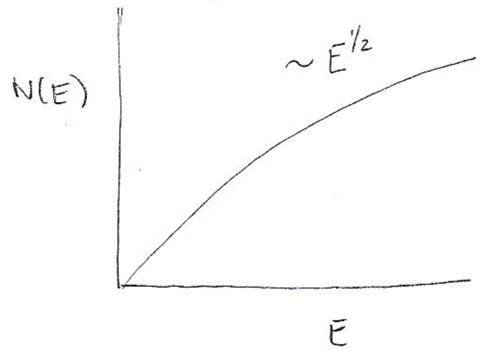
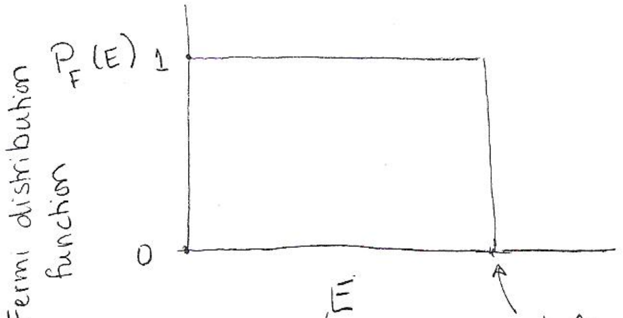
Density of States



Distribution of electrons within available states.

Electrons obey Pauli exclusion principle : Fermions
Probability that an energy level is occupied, P(E)



0 Kelvin

States are sequentially occupied until no more electrons to fill them

define as $\mathcal{E}_f$: Fermi energy.

Free electron metal: $\mathcal{E}_f$ simply fixed by # of electrons available to fill the states.

$$\#\text{ electrons} = N_0 = \underbrace{N_{qs}(\mathcal{E}_f)}_{\#\text{ states up to energy } \mathcal{E}_f} \times 2 \leftarrow \text{spin.}$$

$$\Rightarrow N_0 = L^3 \cdot \frac{\pi}{3}\left(\frac{8m}{h^2}\right)^{3/2} \cdot \mathcal{E}_F^{3/2}$$

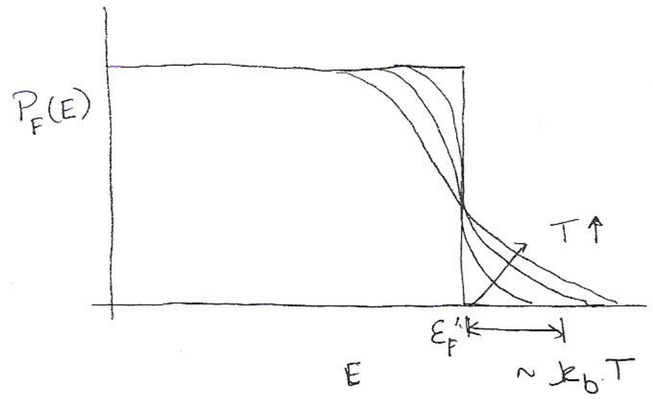
$$\Rightarrow \mathcal{E}_F = \frac{h^2}{8m}\left(\frac{3}{\pi}\frac{N_0}{L^3}\right)^{2/3}$$

$\eta \equiv$ # free electrons / unit volume

e.g. Ca metal $\Rightarrow$ Ca^{2+} $\Rightarrow$ 2 free electrons / atom

from density & structure : atoms / volume for $T > 0, K$ use formal definition of $P_F(E)$

$$P_F(E) = \frac{1}{\exp\left(\frac{E-\mathcal{E}_F}{k_b T}\right) + 1}$$

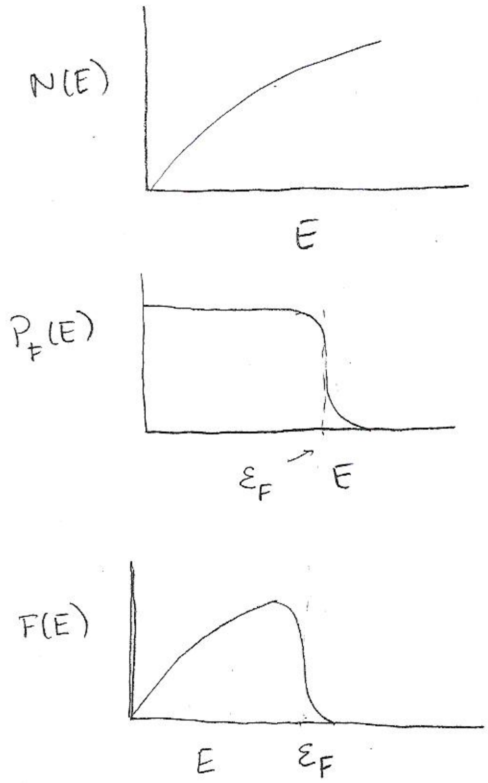


thermal excitation to higher energy states.

