}=\frac{\partial f^{0}}{\partial\varepsilon_{\mathbf{k}}}\hbar\mathbf{v}(\mathbf{k})$$

Therefore,

$$[\mathbf{v}(\mathbf{k})\times\mathbf{B}]\cdot\nabla_{\mathbf{k}}f^{0}=0,$$

and hence

$$-\frac{e}{\hbar}\left(\mathbf{E}+\frac{1}{c}\mathbf{v}(\mathbf{k})\times\mathbf{B}\right)\cdot\nabla_{\mathbf{k}}f^{0}=-\frac{e}{\hbar}\,\mathbf{E}\cdot\nabla_{\mathbf{k}}f^{0.}$$

4.2 ELECTRONIC DISTRIBUTION FUNCTION

4.2.2 Transport under steady-state conditions

$$\mathbf{v}(\mathbf{k})\cdot\nabla_{\mathbf{r}}f^{0}+\mathbf{v}(\mathbf{k})\cdot\nabla_{\mathbf{r}}f^{(1)}-\frac{e}{\hbar}\mathbf{E}\cdot\nabla_{\mathbf{k}}f^{0}-\frac{e}{\hbar}\left(\mathbf{E}+\frac{1}{c}\mathbf{v}(\mathbf{k})\times\mathbf{B}\right)\cdot\nabla_{\mathbf{k}}f^{(1)}=\left(\frac{\partial f^{(1)}}{\partial t}\right)_{\text{coll}}$$

2. In the linear-response regime, $f^{(1)}$, $\mathbf{E}$, ∇T, and $\nabla\mu$ are all first-order quantities. Thus, the term $\mathbf{E}\cdot\nabla_{\mathbf{k}}f^{(1)}$ is of second order and can be neglected. If the magnetic field is retained to describe magnetotransport effects:

$$-\frac{e}{\hbar}\left(\mathbf{E}+\frac{1}{c}\mathbf{v}(\mathbf{k})\times\mathbf{B}\right)\cdot\nabla_{\mathbf{k}}f^{(1)}\simeq-\frac{e}{\hbar c}[\mathbf{v}(\mathbf{k})\times\mathbf{B}]\cdot\nabla_{\mathbf{k}}f^{(1)}.$$

Then we obtain

$$\mathbf{v}(\mathbf{k})\cdot\nabla_{\mathbf{r}}f^{0}+\mathbf{v}(\mathbf{k})\cdot\nabla_{\mathbf{r}}f^{(1)}-\frac{e}{\hbar}\mathbf{E}\cdot\nabla_{\mathbf{k}}f^{0}-\frac{e}{\hbar c}[\mathbf{v}(\mathbf{k})\times\mathbf{B}]\cdot\nabla_{\mathbf{k}}f^{(1)}=\left(\frac{\partial f^{(1)}}{\partial t}\right)_{\text{coll}}$$

For slowly varying perturbations, $f^{(1)}$ is already first order in the spatial gradients. Therefore,

$$\mathbf{v}(\mathbf{k})\cdot\nabla_{\mathbf{r}}f^{(1)}=\mathcal{O}(\nabla^{2}),$$

The linearized Boltzmann equation then becomes

$$\mathbf{v}(\mathbf{k})\cdot\nabla_{\mathbf{r}}f^{0}-\frac{e}{\hbar}\mathbf{E}\cdot\nabla_{\mathbf{k}}f^{0}-\frac{e}{\hbar c}[\mathbf{v}(\mathbf{k})\times\mathbf{B}]\cdot\nabla_{\mathbf{k}}f^{(1)}=\left(\frac{\partial f^{(1)}}{\partial t}\right)_{\text{coll}}.$$

The remaining difficulty is the explicit evaluation of the collision term.

4.2 ELECTRONIC DISTRIBUTION FUNCTION

4.2.3 Relaxation time approximation

The collision term is generally the most difficult contribution to evaluate explicitly. Instead of calculating the full scattering integral, we assume that collisions drive the electronic distribution back toward the local-equilibrium distribution f^0.

The collision term has the dimensions of an inverse time:

$$\left(\frac{\partial f}{\partial t}\right)_{\text{coll}} \sim \frac{f}{\text{s}}.$$

Moreover, as thermal equilibrium is approached,

$f(\mathbf{k},\mathbf{r}) \to f^0(\mathbf{k},\mathbf{r}),$ $\quad f^{(1)}(\mathbf{k},\mathbf{r}) \to 0,$ and therefore $\left(\frac{\partial f}{\partial t}\right)_{\text{coll}} \to 0.$

The simplest phenomenological approximation is to assume that the departure from local equilibrium decays exponentially over a characteristic relaxation time $\tau_{\mathbf{k}}$

$$\left(\frac{\partial f(\mathbf{k},\mathbf{r})}{\partial t}\right)_{\text{coll}} = -\frac{f(\mathbf{k},\mathbf{r}) - f^0(\mathbf{k},\mathbf{r})}{\tau_{\mathbf{k}}} = -\frac{f^{(1)}(\mathbf{k},\mathbf{r})}{\tau_{\mathbf{k}}}$$

For a uniform concentration of scattering centers, $\tau_{\mathbf{k}}$ is independent of position, although it may depend on the electronic state $\mathbf{k}$.

4.2 ELECTRONIC DISTRIBUTION FUNCTION

4.2.3 Relaxation time approximation

$$\left(\frac{\partial f(\mathbf{k},\mathbf{r})}{\partial t}\right)_{\text{coll}} = -\frac{f^{(1)}(\mathbf{k},\mathbf{r})}{\tau_{\mathbf{k}}}$$

The minus sign ensures that collisions restore the local-equilibrium distribution. Once the external perturbation is removed, $f^{(1)} = f - f^0$, and the distribution relaxes toward f^0.

The quantity f^0 is the relaxation time of the electronic state $\mathbf{k}$.

For a spatially uniform system in the absence of external fields, the drift term vanishes. Therefore:

$$\frac{\partial f(\mathbf{k},t)}{\partial t} = \left(\frac{\partial f}{\partial t}\right)_{\text{coll}} = -\frac{f^{(1)}(\mathbf{k},t)}{\tau_{\mathbf{k}}}.$$

Since f^0 is time independent, this gives :

$$\frac{\partial f^{(1)}(\mathbf{k},t)}{\partial t} = -\frac{f^{(1)}(\mathbf{k},t)}{\tau_{\mathbf{k}}},$$

whose solution is $f^{(1)}(\mathbf{k},t) = f^{(1)}(\mathbf{k},0)\exp\left(-\frac{t}{\tau_{\mathbf{k}}}\right).$

Thus, $\tau_{\mathbf{k}}$ sets the characteristic time over which a nonequilibrium distribution relaxes back to equilibrium.

4.2 ELECTRONIC DISTRIBUTION FUNCTION

4.2.3 Relaxation time approximation

$$f^{(1)}(\mathbf{k},t) = f^{(1)}(\mathbf{k},0)\exp\left(-\frac{t}{\tau_{\mathbf{k}}}\right)$$

$$f = f^0 + f^{(1)}$$

The distribution function returns to its equilibrium value on a timescale of the order of $\tau_{\mathbf{k}}$. Thus, $\tau_{\mathbf{k}}$ is the characteristic time required for a perturbed electronic system to relax back to equilibrium after the driving perturbation has been removed.

What changes in the presence of external fields?

Let us return to the linearized Boltzmann equation:

$$\mathbf{v}(\mathbf{k})\cdot\nabla_{\mathbf{r}} f^0 - \frac{e}{\hbar}\mathbf{E}\cdot\nabla_{\mathbf{k}} f^0 - \frac{e}{\hbar c}[\mathbf{v}(\mathbf{k})\times\mathbf{B}]\cdot\nabla_{\mathbf{k}} f^{(1)} = \left(\frac{\partial f^{(1)}}{\partial t}\right)_{\text{coll}}$$

Let us evaluate the spatial-gradient term. The local-equilibrium distribution is

$$f^0(\mathbf{k},\mathbf{r}) = \frac{1}{\exp\left[\dfrac{\varepsilon_{\mathbf{k}} - \mu(\mathbf{r})}{k_B T(\mathbf{r})}\right] + 1} = \frac{1}{\exp\left[\beta(\mathbf{r})\big(\varepsilon_{\mathbf{k}} - \mu(\mathbf{r})\big)\right] + 1},$$

where

$$\beta(\mathbf{r}) = \frac{1}{k_B T(\mathbf{r})}.$$

4.2 ELECTRONIC DISTRIBUTION FUNCTION

4.2.3 Relaxation time approximation

$$\mathbf{v}(\mathbf{k})\cdot\nabla_{\mathbf{r}}f^{0}-\frac{e}{\hbar}\mathbf{E}\cdot\nabla_{\mathbf{k}}f^{0}-\frac{e}{\hbar c}[\mathbf{v}(\mathbf{k})\times\mathbf{B}]\cdot\nabla_{\mathbf{k}}f^{(1)}=\left(\frac{\partial f^{(1)}}{\partial t}\right)_{\text{coll}}$$

$$f^{0}(\mathbf{k},\mathbf{r})=\frac{1}{\exp\left[\beta(\mathbf{r})\left(\varepsilon_{\mathbf{k}}-\mu(\mathbf{r})\right)\right]+1}$$

