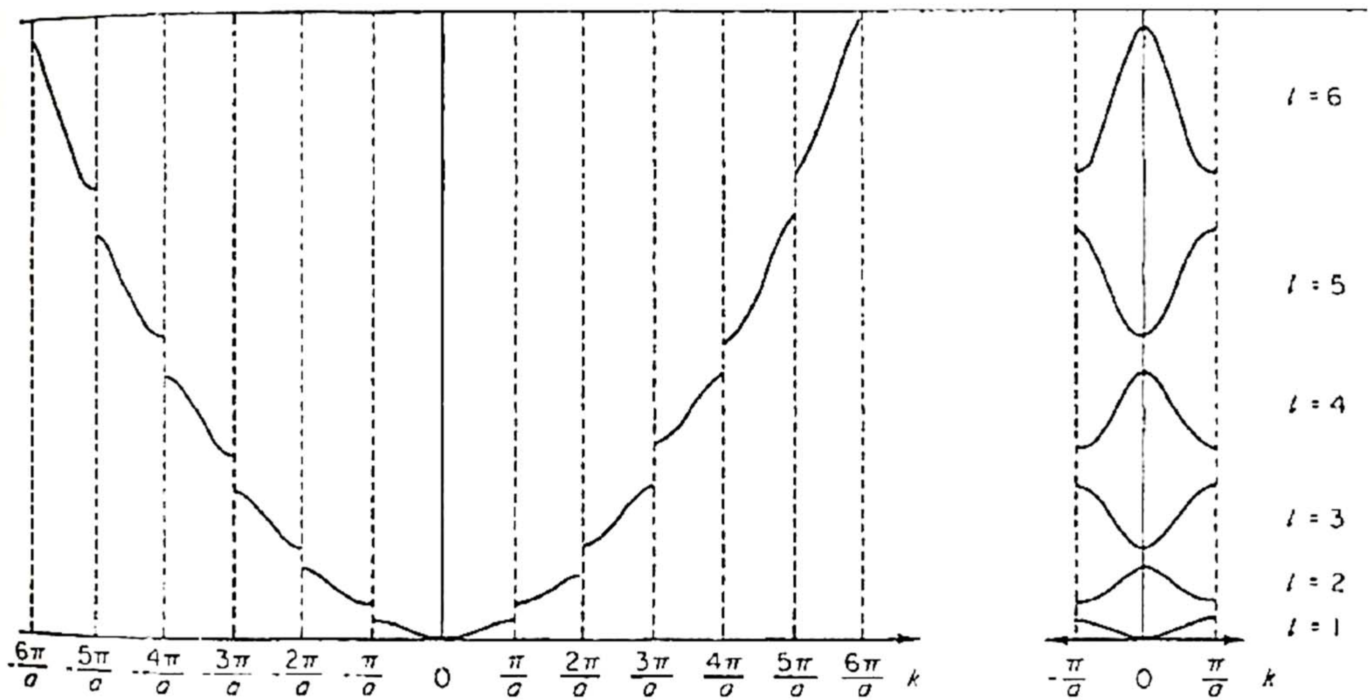
Weak binding model

"Extended" "Reduced"