$P_F(\mathcal{E}_F) = 0.5$ at all T

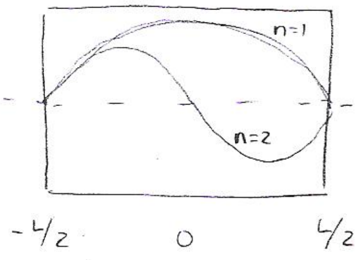
In which energy states are the electrons?

Electron distribution function: $F(E) = 2N(E) \cdot P_F(E)$



Now, consider atom cores.

recall: $\lambda_n = \frac{2L}{n}$

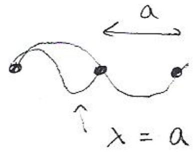


$\psi_n = \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi x}{L}\right)$ even

$\psi_n = \sqrt{\frac{2}{L}} \cos\left(\frac{n\pi x}{L}\right)$ odd

turns out at $\lambda = \frac{2a}{n}$ $\left(k = \frac{2\pi}{\lambda} = \frac{n\pi}{a}\right)$

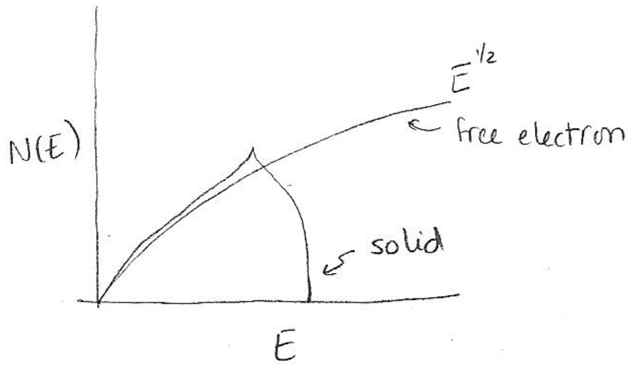
→ discontinuity in N(E)

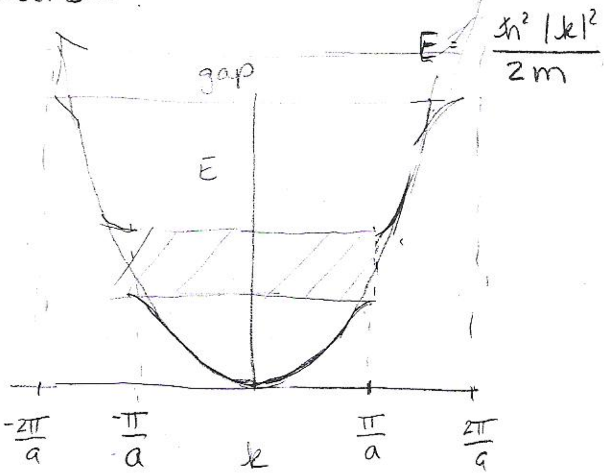


$\lambda = 2a$

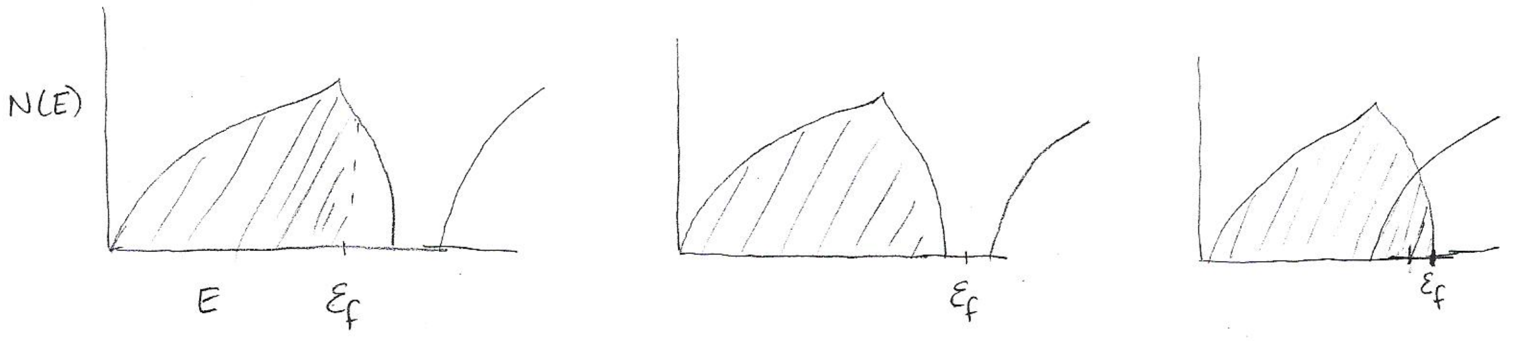
electrons are 'scattered' by atoms.

→ forbidden energies ⇒ bands.





Extend E to higher E like E(k).
& fill states up to $\mathcal{E}_f$ → 3 possibilities (at 0, K)

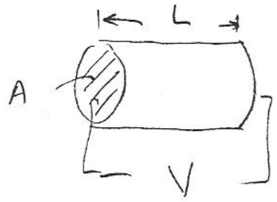


metal

semiconductor/ insulator

metal (alkaline earth metal.