The position dependence of f^0 is entirely contained in the exponent. Therefore:

$$\nabla_{\mathbf{r}}f^{0}=\frac{\partial f^{0}}{\partial[\beta(\varepsilon_{\mathbf{k}}-\mu)]}\nabla_{\mathbf{r}}\left[\beta(\mathbf{r})\left(\varepsilon_{\mathbf{k}}-\mu(\mathbf{r})\right)\right].$$

At fixed position $\mathbf{r}$, $\beta(\mathbf{r})$ and $\mu(\mathbf{r})$ are independent of $\varepsilon_{\mathbf{k}}$. Therefore,

$$\frac{\partial f^{0}}{\partial[\beta(\varepsilon_{\mathbf{k}}-\mu)]}=\frac{1}{\beta}\frac{\partial f^{0}}{\partial\varepsilon_{\mathbf{k}}}.$$

Replacing, we have:

$$\nabla_{\mathbf{r}}f^{0}=\frac{1}{\beta}\frac{\partial f^{0}}{\partial\varepsilon_{\mathbf{k}}}\nabla_{\mathbf{r}}\left[\beta(\mathbf{r})\left(\varepsilon_{\mathbf{k}}-\mu(\mathbf{r})\right)\right]$$

The first driving term becomes

$$\mathbf{v}(\mathbf{k})\cdot\nabla_{\mathbf{r}}f^{0}=\frac{1}{\beta}\frac{\partial f^{0}}{\partial\varepsilon_{\mathbf{k}}}\mathbf{v}(\mathbf{k})\cdot\nabla_{\mathbf{r}}\left[\beta(\mathbf{r})\left(\varepsilon_{\mathbf{k}}-\mu(\mathbf{r})\right)\right].$$

4.2 ELECTRONIC DISTRIBUTION FUNCTION

4.2.3 Relaxation time approximation

$$\mathbf{v}(\mathbf{k})\cdot\nabla_{\mathbf{r}}f^{0}-\frac{e}{\hbar}\mathbf{E}\cdot\nabla_{\mathbf{k}}f^{0}-\frac{e}{\hbar c}[\mathbf{v}(\mathbf{k})\times\mathbf{B}]\cdot\nabla_{\mathbf{k}}f^{(1)}=\left(\frac{\partial f^{(1)}}{\partial t}\right)_{\text{coll}}$$

$$f^{0}(\mathbf{k},\mathbf{r})=\frac{1}{\exp\left[\beta(\mathbf{r})\left(\varepsilon_{\mathbf{k}}-\mu(\mathbf{r})\right)\right]+1}$$

For the electric-field term, since f^0 depends on $\mathbf{k}$ only through $\varepsilon_{\mathbf{k}}$:

$$\nabla_{\mathbf{k}}f^{0}=\frac{\partial f^{0}}{\partial\varepsilon_{\mathbf{k}}}\nabla_{\mathbf{k}}\varepsilon_{\mathbf{k}}=\hbar\,\mathbf{v}(\mathbf{k})\frac{\partial f^{0}}{\partial\varepsilon_{\mathbf{k}}}.$$

$$\mathbf{v}(\mathbf{k})=\frac{1}{\hbar}\nabla_{\mathbf{k}}\varepsilon_{\mathbf{k}}$$

Therefore:

$$-\frac{e}{\hbar}\mathbf{E}\cdot\nabla_{\mathbf{k}}f^{0}=-e\mathbf{E}\cdot\mathbf{v}(\mathbf{k})\frac{\partial f^{0}}{\partial\varepsilon_{\mathbf{k}}}$$

Replacing also the previous expression:

$$\mathbf{v}(\mathbf{k})\cdot\nabla_{\mathbf{r}}f^{0}=\frac{1}{\beta}\frac{\partial f^{0}}{\partial\varepsilon_{\mathbf{k}}}\mathbf{v}(\mathbf{k})\cdot\nabla_{\mathbf{r}}\left[\beta(\mathbf{r})\left(\varepsilon_{\mathbf{k}}-\mu(\mathbf{r})\right)\right]$$

the linearized Boltzmann equation becomes

$$\frac{1}{\beta}\frac{\partial f^{0}}{\partial\varepsilon_{\mathbf{k}}}\mathbf{v}(\mathbf{k})\cdot\nabla_{\mathbf{r}}\left[\beta(\mathbf{r})\left(\varepsilon_{\mathbf{k}}-\mu(\mathbf{r})\right)\right]-e\,\mathbf{E}\cdot\mathbf{v}(\mathbf{k})\frac{\partial f^{0}}{\partial\varepsilon_{\mathbf{k}}}$$
$$=\left(\frac{\partial f^{(1)}}{\partial t}\right)_{\text{coll}}+\frac{e}{\hbar c}[\mathbf{v}(\mathbf{k})\times\mathbf{B}]\cdot\nabla_{\mathbf{k}}f^{(1)}.$$

4.2 ELECTRONIC DISTRIBUTION FUNCTION

4.2.3 Relaxation time approximation

$$\frac{1}{\beta}\frac{\partial f^0}{\partial \varepsilon_{\mathbf{k}}}\,\mathbf{v}(\mathbf{k})\cdot\nabla_{\mathbf{r}}\left[\beta(\mathbf{r})\left(\varepsilon_{\mathbf{k}}-\mu(\mathbf{r})\right)\right]-e\,\mathbf{E}\cdot\mathbf{v}(\mathbf{k})\,\frac{\partial f^0}{\partial \varepsilon_{\mathbf{k}}}\& = \left(\frac{\partial f^{(1)}}{\partial t}\right)_{\text{coll}} + \frac{e}{\hbar c}\left[\mathbf{v}(\mathbf{k})\times\mathbf{B}\right]\cdot\nabla_{\mathbf{k}} f^{(1)}$$

The derivative

$$\frac{\partial f^0}{\partial \mathcal{E}}$$

is strongly peaked around the Fermi energy.

$$f^0(\mathbf{k},\mathbf{r}) = \frac{1}{\exp\left[\dfrac{\varepsilon_{\mathbf{k}}-\mu(\mathbf{r})}{k_B T(\mathbf{r})}\right]+1}$$

We therefore write the nonequilibrium correction as

$$f^{(1)}(\mathbf{k},\mathbf{r}) \equiv -\frac{\partial f^0}{\partial \varepsilon_{\mathbf{k}}}\Phi(\mathbf{k},\mathbf{r})$$

where $\Phi(\mathbf{k},\mathbf{r})$ describes the distortion of the distribution from local equilibrium and has the dimensions of an energy.

The collision term becomes

$$\left(\frac{\partial f^{(1)}}{\partial t}\right)_{coll} = -\frac{f^{(1)}}{\tau_{\mathbf{k}}} = -\frac{\partial f^0}{\partial \varepsilon_{\mathbf{k}}}\frac{\Phi(\mathbf{k},\mathbf{r})}{\tau_{\mathbf{k}}}$$

4.2 ELECTRONIC DISTRIBUTION FUNCTION

4.2.3 Relaxation time approximation

$$\frac{1}{\beta}\frac{\partial f^0}{\partial \varepsilon_{\mathbf{k}}}\,\mathbf{v}(\mathbf{k})\cdot\nabla_{\mathbf{r}}\left[\beta(\mathbf{r})\left(\varepsilon_{\mathbf{k}}-\mu(\mathbf{r})\right)\right]-e\,\mathbf{E}\cdot\mathbf{v}(\mathbf{k})\,\frac{\partial f^0}{\partial \varepsilon_{\mathbf{k}}}\&=\left(\frac{\partial f^{(1)}}{\partial t}\right)_{\text{coll}}+\frac{e}{\hbar c}\left[\mathbf{v}(\mathbf{k})\times\mathbf{B}\right]\cdot\nabla_{\mathbf{k}}f^{(1)}$$

For the magnetic-field term,

$$\nabla_{\mathbf{k}}f^{(1)}=\hbar\,\frac{\partial^2 f^0}{\partial \varepsilon_{\mathbf{k}}^2}\,\mathbf{v}(\mathbf{k})\,\Phi+\frac{\partial f^0}{\partial \varepsilon_{\mathbf{k}}}\,\nabla_{\mathbf{k}}\Phi.$$

$$\left(\frac{\partial f^{(1)}}{\partial t}\right)_{coll}=-\frac{\partial f^0}{\partial \varepsilon_{\mathbf{k}}}\frac{\phi(\mathbf{k},\mathbf{r})}{\tau_{\mathbf{k}}}$$

Since $[\mathbf{v}(\mathbf{k})\times\mathbf{B}]\cdot\mathbf{v}(\mathbf{k})=0,$

we obtain $\frac{e}{\hbar c}[\mathbf{v}(\mathbf{k})\times\mathbf{B}]\cdot\nabla_{\mathbf{k}}f^{(1)}=\frac{\partial f^0}{\partial \varepsilon_{\mathbf{k}}}\frac{e}{\hbar c}[\mathbf{v}(\mathbf{k})\times\mathbf{B}]\cdot\nabla_{\mathbf{k}}\Phi$

