as dopants, the resistivity of ultra-pure GaAs, for example, is no larger than about $1\,\Omega\,\mathrm{m}$. Chromium acts as an acceptor in GaAs with an energy level close to mid-gap. Hence, the residual doping electrons can be removed from the conduction band by a rather small density of Cr doping, which is, however, much higher than the residual n-doping (typical doping densities are of the order of $n_{\mathrm{Cr}} \approx 2 \times 10^{23}\,\mathrm{m}^{-3}$. This way, the resistivities can be increased by more than three orders of magnitude. Therefore, such semiconductor materials are called *semi-insulating*. As a consequence, the Fermi level is typically fixed at the energy of the deep dopant, and one speaks of *pinning of the Fermi level*.

2.6 Diffusive Transport and the Boltzmann Equation

Before we discuss the conventional theory of diffusive transport, we briefly summarize some important facts regarding electrons in solids.

- Neither full nor empty bands carry current.
- The resistance of a perfect, static crystal with at least one partially filled electronic band vanishes. The electrons obey the semiclassical equations of motion

  $$\vec{v}(\vec{k}) = \frac{1}{\hbar}\vec{\nabla}_{\vec{k}} E(\vec{k})$$

  $$\frac{d\vec{k}}{dt} = -\frac{e}{\hbar}(\vec{E} + \vec{v}(\vec{k}) \times \vec{B})$$

  Resistance is generated by deviations from the perfect lattice, such as phonons, impurities, lattice dislocations, but also by surfaces and interfaces.
- Electron–electron scattering changes the total momentum of the electron gas only in exceptional cases, and therefore, to a good approximation, does not contribute to the resistance.
- For small applied electric fields, only a tiny fraction of the electrons with energies close to the Fermi level contribute to the current.

In an introductory solid state physics course, transport usually means diffusive transport: a steady state is established between the external electromagnetic fields and the friction inside the solid, which on a microscopic scale is generated by various scattering events. The sample size investigated is much larger that the mean free path, which is the distance an electron travels before it is scattered. This means we observe a homogeneous friction which stems from averaging over all microscopic scattering events.

The Boltzmann equation plays a central role in the theory of diffusive electronic transport. Even though electron–electron interactions and phase coherence are neglected, the general version of the Boltzmann equation is a nontrivial integro-differential equation. Only after its linearization, the relaxation time approximation and some further assumptions does the equation give us a simple picture of how an electric field acts on the carriers: essentially, the Fermi sphere is displaced in k-space without changing its shape. The relaxation time approximation introduces a phenomenological parameter known as "momentum relaxation time", frequently also referred to as the "Drude scattering time", τ. All important scattering mechanisms are contained in this parameter. We use it in the Drude model to include magnetic field effects.

Anything that disturbs the perfect lattice will lead to scattering of electrons. Lattice imperfections, which we describe by a perturbation Hamiltonian V_p, will scatter electronic waves from the initial state $|\vec{k}\rangle$ into a final state $|\vec{k}'\rangle$. The scattering matrix elements $W_{\vec{k},\vec{k}'}$ have to be calculated from

$$W_{\vec{k},\vec{k}'} \propto |\langle\vec{k}'|V_\mathrm{p}|\vec{k}\rangle|^2 \tag{2.49}$$

A large subfield of transport theory is to calculate such matrix elements for all kinds of scatterers. We will mention some important scattering mechanisms below.

2.6.1 The Boltzmann equation

In general, both external fields as well as scattering will modify the Fermi distribution, which we write here as $f(\vec{k}) = [1 + e^{(E(\vec{k})-\mu)/k_\mathrm{B}\Theta}]^{-1}$. The electron distribution function $\phi(\vec{k},\vec{r},t)$ is, in the most general case, not a Fermi function. It may depend on $\vec{r}$ and on the time t. Note that the points $\{\vec{k},\vec{r}\}$ constitute the phase space, with

$$\frac{2}{(2\pi)^3}\phi(\vec{k},\vec{r},t)\,d\vec{k}\,d\vec{r}$$

being the number of electrons in $d\vec{k}\,d\vec{r}$ for systems with a spin degeneracy of 2.

