Electrons in a periodic potential

Electron transport in bands- a quasi-classical approach

Within this quasi-classical approximation we shall be treating electrons as being in a state of equilibrium, which strictly is not the case but otherwise we would have to find the non-equilibrium charge carrier distribution function to be able to obtain observable macroscopic properties. This simplification comes as alternative to full QM calculations of transport which would be time-consuming and in many macroscopic cases is unnecessary.

This approach treats electronic motion in an electric field *E* using a classical, Newton's 2nd Law, but with a hint of QM:

- The electron mass m_e is replaced by the effective mass *m** (obtained from the QM bandstructures).
- I internal "resistive" force is added, and characterized by a scattering time τ

All QM effects are factored in via *m** and τ. Furthermore, we shall see that *m** can, in principle, be obtained from a bandstructure calculations, while τ can, in principle, be obtained from a combination of Quantum Mechanical & Statistical Mechanical calculations. The scattering time, τ could also be treated as an empirical parameter in this quasi-classical approach.

Let's first see why do we need to replace the electron (or hole) mass with an effective mass *m*.*

If a force ***F*** acts on an electron via an electrical field ***E***, in classical mechanics we can write:

$$F = -e \cdot E = m\frac{d^2r}{dt^2} = \frac{dp}{dt}, p = mv = m\frac{dr}{dt}$$

where $\underline{r}$ is position vector of the electron and *p* is the momentum, and *v* is the velocity. An obvious place where classical description can break down is the momentum – does it have the same meaning in QM and if not – why?

Let's recall that the particle velocity in QM is essentially a *group velocity* of a wave packet:

$$v_g \equiv \frac{\partial\omega}{\partial k} = \frac{1}{\hbar}\frac{\partial\varepsilon}{\partial k}$$

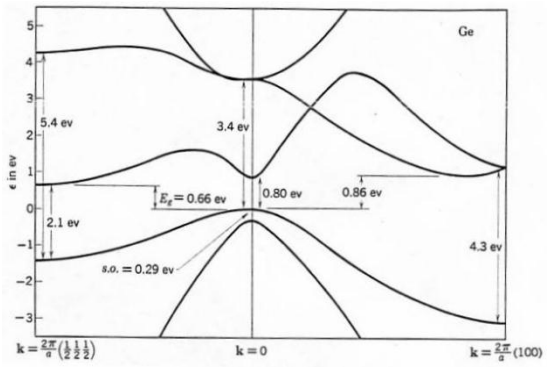
In case of free-electron model:

$$\varepsilon = K = \frac{\hbar^2 k^2}{2m}$$

where *K* is the kinetic energy of a particle. Hence for v_g we obtain:

$$v_g = \frac{1}{\hbar}\frac{\partial\varepsilon}{\partial k} = \frac{1}{\hbar}\frac{\hbar^2\partial k^2}{2m\partial k} = \frac{\hbar k}{m} = \frac{p}{m} = v_{classic}$$

But we observe that the above relationship is based on the assumption that $\hbar k = p = mv_{classic}$ or equivalently, as long as $\varepsilon(k)$ is a parabola all the energy of a particle can be interpreted as a kinetic energy of a particle with mass *m*. However, this is not the case in general for periodic solids within both the nearly-free electron model and the tight-binding approach. We still use notation with the momentum *k*, but that is no longer identical to the momentum of an electron – rather it's *crystal momentum* and $\varepsilon(k)$ is in general a rather complicated function (see example below for *Ge*).



However, we note that we are really only interested in the electrons close to the band edges (e.g. *k=0*) as only those electrons (and holes) would contribute (why?) to the transport properties we are interested in. Hence, only those parts of the dispersion curve that define the *maxima* or *minima* of the valence band or conductance band, respectively, are important. Now we can simply expand any complicated function of $\varepsilon(k)$ into a Taylor series around our points of interest and neglect the terms beyond $\boldsymbol{k^2}$ as an approximation. For conduction band we have:

$$\varepsilon(k) = \varepsilon_C + k \cdot \left.\frac{\partial \varepsilon}{\partial k}\right|_{k=0} + \frac{k^2}{2}\left.\frac{\partial^2 \varepsilon}{\partial k^2}\right|_{k=0} + \cdots$$

and observe that:

$$\left.\frac{\partial \varepsilon}{\partial k}\right|_{k=0} = 0, \varepsilon(k=0) = \varepsilon_C$$

If we now consider ε_C as a zero point of the energy scale, we recover the same quadratic relation in *k* as for the free electron gas, provided that:

$$\left.\frac{k^2}{2}\frac{\partial^2 \varepsilon}{\partial k^2}\right|_{k=0} = \frac{\hbar^2 k^2}{2m^*} \; with \; m^* = \hbar^2 \frac{1}{\frac{\partial^2 \varepsilon}{\partial k^2}}$$

where *m** is the *effective mass* of carriers.

Now, let's go back to our quasi-classical description. An electron in the conduction band in the electric filed *E* will experience the following forces:
F_E = *-eE* = electric force due to the *E* field
F_R = resistance due to scattering (characterised by scattering time *τ*).
$m^*a = m^*(d^2r/dt^2) = -(m^*/\tau)(dr/dt) - eE$ or $m^*(d^2r/dt^2) + (m^*/\tau)(dr/dt) = -eE$, where $-(m^*/\tau)(dr/dt) = -(m^*/\tau)v$ = force due to resistance and out transport problem is now purely classical.

The resistance force: $F_R = -(m^*/\tau)(dr/dt) = -(m^*v)/\tau$ (note that F_R decreases as *v* increases).

The electrical force: $F_e = -eE$ (note that F_e causes v to increase).
Newton's 2nd Law: $m^*(d^2r/dt^2) = m^*(dv/dt) = F_R - F_e$
With the the *"steady state"* condition $a = dv/dt = 0$ and Newton's 2nd Law becomes $F_R = F_e$. Hence, $-eE = (m^*v_d)/\tau$, where v_d is the *drift velocity*.
At the steady state we have:

$$-eE = \frac{m^* v_d}{\tau},$$

Using the definition of mobility μ:

$$v_d \equiv \mu E, \Rightarrow \mu = -\frac{e\tau}{m^*}$$

and the definition of current density *J*:

$$J \equiv -nev_d = -ne\mu E$$

and the definition of the conductivity σ:

$$J \equiv \sigma E \Rightarrow \sigma = -ne\mu = \frac{ne^2\tau}{m^*}$$

Summary of transport properties:

Current density: $J \equiv \sigma E$ (Ohm's "Law")

Conductivity: $\sigma = (nq^2\tau)/m^*$

Mobility: $\mu = (q\tau)/m^*$

$\sigma = nq\mu$

We shall see that the electron concentration *n* is strongly temperature dependent: $n = n(T)$, τ is also strongly temperature dependent $\tau = \tau(T)$. Hence, the conductivity σ is strongly temperature dependent too.

Next topic: Semiconductors