Substituting both expression in the linearized Boltzmann equation

$$\frac{\partial f^0}{\partial \varepsilon_{\mathbf{k}}}\left\{\frac{1}{\beta}\,\mathbf{v}(\mathbf{k})\cdot\nabla_{\mathbf{r}}\left[\beta(\mathbf{r})\left(\varepsilon_{\mathbf{k}}-\mu(\mathbf{r})\right)\right]-e\,\mathbf{E}\cdot\mathbf{v}(\mathbf{k})\right\}$$

$$=\frac{\partial f^0}{\partial \varepsilon_{\mathbf{k}}}\left\{-\frac{\Phi(\mathbf{k},\mathbf{r})}{\tau_{\mathbf{k}}}+\frac{e}{\hbar c}\left[\mathbf{v}(\mathbf{k})\times\mathbf{B}\right]\cdot\nabla_{\mathbf{k}}\Phi(\mathbf{k},\mathbf{r})\right\}.$$

4.2 ELECTRONIC DISTRIBUTION FUNCTION

4.2.3 Relaxation time approximation

$$\frac{\partial f^0}{\partial \varepsilon_{\mathbf{k}}}\left\{\frac{1}{\beta}\,\mathbf{v}(\mathbf{k})\cdot\nabla_{\mathbf{r}}\left[\beta(\mathbf{r})\left(\varepsilon_{\mathbf{k}}-\mu(\mathbf{r})\right)\right]-e\,\mathbf{E}\cdot\mathbf{v}(\mathbf{k})\right\}=\frac{\partial f^0}{\partial \varepsilon_{\mathbf{k}}}\left\{-\frac{\Phi(\mathbf{k},\mathbf{r})}{\tau_{\mathbf{k}}}+\frac{e}{\hbar c}\left[\mathbf{v}(\mathbf{k})\times\mathbf{B}\right]\cdot\nabla_{\mathbf{k}}\Phi(\mathbf{k},\mathbf{r})\right\}$$

All terms contain the common factor $\dfrac{\partial f^0}{\partial \varepsilon_{\mathbf{k}}}$

$$f^0(\mathbf{k},\mathbf{r})=\frac{1}{\exp\left[\dfrac{\varepsilon_{\mathbf{k}}-\mu(\mathbf{r})}{k_B T(\mathbf{r})}\right]+1}$$

At low temperature, the Fermi–Dirac distribution approaches a step function at the chemical potential: $f^0(\varepsilon) \underset{T\to 0}{\to} \Theta(\mu-\varepsilon).$

Consequently,

$$\frac{\partial f^0}{\partial \varepsilon} \underset{T\to 0}{\to} -\delta(\varepsilon-\mu).$$

$$\beta(\mathbf{r})=\frac{1}{k_B T(\mathbf{r})}$$

Therefore, in the low-temperature limit, only electronic states close to the Fermi energy contribute to transport.

The linearized Boltzmann equation becomes

$$-T(\mathbf{r})\,\mathbf{v}(\mathbf{k})\cdot\nabla_{\mathbf{r}}\left[\frac{\varepsilon_{\mathbf{k}}-\mu(\mathbf{r})}{T(\mathbf{r})}\right]+e\,\mathbf{E}\cdot\mathbf{v}(\mathbf{k})=\frac{\phi(\mathbf{k},\mathbf{r})}{\tau_{\mathbf{k}}}-\frac{e}{\hbar c}\left[\mathbf{v}(\mathbf{k})\times\mathbf{B}\right]\cdot\nabla_{\mathbf{k}}\phi(\mathbf{k},\mathbf{r}).$$

Solving this equation $\phi(\mathbf{k},\mathbf{r})$ determines the nonequilibrium correction and hence the transport properties of the crystal.

4.3 ELECTRICAL AND THERMAL CONDUCTIVITY

4.3.1 Isothermal electrical conductivity

$$-T(\mathbf{r})\,\mathbf{v}(\mathbf{k})\cdot\nabla_{\mathbf{r}}\left[\frac{\varepsilon_{\mathbf{k}}-\mu(\mathbf{r})}{T(\mathbf{r})}\right]+e\,\mathbf{E}\cdot\mathbf{v}(\mathbf{k})=\frac{\phi(\mathbf{k},\mathbf{r})}{\tau_{\mathbf{k}}}-\frac{e}{\hbar c}[\mathbf{v}(\mathbf{k})\times\mathbf{B}]\cdot\nabla_{\mathbf{k}}\phi(\mathbf{k},\mathbf{r})$$

Consider an isothermal and spatially homogeneous crystal subjected to a weak, uniform electric field $\mathbf{E}$. The local-equilibrium parameters are uniform.

$$\nabla_{\mathbf{r}}T=0,\qquad \nabla_{\mathbf{r}}\mu=0,\qquad \mathbf{B}=0.$$

The linearized Boltzmann equation then reduces to

$$\frac{\phi(\mathbf{k})}{\tau_{\mathbf{k}}}=-e\,\mathbf{E}\cdot\mathbf{v}(\mathbf{k}).$$

Therefore $\phi(\mathbf{k})=-e\,\tau_{\mathbf{k}}\,\mathbf{E}\cdot\mathbf{v}(\mathbf{k}).$

We then obtain $f^{(1)}(\mathbf{k})=e\,\tau_{\mathbf{k}}\,\mathbf{E}\cdot\mathbf{v}(\mathbf{k})\,\dfrac{\partial f^{0}}{\partial\varepsilon_{\mathbf{k}}}.$

$$f^{(1)}(\mathbf{k},\mathbf{r})\equiv-\frac{\partial f^{0}}{\partial\varepsilon_{\mathbf{k}}}\Phi(\mathbf{k},\mathbf{r})$$

Equivalently, $f^{(1)}(\mathbf{k})=-e\,\tau_{\mathbf{k}}\,\mathbf{E}\cdot\mathbf{v}(\mathbf{k})\left(-\dfrac{\partial f^{0}}{\partial\varepsilon_{\mathbf{k}}}\right).$

The correction $f^{(1)}$ determines the electric current density and, hence, the electrical conductivity tensor.

4.3 ELECTRICAL AND THERMAL CONDUCTIVITY

4.3.1 Isothermal electrical conductivity

$$f^{(1)}(\mathbf{k}) = -e\,\tau_{\mathbf{k}}\,\mathbf{E}\cdot\mathbf{v}(\mathbf{k})\left(-\frac{\partial f^0}{\partial \varepsilon_{\mathbf{k}}}\right)$$

$$\mathbf{j}(\mathbf{r},t) = -\frac{2e}{(2\pi)^3}\int_{\mathrm{BZ}} d^3k\,\mathbf{v}(\mathbf{k})\,f(\mathbf{k};\mathbf{r},t)$$

Let us use the definition of the current density introduced earlier. The equilibrium distribution f^0 produces no current. Therefore, using $f \approx f^{(1)}$,

$$\mathbf{j} = -\frac{2e}{(2\pi)^3}\int_{\mathrm{BZ}} d^3k\,\mathbf{v}(\mathbf{k})\,f^{(1)}(\mathbf{k})$$

Hence $\mathbf{j} = \boldsymbol{\sigma}\cdot\mathbf{E}$,

with $$\sigma_{ij} = \frac{2e^2}{(2\pi)^3}\int_{\mathrm{BZ}} d^3k\,\tau_{\mathbf{k}}\,v_i(\mathbf{k})v_j(\mathbf{k})\left(-\frac{\partial f^0}{\partial \epsilon_{\mathbf{k}}}\right).$$

This expression gives the electrical conductivity tensor within the relaxation-time approximation. The material-specific quantities are the band velocity $\mathbf{v}(\mathbf{k})$ and the relaxation time $\tau_{\mathbf{k}}$.

Since $-\frac{\partial f^0}{\partial \epsilon_{\mathbf{k}}}$ is sharply peaked at the Fermi energy, the geometry of the Fermi surface and the properties of the electronic states close to it are the most relevant factors.