We consider the evolution of $\phi(\vec{k},\vec{r},t)$ in the time interval dt after time t due to an external, static electric field $\vec{E}$. We could add the effect of a magnetic field, which is dealt with in a similar way, although this is somewhat more elaborate [270]. Within dt, an electron located at $(\vec{k},\vec{r})$ in phase space at time t moves to $(\vec{k}+\delta\vec{k},\ \vec{r}+\delta\vec{r})$, which, according to the semiclassical equations of motion, equals $(\vec{k} - (e/\hbar)\vec{E}\,dt,\ \vec{r} + \vec{v}(\vec{k})\,dt)$. This only holds if the electron is not scattered into a different region of the phase space. Also, not all electrons in $(\vec{k}+\delta\vec{k},\ \vec{r}+\delta\vec{r})$ at time $t+dt$ were at $(\vec{k},\vec{r})$ at time t: they could have been scattered into this volume within dt. These scattering events change $\delta\phi$, which

we write as

$$\delta\phi = \left[\frac{\partial\phi(\vec{k},\vec{r},t)}{\partial t}\right]_{\text{scatter}} dt$$

This results in

$$\phi\left(\vec{k} - \frac{e}{\hbar}\vec{E}\,dt,\ \vec{r} + \vec{v}(\vec{k})\,dt,\ t + dt\right) d\vec{k}\,d\vec{r}$$

$$= \phi(\vec{k},\vec{r},t)\,d\vec{k}\,d\vec{r} + \left[\frac{\partial\phi(\vec{k},\vec{r},t)}{\partial t}\right]_{\text{scatter}} dt\,d\vec{k}\,d\vec{r}$$

The size of the volume element $d\vec{k}\,d\vec{r}$ cannot change, which is the statement of Liouville's theorem on the evolution of semiclassical systems in phase space. Now, the *general Boltzmann equation* is obtained by expanding the left-hand side in a Taylor series in dt up to first order:

$$\vec{v}(\vec{k}) \cdot \vec{\nabla}\phi(\vec{k},\vec{r},t) - \frac{e\vec{E}}{\hbar} \cdot \vec{\nabla}_{\vec{k}}\phi(\vec{k},\vec{r},t) + \frac{\partial\phi(\vec{k},\vec{r},t)}{\partial t} = \left[\frac{\partial\phi(\vec{k},\vec{r},t)}{\partial t}\right]_{\text{scatter}} \tag{2.50}$$

In principle, Eq. (2.49) can be calculated from the scattering matrix elements for all scattering mechanisms of relevance (like e.g. electron–phonon scattering or impurity scattering; see [270] for a detailed discussion), each weighted by the corresponding occupation probability of the initial state and the probabilities for finding the final state empty. These probabilities, however, are just the distribution functions $\phi(\vec{k},\vec{r},t)$, and $1-\phi(\vec{k},\vec{r},t)$, respectively. Therefore, the general Boltzmann equation is in fact a complicated integro-differential equation, and models as well as approximations are needed to evaluate the scattering term.

A rather crude approximation consists of putting all these scattering mechanisms together and assuming that they generate an average "relaxation time" τ, which we further assume to be independent of $\vec{k}$ and $\vec{r}$. This is based on the following picture. Provided the system is homogeneous in real space, we can drop the spatial coordinates. If we switch off the external field at time t_0, the distribution function will exponentially relax to $f(\vec{k})$ with a decay time τ:

$$\phi(\vec{k},t) = f(\vec{k}) + (\phi(\vec{k},t_0) - f(\vec{k}))e^{-t/\tau}$$

Since $\vec{E} = 0$, this relaxation will take place exclusively via scattering, and hence

$$\frac{\partial\phi(\vec{k},t)}{\partial t} = \left[\frac{\partial\phi(\vec{k},t)}{\partial t}\right]_{\text{scatter}} = -\frac{\phi(\vec{k},t) - f(\vec{k})}{\tau}$$

which simplifies the general Boltzmann equation considerably. In a stationary state (no time dependence), this now reads

$$-\frac{e\vec{E}}{\hbar} \cdot \nabla_{\vec{k}}\phi(\vec{k}) = -\frac{\phi(\vec{k}) - f(\vec{k})}{\tau} \tag{2.51}$$

