Solid State Physics

Electrical properties

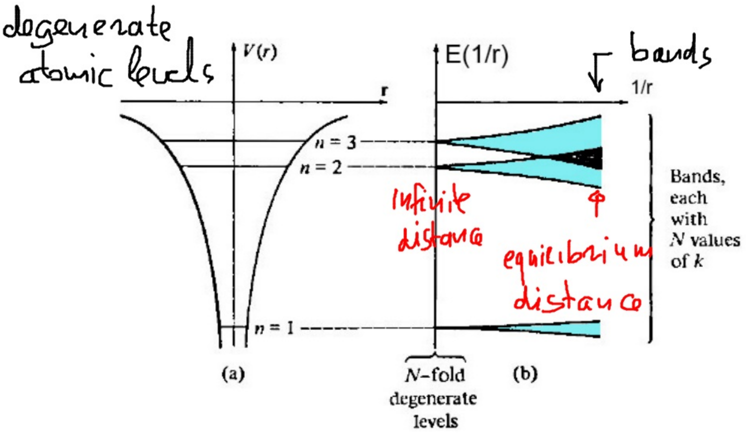
insulators — no/small/negligible overlap

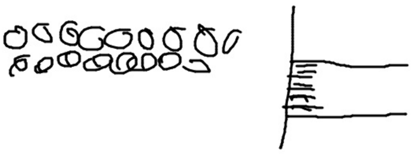
metals — large overlap

of electron orbitals

overlap breaks degeneration

bands form



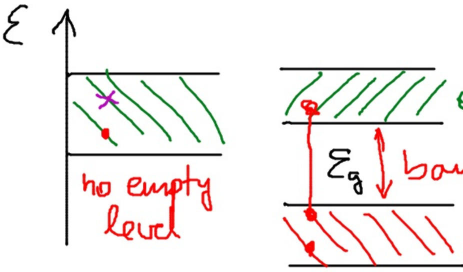


band from one level

$\Rightarrow \Delta\; 10^{-20}\,eV$

$k_b 300\,K = 0.0258\,eV$

insulator



empty ⇔ conduction band

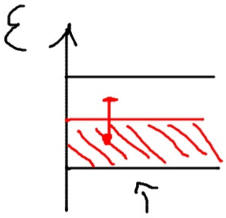
band gap

full valence band

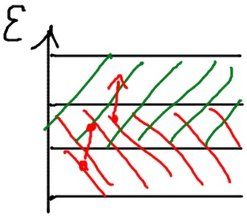
if $\mathcal{E}_g \gg k_bT \Rightarrow$ insulator

if $\mathcal{E}_g \sim k_bT \Rightarrow$ semiconductor (also insulator)

conductor (metal)



half empty band



conduction band

valence band

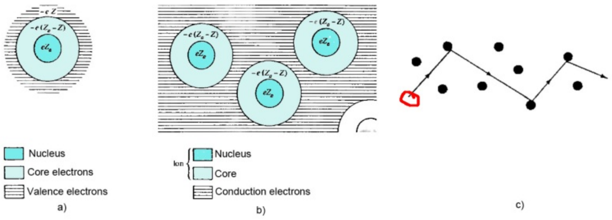
overlapping empty and full bands

classical model of conduction

Drude-model

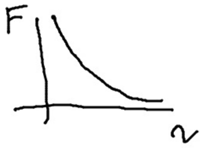
~1900

1. ion cores not moving
2. non-interacting electrons (electron-gas)
3. only electron-ion collisions
4. instantaneous
5. $P_{collision} \sim \Delta t$
6. $v = 0$ after collision



$Q_{electron} = -e$

$\underline{E} \neq 0 \qquad \underline{F} = -e\underline{E} \qquad \xrightarrow{E} \quad \xleftarrow{a}$



$$a = \frac{F}{m_e} = \frac{eE}{m_e}$$

$$v(t) = \cancel{v_0 +}\, a t \quad \longleftrightarrow \quad dv = a\,dt$$

not the electron velocity, just the change caused by $\underline{E}$

collision occures after τ $\qquad v(\tau) = \frac{eE}{m_e}\tau$

after $\quad v(\tau + 0) = 0$

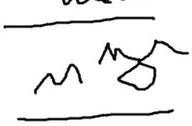
no $\frac{1}{2}$ as τ is average too

$$\langle v \rangle = \frac{1}{\cancel{2}} v_{max} = \frac{eE}{\cancel{2} m_e}\tau = \mu E$$

v_{drift} $\qquad$ average collision time $\qquad$ mobility $\quad \mu = \frac{e\tau}{m_e}$