4.3 ELECTRICAL AND THERMAL CONDUCTIVITY

4.3.1 Isothermal electrical conductivity

The electrical conductivity is temperature-dependent because both $\tau_{\mathbf{k}}$ and $-\frac{\partial f^0}{\partial \epsilon_{\mathbf{k}}}$ depend on temperature.

$$f^{(1)}(\mathbf{k}) = -e\,\tau_{\mathbf{k}}\,\mathbf{E}\cdot\mathbf{v}(\mathbf{k})\left(-\frac{\partial f^0}{\partial \varepsilon_{\mathbf{k}}}\right)$$

The distribution function in the presence of the electric field is:

$$f(\mathbf{k}) = f^0(\mathbf{k}) + f^{(1)}(\mathbf{k}) = f^0(\mathbf{k}) - e\,\tau_{\mathbf{k}}\,[\mathbf{E}\cdot\mathbf{v}(\mathbf{k})]\left(-\frac{\partial f^0}{\partial \epsilon_{\mathbf{k}}}\right)$$

We can write:
$$\frac{\partial f^0}{\partial \epsilon_{\mathbf{k}}}\,\mathbf{v}(\mathbf{k}) = \frac{\partial f^0}{\partial \epsilon_{\mathbf{k}}}\frac{1}{\hbar}\nabla_{\mathbf{k}}\epsilon_{\mathbf{k}} = \frac{1}{\hbar}\nabla_{\mathbf{k}} f^0(\mathbf{k})$$

$$\mathbf{v}(\mathbf{k}) = \frac{1}{\hbar}\nabla_{\mathbf{k}}\epsilon_{\mathbf{k}}$$

Therefore
$$f(\mathbf{k}) = f^0(\mathbf{k}) + \frac{e\,\tau_{\mathbf{k}}}{\hbar}\,\mathbf{E}\cdot\nabla_{\mathbf{k}} f^0(\mathbf{k}).$$

If $\tau_{\mathbf{k}}$ is independent of $\mathbf{k}$, this is the first-order Taylor expansion

$$f(\mathbf{k}) \simeq f^0\left(\mathbf{k} + \frac{e\tau}{\hbar}\mathbf{E}\right)$$

Thus, the electric field shifts the equilibrium distribution in $\mathbf{k}$-space by $-\frac{e\tau}{\hbar}\mathbf{E}$. Equivalently, the centre of the Fermi distribution is displaced towards $-\frac{e\tau}{\hbar}\mathbf{E}$.

4.3 ELECTRICAL AND THERMAL CONDUCTIVITY

4.3.2 Thermoelectric conductivity

$$-T(\mathbf{r})\,\mathbf{v}(\mathbf{k})\cdot\nabla_{\mathbf{r}}\left[\frac{\varepsilon_{\mathbf{k}}-\mu(\mathbf{r})}{T(\mathbf{r})}\right]+e\,\mathbf{E}\cdot\mathbf{v}(\mathbf{k})=\frac{\phi(\mathbf{k},\mathbf{r})}{\tau_{\mathbf{k}}}-\frac{e}{\hbar c}[\mathbf{v}(\mathbf{k})\times\mathbf{B}]\cdot\nabla_{\mathbf{k}}\phi(\mathbf{k},\mathbf{r})$$

Consider a crystal subjected to a uniform electric field $\mathbf{E}$, with its two ends maintained at different temperatures.

The local temperature $T(\mathbf{r})$ and chemical potential $\mu(\mathbf{r})$ are therefore position dependent.

Under steady-state conditions, and assuming $\mathbf{B}=\mathbf{0}$, the linearized Boltzmann equation becomes

$$T(\mathbf{r})\,\mathbf{v}(\mathbf{k})\cdot\nabla_{\mathbf{r}}\left[\frac{\epsilon_{\mathbf{k}}-\mu(\mathbf{r})}{T(\mathbf{r})}\right]-e\,\mathbf{E}\cdot\mathbf{v}(\mathbf{k})=\frac{\phi(\mathbf{k},\mathbf{r})}{\tau_{\mathbf{k}}}.$$

To separate the thermal and chemical-potential contributions, we write

$$\nabla_{\mathbf{r}}\left[\frac{\epsilon_{\mathbf{k}}-\mu(\mathbf{r})}{T(\mathbf{r})}\right]=\nabla_{\mathbf{r}}\left[\frac{\epsilon_{\mathbf{k}}}{T(\mathbf{r})}\right]-\nabla_{\mathbf{r}}\left[\frac{\mu(\mathbf{r})}{T(\mathbf{r})}\right].$$

Using the chain rule,

$$\nabla_{\mathbf{r}}\left[\frac{\epsilon_{\mathbf{k}}}{T(\mathbf{r})}\right]=\nabla_{\mathbf{r}}T(\mathbf{r})\,\frac{\partial}{\partial T}\left(\frac{\epsilon_{\mathbf{k}}}{T}\right).$$

4.3 ELECTRICAL AND THERMAL CONDUCTIVITY

4.3.2 Thermoelectric conductivity

$$-T(\mathbf{r})\,\mathbf{v}(\mathbf{k})\cdot\nabla_{\mathbf{r}}\left[\frac{\varepsilon_{\mathbf{k}}-\mu(\mathbf{r})}{T(\mathbf{r})}\right]+e\,\mathbf{E}\cdot\mathbf{v}(\mathbf{k})=\frac{\phi(\mathbf{k},\mathbf{r})}{\tau_{\mathbf{k}}}-\frac{e}{\hbar c}[\mathbf{v}(\mathbf{k})\times\mathbf{B}]\cdot\nabla_{\mathbf{k}}\phi(\mathbf{k},\mathbf{r})$$

Assuming that the band energy $\epsilon_{\mathbf{k}}$ depends only weakly on temperature,

$$\frac{\partial}{\partial T}\left(\frac{\epsilon_{\mathbf{k}}}{T}\right)\simeq-\frac{\epsilon_{\mathbf{k}}}{T^2}$$

$$\nabla_{\mathbf{r}}\left[\frac{\epsilon_{\mathbf{k}}-\mu(\mathbf{r})}{T(\mathbf{r})}\right]=\nabla_{\mathbf{r}}\left[\frac{\epsilon_{\mathbf{k}}}{T(\mathbf{r})}\right]-\nabla_{\mathbf{r}}\left[\frac{\mu(\mathbf{r})}{T(\mathbf{r})}\right]$$

$$\nabla_{\mathbf{r}}\left[\frac{\epsilon_{\mathbf{k}}}{T(\mathbf{r})}\right]=\nabla_{\mathbf{r}}T(\mathbf{r})\,\frac{\partial}{\partial T}\left(\frac{\epsilon_{\mathbf{k}}}{T}\right)$$

Therefore: $$\nabla_{\mathbf{r}}\left[\frac{\epsilon_{\mathbf{k}}-\mu(\mathbf{r})}{T(\mathbf{r})}\right]\simeq-\frac{\epsilon_{\mathbf{k}}}{T^2}\nabla_{\mathbf{r}}T-\nabla_{\mathbf{r}}\left[\frac{\mu(\mathbf{r})}{T(\mathbf{r})}\right]$$

Substituting it into the linearized Boltzmann equation gives

$$T\,\mathbf{v}(\mathbf{k})\cdot\left[-\frac{\epsilon_{\mathbf{k}}}{T^2}\nabla_{\mathbf{r}}T-\nabla_{\mathbf{r}}\left(\frac{\mu}{T}\right)\right]-e\,\mathbf{E}\cdot\mathbf{v}(\mathbf{k})=\frac{\phi(\mathbf{k},\mathbf{r})}{\tau_{\mathbf{k}}}.$$

Therefore,

$$\phi(\mathbf{k},\mathbf{r})=-\tau_{\mathbf{k}}\,\mathbf{v}(\mathbf{k})\cdot\left[\frac{\epsilon_{\mathbf{k}}}{T}\nabla_{\mathbf{r}}T+T\nabla_{\mathbf{r}}\left(\frac{\mu}{T}\right)+e\,\mathbf{E}\right].$$

4.3 ELECTRICAL AND THERMAL CONDUCTIVITY

4.3.2 Thermoelectric conductivity

$$\phi(\mathbf{k},\mathbf{r}) = -\tau_{\mathbf{k}}\,\mathbf{v}(\mathbf{k})\cdot\left[\frac{\epsilon_{\mathbf{k}}}{T}\nabla_{\mathbf{r}}T + T\nabla_{\mathbf{r}}\left(\frac{\mu}{T}\right) + e\,\mathbf{E}\right]$$

$$\mathbf{j}(\mathbf{r},t) = -\frac{2e}{(2\pi)^3}\int_{\mathrm{BZ}} d^3k\,\mathbf{v}(\mathbf{k})\,f(\mathbf{k};\mathbf{r},t)$$

$$f(\mathbf{k};\mathbf{r},t) = f^0(\mathbf{k};\mathbf{r}) + f^{(1)}(\mathbf{k};\mathbf{r})$$

$$f^{(1)}(\mathbf{k},\mathbf{r}) \equiv -\frac{\partial f^0}{\partial \varepsilon_{\mathbf{k}}}\Phi(\mathbf{k},\mathbf{r})$$

Recalling that f^0 does not give rise to a current density:

$$\mathbf{j}(\mathbf{r},t) = -\frac{2e}{(2\pi)^3}\int_{\mathrm{BZ}} d^3k\,\mathbf{v}(\mathbf{k})\left(-\frac{\partial f^0}{\partial \epsilon_{\mathbf{k}}}\right)\phi(\mathbf{k},\mathbf{r}).$$

Substituting the expression for $\phi(\mathbf{k},\mathbf{r})$:

$$\mathbf{j}(\mathbf{r},t) = \frac{2e}{(2\pi)^3}\int_{\mathrm{BZ}} d^3k\,\mathbf{v}(\mathbf{k})\left(-\frac{\partial f^0}{\partial \epsilon_{\mathbf{k}}}\right)\tau_{\mathbf{k}}\,\mathbf{v}(\mathbf{k})\cdot\left[\frac{\epsilon_{\mathbf{k}}}{T}\nabla_{\mathbf{r}}T + T\nabla_{\mathbf{r}}\left(\frac{\mu}{T}\right) + e\,\mathbf{E}\right].$$

