Semi-Classical Model : Summary

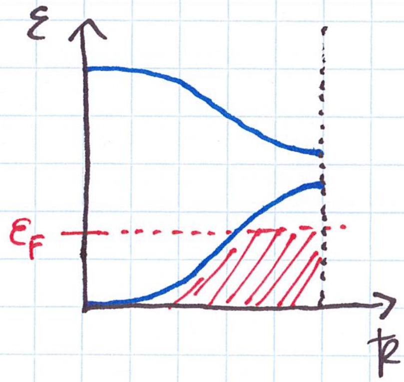
→ quantum particles ($\bar{e}$) in a periodic crystal potential

→ Bloch Theory

→ periodic potential separates Free $\bar{e}$ energies into bands. ⇒ Band gap

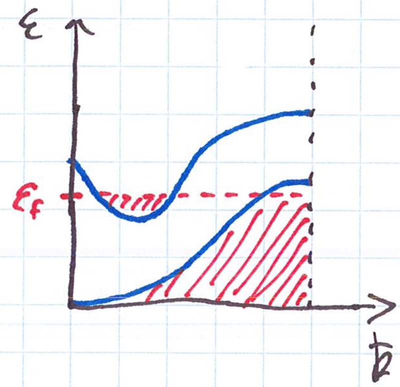
→ Each band contains N k-states ($2N$ $\bar{e}$ states)

Material Types



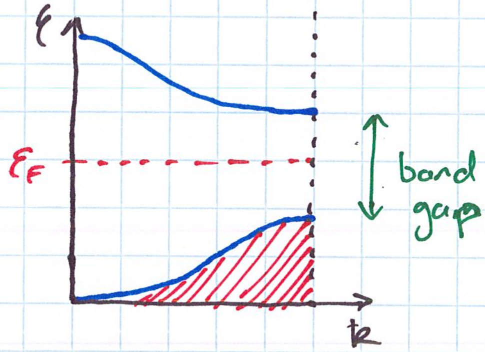
Metal → Fermi energy lies in a band

e.g. Na, Cu, Ag, Au .... a lot



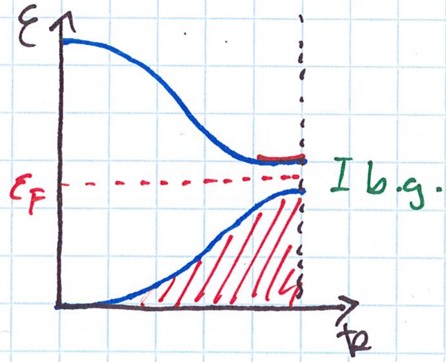
Semi-metal → ε_F lies in two overlapping bands

e.g. Ca



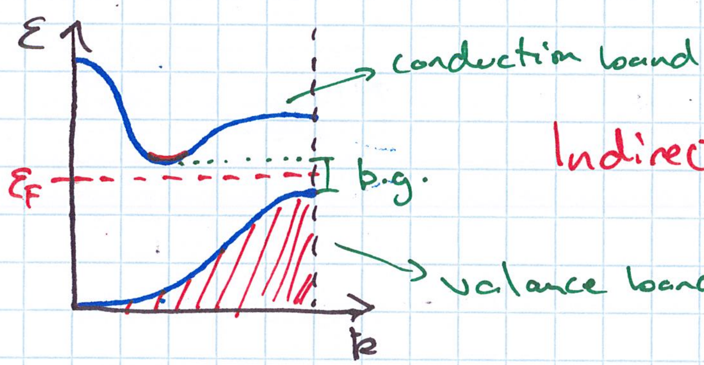
Insulator → ε_F lies between two bands i.e. in the band-gap
→ large band gap.

e.g. C



Direct bandgap e.g. GaAs

Semiconductor → ε_F lies in bandgap
→ small band gap.



Indirect bandgap. e.g. Si

→ Conductivity requires higher-energy states (add energy to $\bar{e}$'s)

→ if none are available → can not conduct.