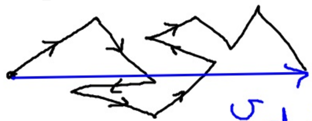
velocity

metal



$$\underline{v}_{drift} = -\frac{eE}{m_e}\tau$$

$v_e \approx 10^5\ m/s$



$v_{drift} \sim 1\ \frac{mm}{s}$

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

conductivity

$$\underline{j} = -ne\underline{v}_{drift} = -n\frac{e^2E}{m_e}\tau = -\underbrace{n\frac{e^2\tau}{m_e}}_{\sigma}\underline{E} = -\sigma\underline{E}$$

can be measured $\rightarrow \sigma = \frac{ne^2\tau}{m_e}$ $\qquad$ calculated

$$\underline{j} = -ne v_{drift} = -ne\mu E$$

$$\boxed{\sigma = ne\mu}$$

Silver $\tau = 4$ [illegible] 10^{-14} s units $[\sigma] = \frac{[j]}{[E]} = \frac{A/m^2}{V/m} = \frac{1}{\Omega m}$ $\rho := \frac{1}{\sigma}$ resistivity $[\rho] = \Omega m$ or $\Omega \frac{mm^2}{m}$

$[\mu] = \frac{[v_{drift}]}{[E]} = \frac{m/s}{V/m} = \frac{m^2}{Vs}$

Calculate n

$$n = L_A \frac{Z \rho_m}{A}$$

# of conduction electrons/atom

mass density kg/m³

Avogadro # 1/mol

atomic mass in kg/mol

$\boxed{\text{example:}}$ Al

$\rho_m = 2700 \frac{kg}{m^3}$

$Z = 3$

$A = 0.02698 \frac{kg}{mol}$

$$n = 6{,}024 \cdot 10^{23} \frac{\cancel{atoms}}{\cancel{mol}} \cdot \frac{3 \frac{el}{\cancel{atoms}} \, 2700 \, \cancel{kg}/m^3}{0{,}02698 \frac{\cancel{kg}}{\cancel{mol}}}$$

$$= 1.807 \cdot 10^{29} \frac{electron}{m^3}$$

τ & calculations hard

using σ : $\sigma = \frac{ne^2}{m}\tau \rightarrow \tau = \frac{m\sigma}{ne^2} = \frac{m}{\rho n e^2}$

$$\tau = \frac{m}{L_A \frac{Z \rho_m}{A} e^2 \cdot \rho} = \frac{m \cdot A}{Z \cdot \rho_m e^2 \cdot L_A}$$

$\boxed{\text{example}}$: Silver (Ag)

$\rho(0°C) = 1.51 \cdot 10^{-8} \Omega m$ $(\rho = \rho(T))$

$Z = 1$ $(5s^1)$

$A = 107.8682 \, g/mol$

$\rho_m = 10.49 \, g/cm^3$

$$\tau = 4.013 \cdot 10^{-14} s$$

mean free path $\bar{\ell}$

$$\tau = \frac{\bar{\ell}}{\langle v \rangle} \qquad \text{Drude: } \langle v \rangle = v_{th} = \sqrt{\frac{3k_B T}{m_e}}$$

$$\sigma = \frac{ne^2\tau}{m_e} \rightarrow \rho = \frac{m_e}{ne^2\tau} \sim \sqrt{T}$$

reality: $\rho \sim T$

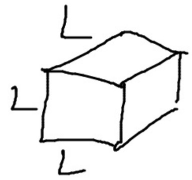
Failures of the Drude model:

$\rho(T)$, C_V, $\frac{K}{\sigma}$

Sommerfeld model

1. cond. e does not interact w. ion cores or e.
2. potential box
3. Pauli principle true