The current density can be separated into a thermoelectric contribution and the contribution driven by the electric field:

$$\mathbf{j}(\mathbf{r},t) = \frac{2e}{(2\pi)^3}\int_{\mathrm{BZ}} d^3k\,\mathbf{v}(\mathbf{k})\left(-\frac{\partial f^0}{\partial \epsilon_{\mathbf{k}}}\right)\tau_{\mathbf{k}}\,\mathbf{v}(\mathbf{k})\cdot\left[\frac{\epsilon_{\mathbf{k}}}{T}\nabla_{\mathbf{r}}T + T\nabla_{\mathbf{r}}\left(\frac{\mu}{T}\right)\right]$$
$$+\frac{2e^2}{(2\pi)^3}\int_{\mathrm{BZ}} d^3k\,\mathbf{v}(\mathbf{k})\left(-\frac{\partial f^0}{\partial \epsilon_{\mathbf{k}}}\right)\tau_{\mathbf{k}}\,\mathbf{v}(\mathbf{k})\cdot\mathbf{E}.$$

4.3 ELECTRICAL AND THERMAL CONDUCTIVITY

4.3.2 Thermoelectric conductivity

$$\mathbf{j}(\mathbf{r},t)=\frac{2e}{(2\pi)^3}\int_{\mathrm{BZ}}d^3\,k\,\mathbf{v}(\mathbf{k})\left(-\frac{\partial f^0}{\partial\epsilon_{\mathbf{k}}}\right)\tau_{\mathbf{k}}\,\mathbf{v}(\mathbf{k})\cdot\left[\frac{\epsilon_{\mathbf{k}}}{T}\nabla_{\mathbf{r}}T+T\nabla_{\mathbf{r}}\left(\frac{\mu}{T}\right)\right]+\frac{2e^2}{(2\pi)^3}\int_{\mathrm{BZ}}d^3\,k\,\mathbf{v}(\mathbf{k})\left(-\frac{\partial f^0}{\partial\epsilon_{\mathbf{k}}}\right)\tau_{\mathbf{k}}\,\mathbf{v}(\mathbf{k})\cdot\mathbf{E}$$

Using the definition of the electrical conductivity tensor, we obtain

$$\sigma_{ij}=\frac{2e^2}{(2\pi)^3}\int_{\mathrm{BZ}}d^3\,k\,v_i(\mathbf{k})v_j(\mathbf{k})\left(-\frac{\partial f^0}{\partial\epsilon_{\mathbf{k}}}\right)\tau_{\mathbf{k}},$$

$$\mathbf{j}(\mathbf{r},t)=\frac{2e}{(2\pi)^3}\int_{\mathrm{BZ}}d^3\,k\,\mathbf{v}(\mathbf{k})\left(-\frac{\partial f^0}{\partial\epsilon_{\mathbf{k}}}\right)\tau_{\mathbf{k}}\,\mathbf{v}(\mathbf{k})\cdot\left[\frac{\epsilon_{\mathbf{k}}}{T}\nabla_{\mathbf{r}}T+T\nabla_{\mathbf{r}}\left(\frac{\mu}{T}\right)\right]+\boldsymbol{\sigma}\cdot\mathbf{E}.$$

In the absence of an externally applied electric field,

$$\mathbf{E}=0,$$

and assuming that the spatial variation of $\frac{\mu}{T}$ is negligible,

$$\nabla_{\mathbf{r}}\left(\frac{\mu(\mathbf{r})}{T(\mathbf{r})}\right)\simeq 0,$$

the current density reduces to the thermoelectric contribution

$$\mathbf{j}_T(\mathbf{r},t)=\frac{2e}{(2\pi)^3}\int_{\mathrm{BZ}}d^3\,k\,\mathbf{v}(\mathbf{k})\left(-\frac{\partial f^0}{\partial\epsilon_{\mathbf{k}}}\right)\tau_{\mathbf{k}}\,\frac{\epsilon_{\mathbf{k}}}{T}\,[\mathbf{v}(\mathbf{k})\cdot\nabla_{\mathbf{r}}T].$$

4.3 ELECTRICAL AND THERMAL CONDUCTIVITY

4.3.2 Thermoelectric conductivity

$$\mathbf{j}_T(\mathbf{r},t) = \frac{2e}{(2\pi)^3}\int_{\mathrm{BZ}} d^3k\, \mathbf{v}(\mathbf{k})\left(-\frac{\partial f^0}{\partial \epsilon_{\mathbf{k}}}\right)\tau_{\mathbf{k}}\,\frac{\epsilon_{\mathbf{k}}}{T}\,[\mathbf{v}(\mathbf{k})\cdot\nabla_{\mathbf{r}}T]$$

Let us define the thermoelectric conductivity tensor:

$$\boldsymbol{\alpha} = -\frac{2e}{(2\pi)^3}\int_{\mathrm{BZ}} d^3k\left(-\frac{\partial f^0}{\partial \epsilon_{\mathbf{k}}}\right)\frac{\epsilon_{\mathbf{k}}\tau_{\mathbf{k}}}{T}\,\mathbf{v}(\mathbf{k})\mathbf{v}(\mathbf{k}).$$

The thermal current density can then be written as:

$$\mathbf{j}_T(\mathbf{r},t) = -\boldsymbol{\alpha}\cdot\nabla_{\mathbf{r}}T.$$

This expression describes a current density driven by a spatial temperature gradient. It is the thermoelectric current underlying the Seebeck effect.

Thus, a temperature gradient can drive a net electric current even in the absence of an externally applied electric field: this is the physical origin of the Seebeck effect.

4.3 ELECTRICAL AND THERMAL CONDUCTIVITY

4.3.3 Thermal conductivity

$$\mathbf{j}(\mathbf{r},t) = -\frac{2e}{(2\pi)^3}\int_{\mathrm{BZ}} d^3\,k\,\mathbf{v}(\mathbf{k})\,f(\mathbf{k},\mathbf{r},t)$$

$$dN = \frac{2}{(2\pi)^3}\,f(\mathbf{k},\mathbf{r},t)\,d^3k\,d^3r$$

Similarly to the electric current density, the heat-current density is defined as the energy transported relative to the local chemical potential:

$$d\mathbf{j}_Q = [\epsilon_{\mathbf{k}} - \mu(\mathbf{r})]\,\mathbf{v}(\mathbf{k})\,dN.$$

Therefore,

$$\mathbf{j}_Q(\mathbf{r},t) = \frac{2}{(2\pi)^3}\int_{\mathrm{BZ}} d^3\,k\,[\epsilon_{\mathbf{k}} - \mu(\mathbf{r})]\,\mathbf{v}(\mathbf{k})\,f(\mathbf{k};\mathbf{r},t).$$

Since the local-equilibrium distribution f^0 produces no net heat current, only the correction $f^{(1)}$ contributes:

$$f^{(1)}(\mathbf{k},\mathbf{r}) \equiv -\frac{\partial f^0}{\partial \varepsilon_{\mathbf{k}}}\Phi(\mathbf{k},\mathbf{r})$$

$$\mathbf{j}_Q(\mathbf{r},t) = \frac{2}{(2\pi)^3}\int_{\mathrm{BZ}} d^3\,k\,[\epsilon_{\mathbf{k}} - \mu(\mathbf{r})]\,\mathbf{v}(\mathbf{k})\,f^{(1)}(\mathbf{k},\mathbf{r}),$$

giving:

$$\mathbf{j}_Q(\mathbf{r},t) = \frac{1}{4\pi^3}\int_{\mathrm{BZ}} d^3\,k\,[\epsilon_{\mathbf{k}} - \mu(\mathbf{r})]\,\mathbf{v}(\mathbf{k})\left(-\frac{\partial f^0}{\partial \epsilon_{\mathbf{k}}}\right)\phi(\mathbf{k},\mathbf{r}).$$

4.3 ELECTRICAL AND THERMAL CONDUCTIVITY

4.3.3 Thermal conductivity

$$\mathbf{j}_Q(\mathbf{r},t) = \frac{1}{4\pi^3}\int_{\mathrm{BZ}} d^3k\,[\epsilon_{\mathbf{k}} - \mu(\mathbf{r})]\,\mathbf{v}(\mathbf{k})\left(-\frac{\partial f^0}{\partial \epsilon_{\mathbf{k}}}\right)\phi(\mathbf{k},\mathbf{r})$$

Let's recall the expression for $\phi(\mathbf{k},\mathbf{r})$ and use again the assumption

$$\nabla_{\mathbf{r}}\left(\frac{\mu(\mathbf{r})}{T(\mathbf{r})}\right) \simeq 0,$$

$$\phi(\mathbf{k},\mathbf{r}) = -\tau_{\mathbf{k}}\,\mathbf{v}(\mathbf{k})\cdot\left[\frac{\epsilon_{\mathbf{k}}}{T}\nabla_{\mathbf{r}}T + T\nabla_{\mathbf{r}}\left(\frac{\mu}{T}\right) + e\,\mathbf{E}\right]$$

When the chemical potential is spatially uniform, a temperature gradient changes the local occupation according to the energy of each state measured relative to μ; therefore, the thermal driving term in $\phi(\mathbf{k},\mathbf{r})$ is proportional to $\epsilon_{\mathbf{k}} - \mu$.