Electrical Conductivity



voltage — current, charge/time.

apply V, measure I.

Ohm's Law $I = V/R$ ← resistance

definitions: $\rho = \frac{R \cdot A}{L} = \frac{1}{\sigma}$ $\qquad \mathcal{E} = \frac{V}{L}$ $\qquad J = \frac{I}{A}$

resistivity, conductivity, field, current density

rewrite Ohm's Law: $J = \sigma \cdot \mathcal{E}$

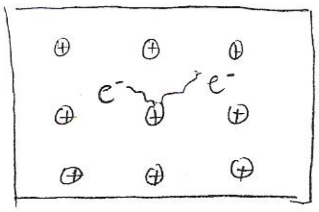
charge/area·time — want to evaluate.

by definition: $J = \eta \cdot e \, V_d$

$\frac{N}{L^3}$ ← #/vol — charge — net velocity: dist/time

if we have how V_d responds to $\mathcal{E}$ → have σ.

<u>free electron gas model</u>

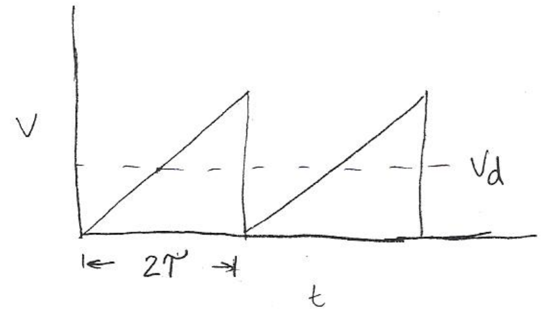


apply $\mathcal{E} \Rightarrow F = |e|\mathcal{E} = ma$

$F = ma \Rightarrow a = \frac{|e|\mathcal{E}}{m}$

electron should accelerate infinitely...
→ collisions.

$V_d = a \cdot \tau = \frac{|e|\mathcal{E}}{m} \cdot \tau$



$\Rightarrow J = \underbrace{\eta \cdot \frac{e^2}{m} \cdot \tau}_{\to \sigma} \cdot \mathcal{E}$

$\bar{l}$ = dist btw collisions $\Rightarrow V_d = \bar{l}/\tau$

$\Rightarrow \sigma = \eta \frac{e^2}{m} \tau = \eta \frac{e^2}{m} \frac{\bar{l}}{V_d}$

turns out - only electrons w/ energy close to $\mathcal{E}_F$ participate

$\Rightarrow \quad v_d \rightarrow v_F$ velocity of electrons at the Fermi level

classical: $E = \frac{1}{2} m v^2 \quad \Rightarrow \quad v = \left(\frac{2E}{m}\right)^{1/2}$

insert $E = \mathcal{E}_F = \frac{h^2}{8m}\left(\frac{3}{\pi}\eta\right)^{2/3}$

$\Rightarrow \quad v_F \cong \frac{h}{2m}\left(\frac{3\eta}{\pi}\right)^{1/3}$

under applied $\mathcal{E}$ retain $v = (2\mathcal{E}_F/m)^{1/2}$ but note $\mathcal{E}_F$ changes.

<u>more definitions</u>: $\quad J = \sigma \mathcal{E} = \eta\, |e| \cdot v_d$ } previously.

$\sigma = J/\mathcal{E} = \eta\, |e| \frac{v_d}{\mathcal{E}} = \eta\, |e| \cdot \mu$

$\rho = 1/\sigma$

mobility.

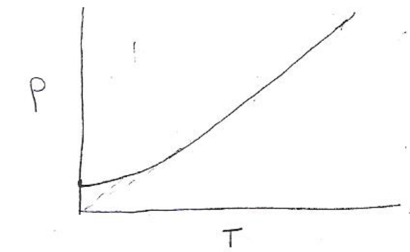
<u>metals</u> $\quad \eta \sim$ constant electrons in the 'free electron gas'

$Ca \rightarrow Ca^{2+} + 2e^-$, also $\mathcal{E}_F$

$\mu \sim \bar{l}$ mean free path between collisions.

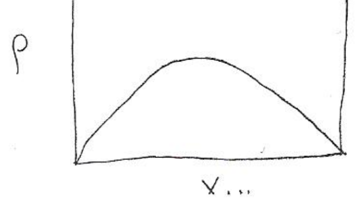
contributions to collisions: lattice (thermal) vibrations, impurities, grain boundaries.

$\frac{1}{\bar{l}_{tot}} = \sum_i \frac{1}{\bar{l}_i} \Rightarrow \rho_{tot} = \sum_i \rho_i$



$\rho_{th}: \bar{l}_{th} = \frac{C}{T} \Rightarrow \rho_{th} \propto T$

$\rho_{imp}: \bar{l}_{imp} = \frac{C}{X_{imp}} \Rightarrow \rho_{imp} \propto X_{imp}$



Ni-Cu solution

$\rho \propto X_{Ni}(1 - X_{Ni})$