Eq. (2.51) can be further evaluated by considering small electric fields only. In this regime, the deviation of ϕ from the Fermi function should be roughly linear in $\vec{E}$, and we can thus write $\vec{\nabla}_{\vec{k}}\phi(\vec{k}) \approx \vec{\nabla}_{\vec{k}} f(\vec{k})$. Now, Eq. (2.43) represents a Taylor expansion of $\phi(\vec{k})$ in $(e\tau\vec{E}/\hbar)$ up to first order:

$$\phi(\vec{k}) = f(\vec{k}) + \vec{\nabla}_{\vec{k}} f(\vec{k}) \frac{e\tau\vec{E}}{\hbar}$$

The right-hand side is a good approximation for $f(\vec{k} + e\tau\vec{E}/\hbar)$, provided that $e\tau\vec{E}/\hbar \ll \vec{k}$. We thus finally find a *simplified Boltzmann equation*, which states that, under all the approximations made, small electric fields displace the Fermi surface in k-space by $e\tau\vec{E}/\hbar$ (Fig. 2.12):

$$\phi(\vec{k}) = f\left(\vec{k} + \frac{e\tau\vec{E}}{\hbar}\right) \tag{2.52}$$

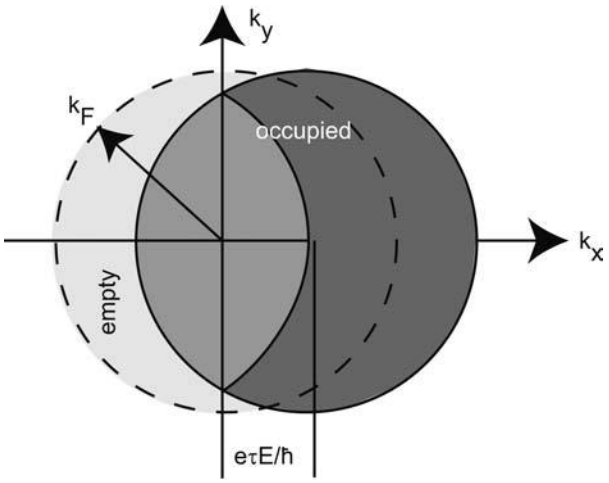

Fig. 2.12 The displaced Fermi sphere as obtained from the Boltzmann equation. The electrons in the dark gray region carry the net current.

Electrons get accelerated and scatter into empty states via elastic or inelastic processes, which emphasizes again the diffusive and dissipative character of the Boltzmann model. As a consequence, this displacement is quasi-static. In addition, we see that only electrons close to the surface of the Fermi sphere contribute to the current. For states deep inside the Fermi sphere, the partial current generated by an electron with momentum $\hbar\vec{k}$ is canceled by the electron with momentum $-\hbar\vec{k}$.

2.6.2 The conductance predicted by the simplified Boltzmann equation

It remains to calculate the conductance σ predicted by the assumptions leading to Eq. (2.52). In general, σ is a tensor defined by

$$\vec{j} = \sigma \vec{E}$$

However, it makes sense to assume $\vec{j} \parallel \vec{E}$, such that σ is actually a scalar. It is obtained from the current density via

$$\vec{j} = \sigma \vec{E} \qquad \Longrightarrow \qquad \sigma = \frac{\vec{j}\vec{E}}{\vec{E}^2} \tag{2.53}$$

In order to calculate $\vec{j}$, we have to integrate over the $\vec{k}$-space, weighting each state by its occupation probability. State $\vec{k}$ contributes a partial current of

$$\vec{j}(\vec{k}) = -e\phi(\vec{k})\vec{v}(\vec{k}) = -\frac{e\hbar}{m^*}\vec{k}\phi(\vec{k})$$