→ since each band can hold $2N$ $\bar{e}$, an even # of $\bar{e}$/atom is required for an insulator

Conductivity:

recall $\rightarrow$ $\bar{v}_n(\mathbf{k}) = \frac{1}{\hbar} \nabla_{\mathbf{k}} \mathcal{E}(\mathbf{k})$

Recall: current density $\bar{j} = -e\bar{v}$

$$\bar{j} = -e \sum_{\mathbf{k}} \bar{v}_{\mathbf{k}}$$

$$= \frac{-e}{\hbar} \int \frac{1}{4\pi^3} \nabla_{\mathbf{k}} \mathcal{E}_{\mathbf{k}} \, d\mathbf{k}$$

→ for a filled band, $\mathcal{E}_{\mathbf{k}}$ is periodic, integral over all $\mathbf{k}$ yields $= 0$. App. I for proof. *

→ only $\bar{e}$ in partially filled bands contribute to conductivity → electrical & $\bar{e}$ part of thermal

→ $\boxed{\text{Filled bands are inert}}$

→ partially filled band:

$$j = \frac{-e}{4\pi^3} \int_{\text{occupied}} v(\mathbf{k}) \, d\mathbf{k}$$

* → generally: integral over complete Brillouin zone of the gradient of a periodic function is 0.

Holes:

$\rightarrow \quad j = \frac{-e}{4\pi^3} \int_{\text{occupied}} \bar{v}_k \, dk$

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Filled band: $j = 0$

$$0 = \int_{\text{zone}} v_k \, dk = \int_{\text{occ.}} v_k \, dk + \int_{\text{unocc.}} v_k \, dk$$

$$\therefore \quad j = \frac{-e}{4\pi^3} \int_{\text{occ.}} v_k \, dk = \frac{+e}{4\pi^3} \int_{\text{unocc.}} v_k \, dk$$

-> current carried by (−) charge carries occupying "filled" states equivalent to (+) charge carries occupying "unfilled" states.

-> hole = absence of $\bar{e}$ (& viceversa)

-> holes, (+) charge carriers, critical to semi-conductor physics => doping.

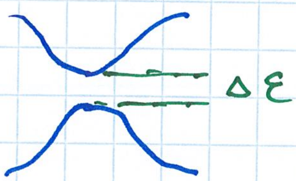
-> holes & $\bar{e}$ can interact & bind => exciton

Semi-conductors

→ require heat or optical energy (i.e. photon) to promote $\bar{e}$ into conduction band.

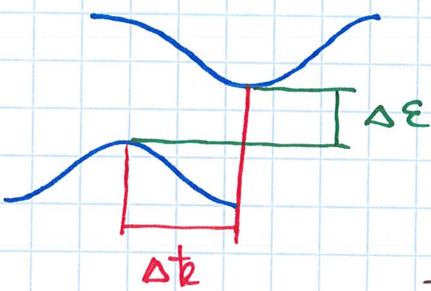
⇒ photovoltaics

Direct band gap: only a photon is req'd to move from valance to conduction band.



i.e. transition → absorb/emit photon.
$\Delta \mathcal{E}$

Indirect band gap: transition also requires a momentum transfer. Δk and $\Delta \mathcal{E}$



→ since photons carry almost no momentum... phonons are req'd. (lattice vibrations).

→ reduced efficiency.

Final Notes:

1) $\bar{p} \neq \hbar k$ ⇒ momentum is not just $\hbar k$, but is still related to k. ⇒ $\bar{p} = m\bar{v}_k = \frac{m}{\hbar} \nabla_k \mathcal{E}_k$

2) Insulator requires even # of $\bar{e}$ / atom
↳ otherwise $\mathcal{E}_F$ guaranteed to lie in band. (2N $\bar{e}$ per band).

3) Still nothing about τ: Bloch's Theory accounts for interaction of $\bar{e}$ $\bar{w}$ stationary lattice
→ need dynamic lattice (phonons) to account for scattering!