0.1 Electronic Band Structure of Solids

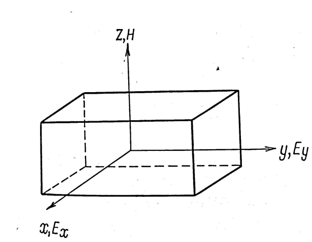
0.1.1 Free electron model

Drude model (classical approach)

- Electrons are free: no electron-electron and no electon-phonon interactions.
- Electrons collide with ionic cores with probability per unit time τ; such collisions are instantaneous and inelastic (all of electron's momentum is transfered to the lattice).

In this approximation, the change in the momentum $\mathbf{p}$ within $\mathrm{d}t$ is

$$\mathrm{d}\mathbf{p} = \overbrace{\left(1 - \frac{\mathrm{d}t}{\tau}\right)\mathbf{F}\mathrm{d}t}^{\text{no collision: Newton's second law}} + \frac{\mathrm{d}t}{\tau}\underbrace{(-\mathbf{p})}_{\text{collision: all momentum transferred to the lattice}}$$

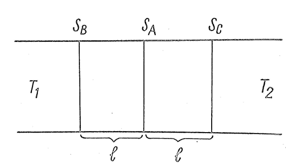


Hence, the equation of motion is $\mathrm{d}\mathbf{p}/\mathrm{d}t = -\mathbf{p}/\tau + \mathbf{F}$.

Assume that a field $\mathbf{E}$ is applied along a metallic wire. The field acts on the electron with a force $\mathbf{F} = -e\mathbf{E}$. In the steady-state case ($\mathrm{d}\mathbf{p}/\mathrm{d}t = 0$), we get $\mathbf{v} = -e\mathbf{E}\tau\,/\,2m$. The current density is thus $\mathbf{j} = -ne\mathbf{v} = ne^2\tau\mathbf{E}\,/\,2m$, and the specific electric conductivity is $\sigma = ne^2\tau\,/\,2m$.

Suppose now that our wire (aligned along x-axis) is placed in a magnetic field $\mathbf{H}$ oriented along the z-axis. An electron is then subject to the sum of Coulomb and Lorentz forces $\mathbf{F} = -e\mathbf{E} - e/c\,\mathbf{v} \times \mathbf{H}$. Hall voltage is developed in the y-direction and Hall coefficient $R_H \equiv E_y\,/\,j_x H = -1\,/\,ne$.

The Drude model achieved complete success in the derivation of the Wiedermann-Franz law, according to which the ratio of thermal and electrical conductivities is a universal linear function of temperature for many metals: $\kappa/\sigma = LT$ (L here is called Lorentz number). Say, T depends on x only. Then the heat transfer $W = \kappa\partial T/\partial x$. The number of electrons passing through unit cross section S_A per unit time is n|v_x|/2. S_B and S_C are cross sections on which the electrons, on average, have suffered the last collisions. $l = 2\tau\bar{v}/3$ is the mean-free path[1]. From the equipartition of energy, we get $1/2m\bar{v}^2 = 3/2k_BT(x)$.[2] Hence,



$$W = \frac{1}{2}n|v_x|\left(\left.\frac{mv^2}{2}\right|_{x-l} - \left.\frac{mv^2}{2}\right|_{x+l}\right) \approx \frac{1}{2}nk_B\bar{v}^2\tau\frac{\partial T}{\partial x}$$

and we get that $\kappa = 3k_B^2 n\tau T\,/\,2m$. Finally, $\kappa/\sigma = 3(k_B/e)^2T$.

Sommerfeld model (quantum mechanical approach)

- Electrons are still free: no electron-electron and no electron-phonon interaction.
- Electrons are fermions obeying the Fermi-Dirac distribution.

In this system, electrons move within a metal, i.e. a potential box with a rectangular potential barrier. The motion of the electron is then defined by the Schriödinger equation and the boundary conditions on the surface of the metal. Solutions are plain waves $\psi_{\mathbf{k}\sigma}(\mathbf{r}, \sigma_z) = \alpha\exp(i\mathbf{k}\cdot\mathbf{r})\phi_\sigma(s)$. The spectrum is $E(\mathbf{k}) = \hbar^2k^2\,/\,2m^*$. $\mathbf{k}$ varies quasi-continuously since $k_x = \pi\kappa_x/L_x$, $k_y = \pi\kappa_y/L_y$,

[1] This is known from the kinetic theory of gases.
[2] $\bar{v}$ is the average velocity and we assume that $|v_x|^2 \approx \bar{v}^2/3$

$k_z = \pi\kappa_z/L_z$, and $\kappa_x, \kappa_y, \kappa_z \in \mathbb{Z}$. To calculate the degree of degeneracy $g(E)$, we calculate the volume of a small shell $4\pi p^2 \mathrm{d}p = 2^{5/2}\pi m^{*3/2}E^{1/2}$ and divide it by the unit phase cell volume $\Delta p_x \Delta p_y \Delta p_z$ which is determined from the Heisenberg uncertainty principle $\underbrace{\Delta x \Delta y \Delta y}_{V} \Delta p_x \Delta p_y \Delta p_z \sim h^3$. This yields[3]

$$g(E) = \frac{1}{h^3} 4\pi (2m^*)^{3/2} V E^{1/2} \equiv C E^{1/2}$$

0.1.2 Nearly-Free electron model

0.1.3 Tight-binding model

0.2 References

[3]Additional coefficient 2 comes from the spin degeneracy.