Therefore, it becomes

$$\phi(\mathbf{k},\mathbf{r}) = -\tau_{\mathbf{k}}\,\mathbf{v}(\mathbf{k})\cdot\left[\frac{\epsilon_{\mathbf{k}} - \mu}{T}\,\nabla_{\mathbf{r}}T + e\,\mathbf{E}\right].$$

Then, we obtain the final expression:

$$\mathbf{j}_Q(\mathbf{r},t) = -\frac{1}{4\pi^3}\int_{\mathrm{BZ}} d^3k\,[\epsilon_{\mathbf{k}} - \mu(\mathbf{r})]\,\mathbf{v}(\mathbf{k})\left(-\frac{\partial f^0}{\partial \epsilon_{\mathbf{k}}}\right)\tau_{\mathbf{k}}\,\frac{\epsilon_{\mathbf{k}}}{T}\,[\mathbf{v}(\mathbf{k})\cdot\nabla_{\mathbf{r}}T]$$
$$-\frac{e}{4\pi^3}\int_{\mathrm{BZ}} d^3k\,[\epsilon_{\mathbf{k}} - \mu(\mathbf{r})]\,\mathbf{v}(\mathbf{k})\left(-\frac{\partial f^0}{\partial \epsilon_{\mathbf{k}}}\right)\tau_{\mathbf{k}}\,[\mathbf{v}(\mathbf{k})\cdot\mathbf{E}].$$

4.3 ELECTRICAL AND THERMAL CONDUCTIVITY

4.3.3 Thermal conductivity

$$\mathbf{j}_Q(\mathbf{r},t) = -\frac{1}{4\pi^3}\int_{\mathrm{BZ}} d^3k\,[\epsilon_{\mathbf{k}} - \mu(\mathbf{r})]\,\mathbf{v}(\mathbf{k})\left(-\frac{\partial f^0}{\partial \epsilon_{\mathbf{k}}}\right)\tau_{\mathbf{k}}\,\frac{\epsilon_{\mathbf{k}}}{T}\,[\mathbf{v}(\mathbf{k})\cdot\nabla_{\mathbf{r}}T]$$
$$-\frac{e}{4\pi^3}\int_{\mathrm{BZ}} d^3k\,[\epsilon_{\mathbf{k}} - \mu(\mathbf{r})]\,\mathbf{v}(\mathbf{k})\left(-\frac{\partial f^0}{\partial \epsilon_{\mathbf{k}}}\right)\tau_{\mathbf{k}}\,[\mathbf{v}(\mathbf{k})\cdot\mathbf{E}]$$

It is convenient to introduce the transport tensors:

$$\mathbf{L}^{(n)} = \frac{1}{4\pi^3}\int_{\mathrm{BZ}} d^3k\,(\epsilon_{\mathbf{k}} - \mu)^n\,\mathbf{v}(\mathbf{k})\mathbf{v}(\mathbf{k})\left(-\frac{\partial f^0}{\partial \epsilon_{\mathbf{k}}}\right)\tau_{\mathbf{k}}.$$

The heat-current density can then be written in the compact form:

$$\mathbf{j}_Q(\mathbf{r},t) = -e\,\mathbf{L}^{(1)}\cdot\mathbf{E} - \mathbf{L}^{(2)}\cdot\frac{\nabla_{\mathbf{r}}T}{T}.$$

$$\mathbf{j}(\mathbf{r},t) = \frac{2e}{(2\pi)^3}\int_{\mathrm{BZ}} d^3k\,\mathbf{v}(\mathbf{k})\left(-\frac{\partial f^0}{\partial \epsilon_{\mathbf{k}}}\right)\tau_{\mathbf{k}}\,\mathbf{v}(\mathbf{k})\cdot\left[\frac{\epsilon_{\mathbf{k}}}{T}\nabla_{\mathbf{r}}T\right] + \frac{2e^2}{(2\pi)^3}\int_{\mathrm{BZ}} d^3k\,\mathbf{v}(\mathbf{k})\left(-\frac{\partial f^0}{\partial \epsilon_{\mathbf{k}}}\right)\tau_{\mathbf{k}}\,\mathbf{v}(\mathbf{k})\cdot\mathbf{E}$$

With the same notation, the electric current density becomes

$$\mathbf{j}(\mathbf{r},t) = e^2\,\mathbf{L}^{(0)}\cdot\mathbf{E} + e\,\mathbf{L}^{(1)}\cdot\frac{\nabla_{\mathbf{r}}T}{T}.$$

4.3 ELECTRICAL AND THERMAL CONDUCTIVITY

4.3.3 Thermal conductivity

$$\mathbf{j}(\mathbf{r},t) = e^2\,\mathbf{L}^{(0)}\cdot\mathbf{E} + e\,\mathbf{L}^{(1)}\cdot\frac{\nabla_{\mathbf{r}}T}{T}$$

$$\mathbf{j}_Q(\mathbf{r},t) = -e\,\mathbf{L}^{(1)}\cdot\mathbf{E} - \mathbf{L}^{(2)}\cdot\frac{\nabla_{\mathbf{r}}T}{T}$$

The thermal conductivity of a crystal is defined from the heat current flowing in response to a temperature gradient under open-circuit conditions, i.e..

$$\mathbf{j}(\mathbf{r},t) = 0.$$

Although no external electric field is applied, a temperature gradient induces an internal electric field that prevents a net electric current from flowing.

Therefore:

$$e\,\mathbf{L}^{(0)}\cdot\mathbf{E} = -\mathbf{L}^{(1)}\cdot\frac{\nabla_{\mathbf{r}}T}{T},$$

Multiplying by $\left[\mathbf{L}^{(0)}\right]^{-1}$, the inverse of the zeroth-order transport tensor, gives

$$e\,\mathbf{E} = -\left[\mathbf{L}^{(0)}\right]^{-1}\cdot\mathbf{L}^{(1)}\cdot\frac{\nabla_{\mathbf{r}}T}{T}.$$

Therefore,

$$e\,\mathbf{L}^{(1)}\cdot\mathbf{E} = -\mathbf{L}^{(1)}\cdot\left[\mathbf{L}^{(0)}\right]^{-1}\cdot\mathbf{L}^{(1)}\cdot\frac{\nabla_{\mathbf{r}}T}{T}.$$

4.3 ELECTRICAL AND THERMAL CONDUCTIVITY

4.3.3 Thermal conductivity

$$\mathbf{j}(\mathbf{r},t) = e^2\,\mathbf{L}^{(0)}\cdot\mathbf{E} + e\,\mathbf{L}^{(1)}\cdot\frac{\nabla_{\mathbf{r}}T}{T}$$

$$\mathbf{j}_Q(\mathbf{r},t) = -e\,\mathbf{L}^{(1)}\cdot\mathbf{E} - \mathbf{L}^{(2)}\cdot\frac{\nabla_{\mathbf{r}}T}{T}$$

$$e\,\mathbf{L}^{(1)}\cdot\mathbf{E} = -\mathbf{L}^{(1)}\cdot\left[\mathbf{L}^{(0)}\right]^{-1}\cdot\mathbf{L}^{(1)}\cdot\frac{\nabla_{\mathbf{r}}T}{T}$$

Substituting this result into $\mathbf{j}_Q(\mathbf{r},t)$, we obtain

$$\mathbf{j}_Q(\mathbf{r},t) = \left[\mathbf{L}^{(1)}\cdot\left[\mathbf{L}^{(0)}\right]^{-1}\cdot\mathbf{L}^{(1)} - \mathbf{L}^{(2)}\right]\cdot\frac{\nabla_{\mathbf{r}}T}{T}.$$

or equivalently

$$\mathbf{j}_Q(\mathbf{r},t) = -\left[\mathbf{L}^{(2)} - \mathbf{L}^{(1)}\cdot\left[\mathbf{L}^{(0)}\right]^{-1}\cdot\mathbf{L}^{(1)}\right]\cdot\frac{\nabla_{\mathbf{r}}T}{T}.$$

We define the thermal-conductivity tensor as

$$\boldsymbol{\kappa}_{\text{th}} = \frac{1}{T}\left[\mathbf{L}^{(2)} - \mathbf{L}^{(1)}\cdot\left[\mathbf{L}^{(0)}\right]^{-1}\cdot\mathbf{L}^{(1)}\right].$$

Therefore, $\mathbf{j}_Q(\mathbf{r},t) = -\boldsymbol{\kappa}_{\text{th}}\cdot\nabla_{\mathbf{r}}T.$

This is Fourier's law of heat conduction in a crystal.