$-\frac{\pi}{a} < k < \frac{\pi}{a}$: 1st Brillouin Zone

Weak binding model

$$(E_{max} - E) = \frac{\hbar^2 (k_{max} - k)^2}{2m_t^*}$$

k_{max}: k at the top of band

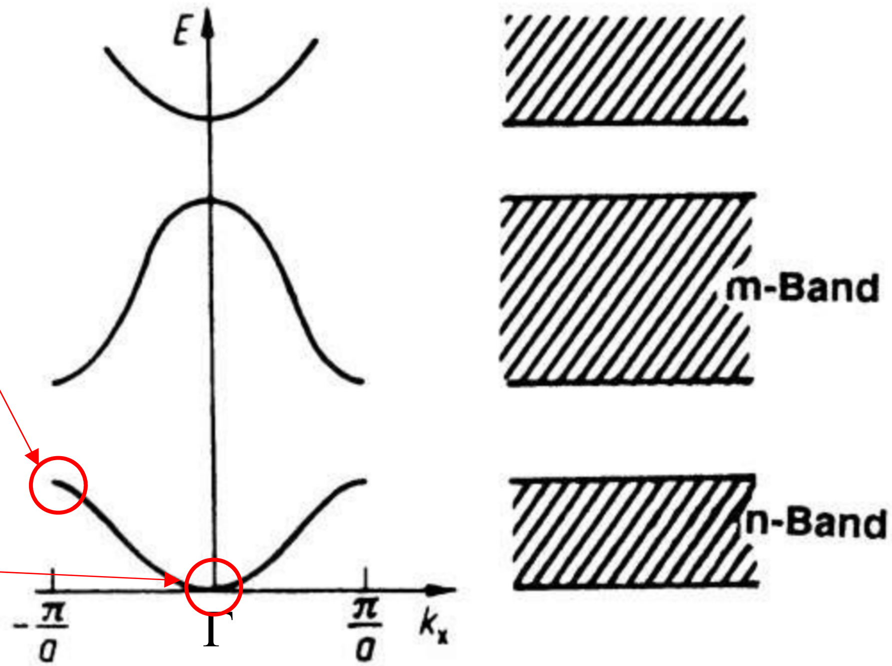
m_t^*: effective mass at the top of band

$$(E_{max} - E) = \frac{\hbar^2 {k_{min}}^2}{2m_b^*}$$

: Free electron like behavior

k_{min}: k at the bottom of band

m_b^*: effective mass at the bottom of band



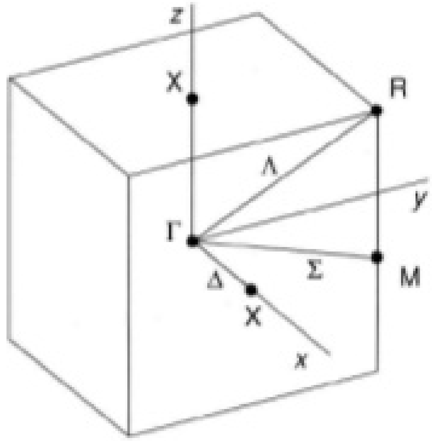
Γ Point : extrema in energy band

$N(E) \propto E^{1/2}$ near the bottom of the band
$N(E) \propto (E_{max} - E)^{1/2}$ near the top of the band

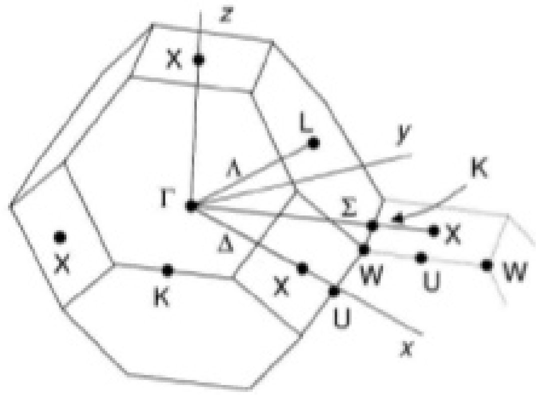
(Nearly free electron model)