3D



N electron

$$V(x,y,z) = \begin{cases} 0 & 0 \le x \le L \text{ and } 0 \le y \le L,\ 0 \le z \le L \\ \infty & x > L \text{ or } y > L \text{ or } z > L \\ & x < 0 \quad y < 0 \quad z < 0 \end{cases}$$

$$\psi(\underline{r}_1, \underline{r}_2 \dots, \underline{r}_N) = \sum_{i=1}^{N} \phi_i(\underline{r}_i)$$

$$\phi_i(\underline{r}_i) \equiv \underbrace{\phi_{i,x}(x)}_{\phi(x)} \cdot \underbrace{\phi_{i,y}(y)}_{\phi(y)} \cdot \underbrace{\phi_{i,z}(z)}_{\phi(z)}$$

$$\phi(x) = \sqrt{\frac{2}{L}} \sin k_x x \quad , k_x = \frac{\pi}{L} \cdot n_x \ , n_x = 1,2,3$$

$$\phi(y) = \sqrt{\frac{2}{L}} \sin k_y y \quad , k = \frac{\pi}{L} \cdot n_y \ , n_y = 1,2,3$$

$$\phi(z) = \sqrt{\frac{2}{L}} \sin k_z z \quad , k = \frac{\pi}{L} \cdot n_z \ , n_z = 1,2,3$$

1D a – lattice const
N – atoms

$$L = N \cdot a \ , \Delta k = \frac{\pi}{L} \sim 10^{-13} - 10^{-15} \frac{1}{m}$$

$$\mathcal{E}_n(k) = \frac{\hbar^2 k^2}{2m_e} = \frac{\hbar^2 \left(\frac{\pi}{L}\right)^2 n^2}{2m_e} = \frac{\hbar^2 \pi^2}{2m_e N^2 a^2} \cdot n^2$$

3D $\psi(x,y,z) = \left(\frac{2}{L}\right)^{3/2} \sin k_x x \cdot \sin k_y y \cdot \sin k_z z$

$$\mathcal{E} = \frac{\hbar^2 k^2}{2m_e} = \frac{\hbar^2}{2m_e} \cdot (k_x^2 + k_y^2 + k_z^2)$$

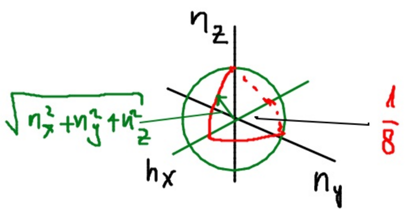
$\mathcal{E}_F$

$$\Delta V_k = \left(\frac{2\pi}{L}\right)\left(\frac{2\pi}{L}\right)\left(\frac{2\pi}{L}\right) = \left(\frac{2\pi}{L}\right)^3 = \frac{8\pi^3}{V}$$

# of k points in Ω_k : $n = \frac{\Omega_k}{\Delta V_k} = \frac{V}{\pi^3} \cdot \Omega_k$

density of levels =

$$g_{el,levels} = \frac{n}{\Omega_k} = \frac{V}{\pi^3}$$



for N k-states ($N \gg 1$) $\Longrightarrow$ $\Omega(N)$ is a sphere

$\Omega(N) = \frac{4}{3} k_F^3 \pi$ but $n_x, n_y, n_z > 0 \Longrightarrow \frac{1}{8} \times \Omega(N)$

$$N_{states} = g_{e,levels} \cdot \frac{\Omega(\mathcal{N})}{8}$$

$$N_{states} = \frac{V}{\pi^{3}} \cdot \frac{1}{8} \cdot \frac{4}{3} k_F^3 \pi = \frac{V}{6\pi^2} k_F^3$$

Z electrons/atom $\quad N_{electrons} = Z \cdot \mathcal{N}$

Pauli $\rightarrow$ $\quad N_{states} = \frac{N_{electrons}}{2}$

$$\frac{V}{6\pi^2} k_F^3 = \frac{N_{electrons}}{2}$$

$N_e \equiv N_{electrons}$

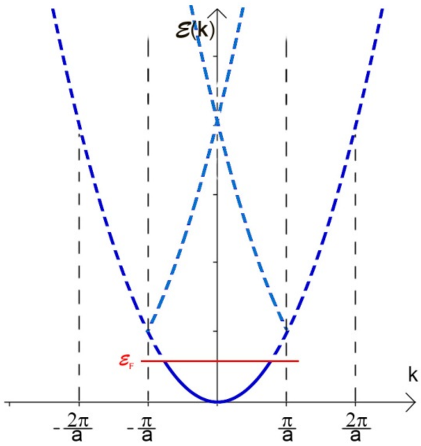
$$N_e = \frac{V}{3\pi^2} k_F^3 \qquad n = \frac{N_e}{V} = \frac{k_F^3}{3\pi^2}$$

$$k_F = \frac{2\pi}{a} \Rightarrow k \leq k_F \text{ values} \quad k \in \left[0, \frac{2\pi}{a}\right]$$

$$\varepsilon_F = \frac{\hbar^2 k_F^2}{2m} \rightarrow k_F = \sqrt{\frac{2m\,\varepsilon_F}{\hbar^2}}$$

$$v_F = \frac{\hbar k_F}{m_e}$$

$$n = \frac{1}{3\pi^2}\left(\frac{2m\varepsilon_F}{\hbar^2}\right)^{3/2} = \frac{(2m\varepsilon_F)^{3/2}}{3\pi^2\hbar^3}$$