The total current density is obtained by summing up the contributions of all states. Since, for a spin degeneracy of 2, each state occupies a volume of $4\pi^3$ in $\vec{k}$-space, this summation can be written as the integral

$$\vec{j} = \int \vec{j}(\vec{k})\, d\vec{k} = -\frac{e\hbar}{4\pi^3 m^*} \underbrace{\int \vec{k} f(\vec{k})\, d\vec{k}}_{=0} + \int \vec{k} \vec{\nabla}_{\vec{k}} f(\vec{k}) \frac{e\tau\vec{E}}{\hbar}\, d\vec{k}$$

Since

$$\vec{\nabla}_{\vec{k}} f(\vec{k}) = \frac{\partial f(\vec{k})}{\partial E} \vec{\nabla}_{\vec{k}} E(\vec{k}) = \frac{\partial f(\vec{k})}{\partial E} \frac{\hbar^2 \vec{k}}{m^*}$$

the current density equals

$$\vec{j} = -\frac{e^2\tau\hbar^2}{4\pi^3 m^{*2}} \int \vec{k} \frac{\partial f(\vec{k})}{\partial E} [\vec{k}\vec{E}]\, d\vec{k}$$

With Eq. (2.53), we can write

$$\sigma = -\frac{e^2\tau\hbar^2}{4\pi^3 m^{*2}} \int \frac{(\vec{k}\vec{E})^2}{\vec{E}^2} \frac{\partial f(\vec{k})}{\partial E}\, d\vec{k}$$

For sufficiently low temperatures,

$$-\frac{\partial f(E)}{\partial E} = \delta(E - E_\mathrm{F}) = \delta(k - k_\mathrm{F}) \frac{m^*}{\hbar^2 k}$$

which results in the surface integral

$$\sigma = \frac{e^2\tau}{4\pi^3 m^*} \int \frac{(\vec{k}\vec{E})^2}{\vec{E}^2} \delta(k - k_\mathrm{F}) \frac{1}{k}\, d\vec{k}$$
$$= \frac{e^2\tau}{4\pi^3 m^*} \int_{\theta=0}^{2\pi} \int_{\varphi=0}^{\pi} k_\mathrm{F}^3 \cos^2\varphi \sin\varphi \, d\varphi \, d\theta = \frac{e^2\tau k_\mathrm{F}^3}{3\pi^2 m^*}$$

Since the electron density n is given by $n = 3\pi^2 k_\mathrm{F}^3$, we find

$$\sigma = \frac{ne^2\tau}{m^*} = ne\mu \tag{2.54}$$

Here, we have defined the electron mobility by $\mu \equiv e\tau/m^*$.

Question 2.7: *Prove that $\sigma = ne\mu$ also holds in two dimensions.*

Result (2.54) is at first sight quite strange: the conductivity is proportional to the total electron density, and it seems like all electrons would contribute equally to the current. However, we know that only the electrons at the Fermi surface carry current. The explanation is that a higher electron density increases the number of electrons and the electron velocity at the Fermi surface, which turns out to give a conductivity proportional to n.

We can use Eq. (2.54) to define a useful quantity, the drift velocity $\vec{v}_\mathrm{d}$ as

$$\vec{v}_\mathrm{d} = -\frac{\vec{j}}{en} = -\mu\vec{E} \tag{2.55}$$

The drift velocity is thus an effective average velocity, which leads to an equation for the current density that is formally identical to the Drude expression, which was derived by assuming that all electrons contribute equally to the current and move through the crystal with an average drift velocity.

Along similar lines, it can be shown that, in the additional presence of magnetic fields, the current density can be written as

$$\vec{j} = \sigma(\vec{E} + \vec{v}_\mathrm{d} \times \vec{B}) \tag{2.56}$$

This current density corresponds to the stationary solution of the classical equation of motion

$$m^* \frac{d^2\vec{r}}{dt^2} + \frac{m^*}{\tau}\vec{v}_\mathrm{d} = -e(\vec{E} + \vec{v}_\mathrm{d} \times \vec{B}) \tag{2.57}$$

Thus, electrons are moving at velocity $\vec{v}_\mathrm{d}$ through the crystal and experience a Stokes-type friction term given by $m^*\vec{v}_\mathrm{d}/\tau$.