4.4 DRIFT-DIFFUSION EQUATIONS

4.4.1 Diffusion equation

Let us return to the stationary, linearized Boltzmann equation:

$$\mathbf{v}(\mathbf{k}) \cdot \nabla_{\mathbf{r}} f^0 - \frac{e}{\hbar}\mathbf{E} \cdot \nabla_{\mathbf{k}} f^0 = \left(\frac{\partial f^{(1)}}{\partial t}\right)_{\text{coll}} + \frac{e}{\hbar c}[\mathbf{v}(\mathbf{k}) \times \mathbf{B}] \cdot \nabla_{\mathbf{k}} f^{(1)}.$$

In the absence of a magnetic field, the last term vanishes. Therefore,

$$\mathbf{v}(\mathbf{k}) \cdot \nabla_{\mathbf{r}} f^0 - \frac{e}{\hbar}\mathbf{E} \cdot \nabla_{\mathbf{k}} f^0 = \left(\frac{\partial f^{(1)}}{\partial t}\right)_{\text{coll}}$$

The electric current density is the net electric charge crossing a unit area per unit time. For electrons, whose charge is $-e$,

$$\mathbf{j}(\mathbf{r}) = -\frac{2e}{(2\pi)^3}\int_{\text{BZ}} d^3\,k\,\mathbf{v}(\mathbf{k})\,f(\mathbf{k},\mathbf{r}).$$

For a one-dimensional system oriented along the x −axis,

$$j(x) = -\frac{2e}{2\pi}\int d\,k\,v(k)\,f(k,x).$$

4.4 DRIFT-DIFFUSION EQUATIONS

4.4.1 Diffusion equation

$$j(x) = -\frac{e}{\pi}\int d\,k\, v(k)\, f(k,x)$$

Let us rewrite the current integral using the velocity as the integration variable. Recall that:

$$v(k) = \frac{1}{\hbar}\frac{d\epsilon(k)}{dk}$$

Differentiating with respect to k, we obtain:

$$\frac{dv}{dk} = \frac{1}{\hbar}\frac{d^2\epsilon(k)}{dk^2}.$$

For a parabolic band, the curvature is constant and defines the effective mass:

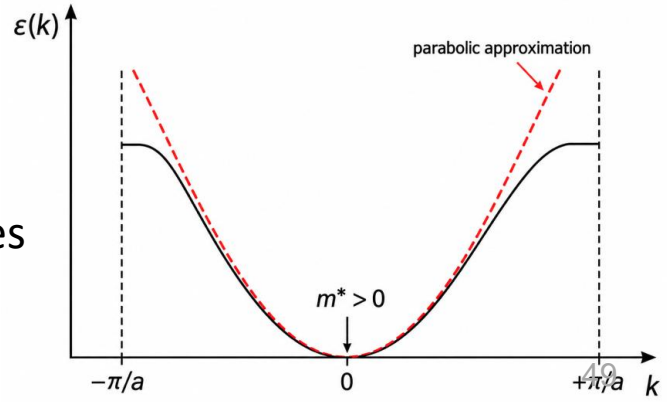
$$\frac{1}{m^*} = \frac{1}{\hbar^2}\frac{d^2\epsilon(k)}{dk^2} \qquad \text{and so:} \qquad \frac{dv}{dk} = \frac{\hbar}{m^*}.$$

For a parabolic band centred at k_0, introduce

$$q = k - k_{0.}$$

Since $dk = dq$, the relation obtained above gives

$$dk = \frac{m^*}{\hbar}\,dv, \qquad q = \frac{m^*}{\hbar}\,v.$$



4.4 DRIFT-DIFFUSION EQUATIONS

4.4.1 Diffusion equation

$$j(x) = -\frac{e}{\pi}\int d\,k\,v(k)\,f(k,x) \qquad dk = \frac{m^* dv}{\hbar} \qquad q = \frac{m^* v}{\hbar} \qquad q = k - k_0$$

Substituting into the expression for the current density yields:

$$j(x) = -\frac{2e}{2\pi}\frac{m^*}{\hbar}\int d\,v\,v\,f\left(k_0 + \frac{m^* v}{\hbar}, x\right).$$

We now define the distribution in velocity space as:

$$F(v,x) \equiv \frac{m^*}{\pi\hbar}\,f\left(k_0 + \frac{m^* v}{\hbar}, x\right).$$

The current density can therefore be written as:

$$j(x) = -e\int d\,v\,v\,F(v,x).$$

Thus, apart from the electron charge, the current density is the first velocity moment of the distribution $F(v,x)$.

4.4 DRIFT-DIFFUSION EQUATIONS

4.4.1 Diffusion equation

Let us now express the linearized Boltzmann equation in terms of the velocity variable. For a one-dimensional system, with the electric field directed along x,

$$v\frac{\partial F^0}{\partial x} - \frac{eE}{\hbar}\frac{\partial F^0}{\partial k} = \left(\frac{\partial F^{(1)}}{\partial t}\right)_{\text{coll}}$$

$$\mathbf{v}(\mathbf{k}) \cdot \nabla_{\mathbf{r}} f^0 - \frac{e}{\hbar}\mathbf{E} \cdot \nabla_{\mathbf{k}} f^0 = \left(\frac{\partial f^{(1)}}{\partial t}\right)_{\text{coll}}$$

For a parabolic band,

$$\frac{\partial}{\partial k} = \frac{dv}{dk}\frac{\partial}{\partial v} = \frac{\hbar}{m^*}\frac{\partial}{\partial v}.$$

$$dk = \frac{m^* dv}{\hbar}$$

Therefore,

$$v\frac{\partial F^0}{\partial x} - \frac{eE}{m^*}\frac{\partial F^0}{\partial v} = \left(\frac{\partial F^{(1)}}{\partial t}\right)_{\text{coll}}.$$

Within the relaxation-time approximation, $\left(\frac{\partial F^{(1)}}{\partial t}\right)_{\text{coll}} = -\frac{F - F^0}{\tau} = \frac{F^0 - F}{\tau}.$

Hence,

$$v\frac{\partial F^0}{\partial x} - \frac{eE}{m^*}\frac{\partial F^0}{\partial v} = \frac{F^0 - F}{\tau}.$$

4.4 DRIFT-DIFFUSION EQUATIONS

4.4.1 Diffusion equation

$$j(x) = -e \int d\,v\, v\, F(v,x)$$

$$v\frac{\partial F^0}{\partial x} - \frac{eE}{m^*}\frac{\partial F^0}{\partial v} = \frac{F^0 - F}{\tau}$$

To relate the current to the linearized Boltzmann equation, multiply both sides by v and integrate over all velocities.

$$\int d\,v\, v \left[v\frac{\partial F^0}{\partial x} - \frac{eE}{m^*}\frac{\partial F^0}{\partial v} \right] = \int d\,v\, v\, \frac{F^0 - F}{\tau}.$$

Let us first evaluate the collision term on the right-hand side.

Assuming a velocity-independent relaxation time,

$$\int d\,v\, v\, \frac{F^0 - F}{\tau} = \frac{1}{\tau}\left[\int d\,v\, vF^0 - \int d\,v\, vF \right].$$

Since the local-equilibrium distribution F^0 is even in v, $\int d\,v\, vF^0 = 0.$

Therefore,

$$\int d\,v\, v\, \frac{F^0 - F}{\tau} = -\frac{1}{\tau}\int d\,v\, vF = \frac{j(x)}{e\tau}.$$

4.4 DRIFT-DIFFUSION EQUATIONS

4.4.1 Diffusion equation

We now evaluate the left-hand side of the linearized Boltzmann equation. Multiplying it by v and integrating over all velocities gives:

$$\int d\,v\,v^2\frac{\partial F^0(v,x)}{\partial x}-\frac{eE}{m^*}\int d\,v\,v\frac{\partial F^0(v,x)}{\partial v}=\frac{j(x)}{e\tau}.$$

$$\int d\,v\,v\frac{F^0-F}{\tau}=\frac{j(x)}{e\tau}$$

$$v\frac{\partial F^0}{\partial x}-\frac{eE}{m^*}\frac{\partial F^0}{\partial v}=\frac{F^0-F}{\tau}$$

Therefore,

$$j(x)=e\tau\,\frac{\partial}{\partial x}\int d\,v\,v^2F^0(v,x)-\frac{e^2\tau E}{m^*}\int d\,v\,v\frac{\partial F^0(v,x)}{\partial v}.$$

The second integral can be evaluated by parts:

$$\int d\,v\,v\frac{\partial F^0(v,x)}{\partial v}=[vF^0(v,x)]_{-\infty}^{+\infty}-\int d\,v\,F^0(v,x).$$

Since $F^0(v,x)\to 0$ for $|v|\to\infty$

$$\int d\,v\,v\frac{\partial F^0(v,x)}{\partial v}=-n(x),$$

where $n(x)\equiv\int d\,v\,F^0(v,x)$ is the local electron density.