The first Brillouin zones

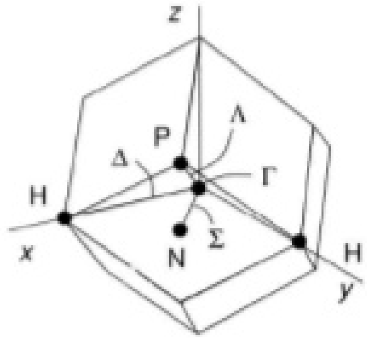
Simple cubic



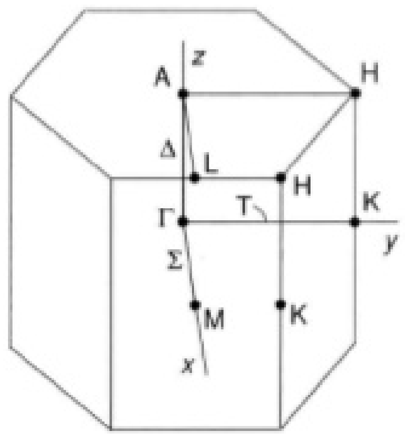
FCC



BCC

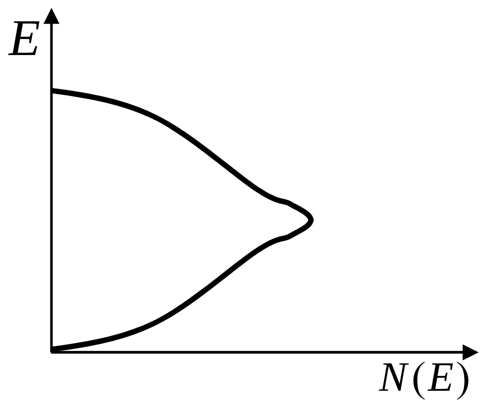


Hexagonal



- The k values in the Brillouin zone depend on the crystal symmetry.
- The first Brillouin zone = unit cell of reciprocal lattice
  ex) FCC crystal has BCC Brillouin zone.
- Greek and Latin letters indicate the directions and zone faces.

Density of states in a band



Near the bottom of the band

$$N(E) \propto E^{\frac{1}{2}}$$

$$N(E) = \frac{1}{4\pi^2}\left(\frac{2m_b^*}{\hbar^2}\right)^{\frac{3}{2}}E^{\frac{1}{2}}$$

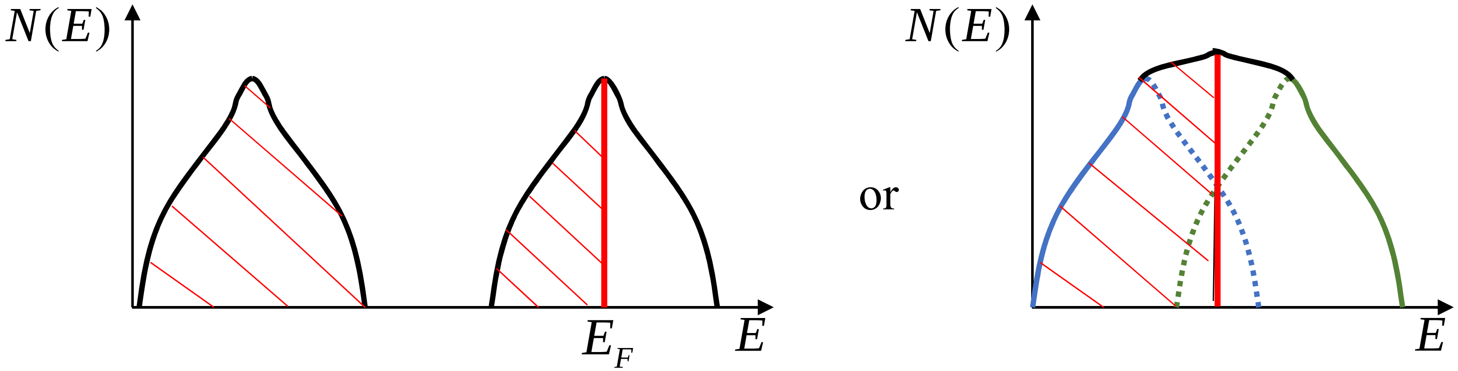
Near the top of the band

$$N(E) \propto (E_{max} - E)^{1/2}$$

$$N(E) = \frac{1}{4\pi^2}\left(\frac{2m_t^*}{\hbar^2}\right)^{\frac{3}{2}}(E_{max} - E)^{1/2}$$