$(k_F) \sim 0{,}1\,nm$ ✓

$v_F \sim 0{,}001 \cdot c$ ✗

$\varepsilon_F \sim$ binding energy

$\boxed{\text{example}}$ $\quad$ Cu $\quad \varepsilon_F = 4.1\,eV$

$$n = \frac{(2m_e\varepsilon_F)^{3/2}}{3\pi^2\hbar^3} = \frac{\left(2\cdot 9.1\cdot 10^{-31}kg \cdot 4.1eV \cdot 1.6\cdot 10^{-19} J/eV\right)^{3/2}}{3\pi^2\left(1.57\cdot 10^{-34}\right)^3}$$

$$= 3.77\cdot 10^{28}\,\frac{\text{electrons}}{m^3} \quad \leftarrow \text{wrong}$$

$$v_F = 1.2\cdot 10^6\, m/s = 0.004c$$

Specific heat of metals

of electrons in $\Delta\varepsilon$

$$\Delta n_{states} = g(\varepsilon)\Delta\varepsilon$$

$$g(\varepsilon) = \frac{8\pi\,(2m_e^3)^{1/2}}{h^3}\cdot\sqrt{\varepsilon}$$

$$f_{F-D} = \frac{1}{e^{(\varepsilon-\varepsilon_F)/k_BT}+1}$$

$$dn = f_{F-D}(\varepsilon)\, g(\varepsilon)\, d\varepsilon$$

$$U = \int_0^\infty \varepsilon\, dn = \int_0^\infty \varepsilon \cdot g(\varepsilon)\, f_{F-D}(\varepsilon)\, d\varepsilon$$

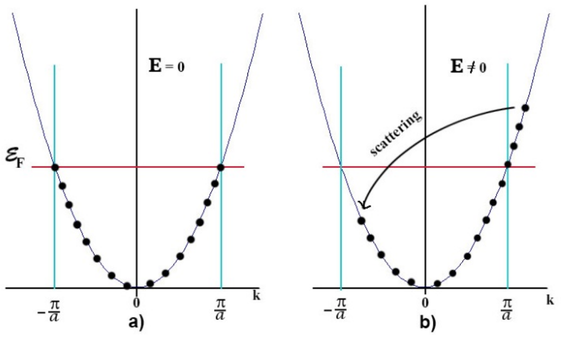
$$U = \int_0^\infty \frac{\varepsilon \cdot g(\varepsilon)}{e^{(\varepsilon-\varepsilon_F)/k_BT}+1}\, d\varepsilon =$$

$$= \underset{\sim \text{const}}{\int_0^{\varepsilon_F - k_BT} (\ )\, d\varepsilon} + \int_{\varepsilon_F-k_BT}^{\varepsilon_F+k_BT} (\ )\, d\varepsilon + \underset{\sim 0}{\int_{\varepsilon + k_BT}^{\infty} (\ )\, d\varepsilon}$$

$$C_V = \frac{\pi^2}{3} k_B^2\, g(\varepsilon_F)\, T$$

$$U = \text{const} + \underbrace{\int \frac{g(\varepsilon)\,\varepsilon}{(\quad)}\, d\varepsilon}$$

$$\approx g(\varepsilon_F) \cdot \int_{\varepsilon_F-k_BT}^{\varepsilon_F+k_BT} \frac{\varepsilon}{e^{(\varepsilon-\varepsilon_F)/k_BT}+1}\, d\varepsilon$$



$$v \sim v_F$$

$$\tau = \frac{\bar{l}}{v_F}\ , \quad \sigma = \frac{ne^2\tau}{m_e} = \frac{ne^2}{m_e}\,\frac{\bar{l}}{v_F}$$

$$v_F \neq v_F(T) \quad \bar{l} \sim \frac{1}{T} \Rightarrow \rho \sim T \ \checkmark$$

Problems:
- $v_F \sim 10 \times v_T^{(\text{Drude})}$ $\times$
- $\bar{l} = 10^{-7}\,m$ $\times$ $\quad \bar{l} \sim 10^{-9}\,m$
- insulators ?
- Hall effect
- magnetoresistance