4.4 DRIFT-DIFFUSION EQUATIONS

4.4.1 Diffusion equation

$$j(x) = e\tau \frac{\partial}{\partial x}\int d\,v\, v^2 F^0(v,x) - \frac{e^2\tau E}{m^*}\int d\,v\, v \frac{\partial F^0(v,x)}{\partial v}$$

$$\int d\,v\, v \frac{\partial F^0(v,x)}{\partial v} = -n(x)$$

$$n(x) \equiv \int d\,v\, F^0(v,x)$$

Let us express the second velocity moment of the local-equilibrium distribution as:

$$\langle v^2\rangle_0(x) \equiv \frac{\int d\,v\, v^2 F^0(v,x)}{\int d\,v\, F^0(v,x)} = \frac{1}{n(x)}\int d\,v\, v^2 F^0(v,x),$$

Therefore,

$$\int d\,v\, v^2 F^0(v,x) = n(x)\langle v^2\rangle_0(x).$$

The current density becomes:

$$j(x) = \frac{e^2\tau}{m^*}\, n(x)E + e\tau\, \frac{\partial}{\partial x}[n(x)\langle v^2\rangle_0(x)].$$

For an isothermal system, the result becomes

$$j(x) = \frac{e^2\tau}{m^*}\, n(x)E + e\tau\langle v^2\rangle_0 \frac{\partial n(x)}{\partial x}.$$

4.4 DRIFT-DIFFUSION EQUATIONS

4.4.1 Diffusion equation

$$j(x) = \frac{e^2\tau}{m^*} n(x)E + e\tau\langle v^2\rangle_0 \frac{\partial n(x)}{\partial x}$$

Let us introduce the electron mobility: $\mu = \frac{e\tau}{m^*}$

In the classical, non-degenerate limit, local thermal equilibrium gives, in one dimension,

$$\frac{1}{2}m^*\langle v^2\rangle_0 = \frac{1}{2}k_B T, \qquad \text{and therefore} \quad \langle v^2\rangle_0 = \frac{k_B T}{m^*}.$$

Substituting this result into the expression for the current density yields:

$$j(x) = e\mu n(x)E + \mu k_B T \frac{\partial n(x)}{\partial x}.$$

Let's introduce the diffusion coefficient as $D_n = \frac{\mu_n k_B T}{e}$.

The electron current density can therefore be written as

$$j_n(x) = e\mu_n n(x)E + eD_n \frac{\partial n(x)}{\partial x}.$$

4.4 DRIFT-DIFFUSION EQUATIONS

4.4.1 Diffusion equation

For an isotropic three-dimensional system, the electron drift-diffusion equation is:

$$\mathbf{j}(\mathbf{r}) = e\mu\, n(\mathbf{r})\, \mathbf{E}(\mathbf{r}) + eD\, \boldsymbol{\nabla} n(\mathbf{r}).$$

This expression follows from the linearized Boltzmann equation under the assumptions of a parabolic band, the relaxation-time approximation, and local thermal equilibrium in the low-field regime.

At higher electric fields, the transport coefficients may become field-dependent. In this case, $\mu(E)$ and $D(E)$ are generally introduced through empirical models or more detailed transport calculations.

To determine the electron density $n(\mathbf{r})$ and the electric field $\mathbf{E}(\mathbf{r})$ in a device, the drift-diffusion equation must be coupled to the **continuity equation** and **Poisson's equation**.

Throughout this section, $\mathbf{j}(\mathbf{r})$ denotes the conventional current density associated with the electron distribution.

The electric current through an oriented open surface $\mathcal{S}$ is the flux of the current density through that surface:

$$I_{\mathcal{S}}(t) = \int_{\mathcal{S}} \mathbf{j}\,(\mathbf{r}, t) \cdot \hat{\mathbf{n}}\, dS,$$

where $\hat{\mathbf{n}}$ is the unit normal vector that specifies the orientation of $\mathcal{S}$.

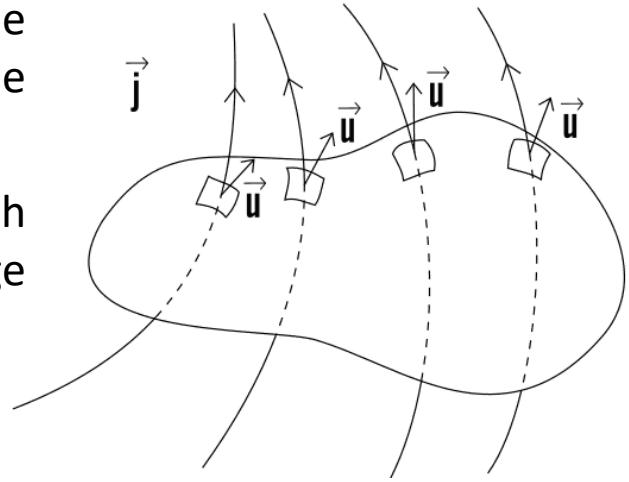
4.4 DRIFT-DIFFUSION EQUATIONS

4.4.2 Continuity equation

Let us now consider a closed surface $\partial\mathcal{V}$. By convention, the unit normal vector $\hat{\mathbf{n}}$ is directed outward at every point of the surface.

$$I_S(t) = \int_S \mathbf{j}(\mathbf{r},t)\cdot\hat{\mathbf{n}}\,dS$$

A net outward current corresponds to charge leaving the volume $\mathcal{V}$; therefore, the total charge enclosed by the surface $Q_{\text{in}}(t)$, may vary with time.



Charge conservation relates the net outward current through a closed surface $\partial\mathcal{V}$ to the rate of change of the charge enclosed within the volume $\mathcal{V}$:

$$\oint_{\partial\mathcal{V}} \mathbf{j}(\mathbf{r},t)\cdot\hat{\mathbf{n}}\,dS = -\frac{dQ_{\text{in}}}{dt}.$$

For electrons, $\quad Q_{\text{in}}(t) = \int_{\mathcal{V}} \rho_e(\mathbf{r},t)\,dV, \qquad \rho_e(\mathbf{r},t) = -e\,n(\mathbf{r},t).$

Therefore, $\quad \oint_{\partial\mathcal{V}} \mathbf{j}(\mathbf{r},t)\cdot\hat{\mathbf{n}}\,dS = -\frac{d}{dt}\int_{\mathcal{V}} \rho_e(\mathbf{r},t)\,dV.$

Using the divergence theorem, $\quad \int_{\mathcal{V}} \boldsymbol{\nabla}\cdot\mathbf{j}(\mathbf{r},t)\,dV = -\frac{d}{dt}\int_{\mathcal{V}} \rho_e(\mathbf{r},t)\,dV.$

4.4 DRIFT-DIFFUSION EQUATIONS

4.4.3 Poisson equation

Since the integration volume $\mathcal{V}$ is arbitrary, the integrands must satisfy:

$$\int_{\mathcal{V}} \boldsymbol{\nabla} \cdot \mathbf{j}(\mathbf{r},t)\, dV = -\frac{d}{dt}\int_{\mathcal{V}} \rho_e(\mathbf{r},t)\, dV$$

$$\frac{\partial \rho_e(\mathbf{r},t)}{\partial t} + \boldsymbol{\nabla} \cdot \mathbf{j}(\mathbf{r},t) = 0.$$

This is the local continuity equation for electric charge. For electrons, in the absence of carrier generation and recombination,

$$\frac{\partial n(\mathbf{r},t)}{\partial t} = \frac{1}{e}\,\boldsymbol{\nabla} \cdot \mathbf{j}(\mathbf{r},t)$$

$$\rho_e(\mathbf{r},t) = -e\, n(\mathbf{r},t)$$

Let us derive the Poisson equation. For a homogeneous medium with permittivity ε, Gauss's law in differential form is

$$\boldsymbol{\nabla} \cdot \mathbf{E}(\mathbf{r},t) = \frac{\rho(\mathbf{r},t)}{\varepsilon}.$$

The electric field is related to the electrostatic potential $\mathrm{V}(\mathbf{r},t)$ by

$$\mathbf{E}(\mathbf{r},t) = -\boldsymbol{\nabla} V(\mathbf{r},t).$$

4.4 DRIFT-DIFFUSION EQUATIONS

5.4.3 Poisson equation

$$\boldsymbol{\nabla} \cdot \mathbf{E}(\mathbf{r}, t) = \frac{\rho(\mathbf{r}, t)}{\varepsilon} \qquad \mathbf{E}(\mathbf{r}, t) = -\boldsymbol{\nabla} V(\mathbf{r}, t)$$

Therefore,

$$\boldsymbol{\nabla} \cdot \mathbf{E} = -\boldsymbol{\nabla}^2 V,$$

and Poisson's equation is

$$\boldsymbol{\nabla}^2 V(\mathbf{r}, t) = -\frac{\rho(\mathbf{r}, t)}{\varepsilon}.$$

The coupled equations to be solved for the transport in a crystal are therefore

$$\begin{cases} \mathbf{j} = e\mu n\, \mathbf{E} + eD\, \boldsymbol{\nabla} n \\ \dfrac{\partial n}{\partial t} = \dfrac{1}{e}\, \boldsymbol{\nabla} \cdot \mathbf{j}, \\ \boldsymbol{\nabla}^2 V = -\dfrac{\rho}{\varepsilon}. \end{cases}$$