Density of states in a band

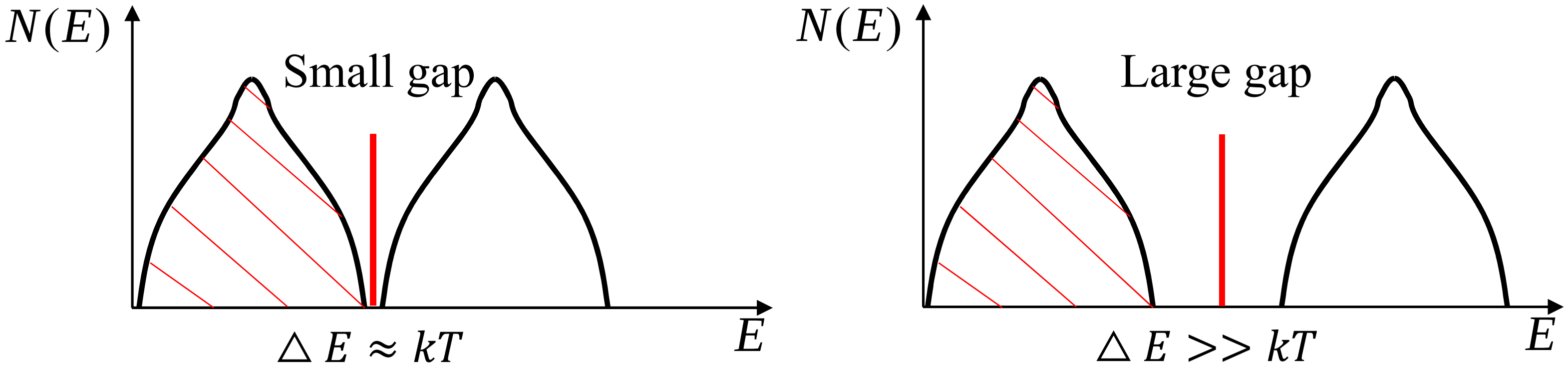
- Metal



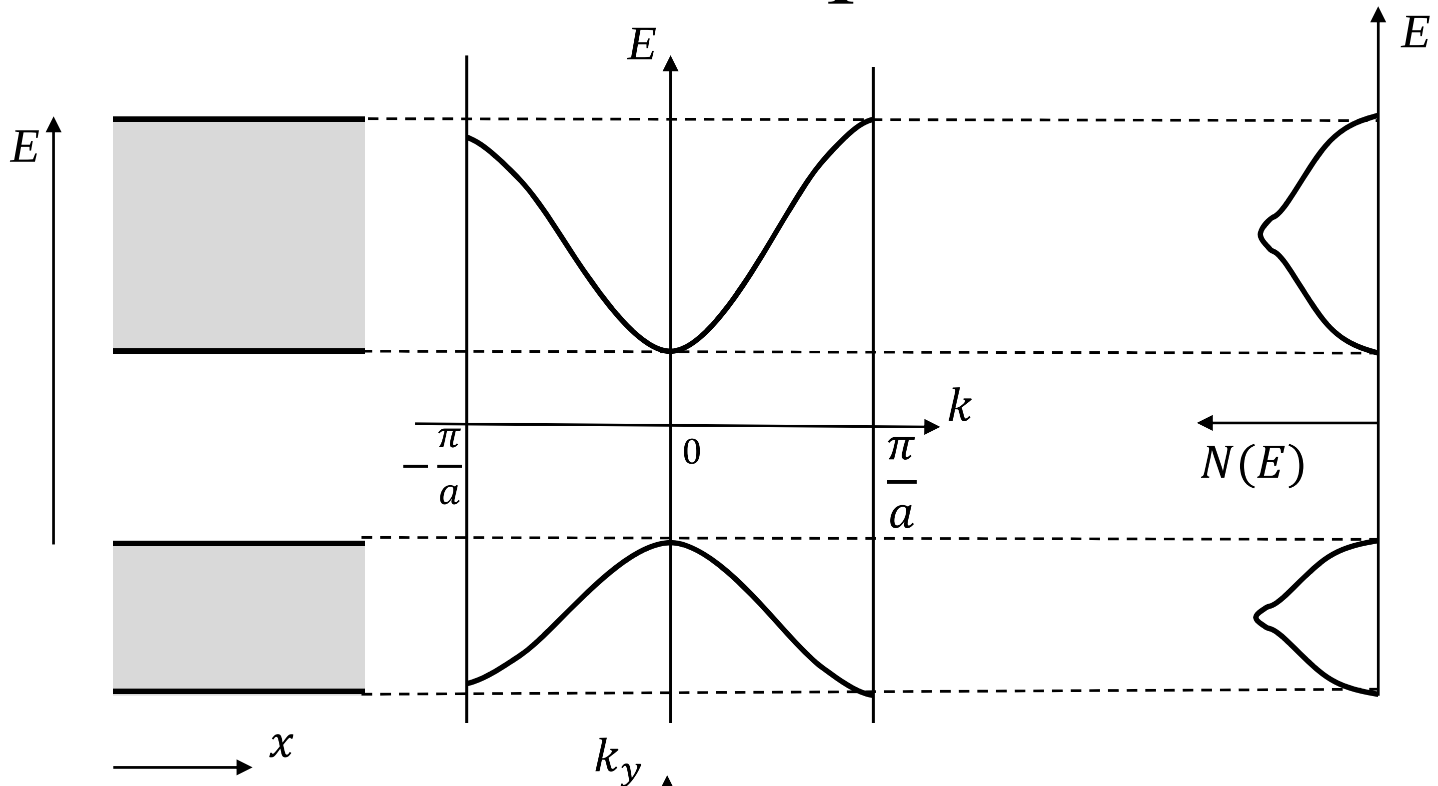
Partially occupied

Bands overlap

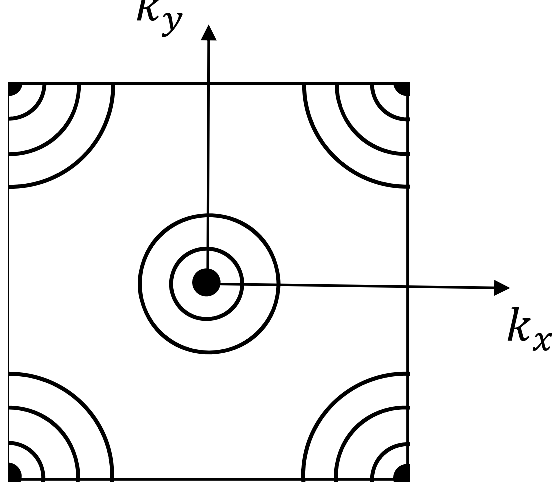
- Semiconductor or Insulator



Different band representation



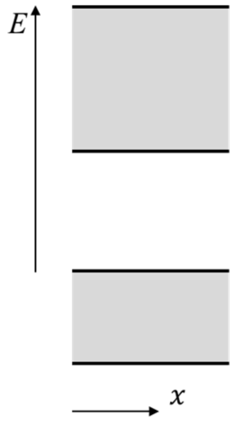
Equal energy surfaces

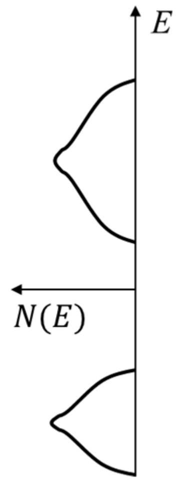


Different band representations

- E *vs* x χ

: Flat band diagram that emphasizes the non-localized nature of the band states



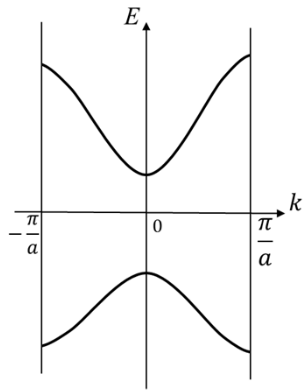


- $N(E)$ *vs* E

: Variation of the DOS within a band important when describing a variety of electron transport processes, optical excitations, *etc*.

- E *vs* k

: Dispersion relation for electron waves that is useful in describing the transport



- Free electron like behavior

1. $E \propto |k^2|$ (parabolic E-k)
2. $N(E) \propto E^{\frac{1}{2}}$
3. Spherical equal energy surfaces

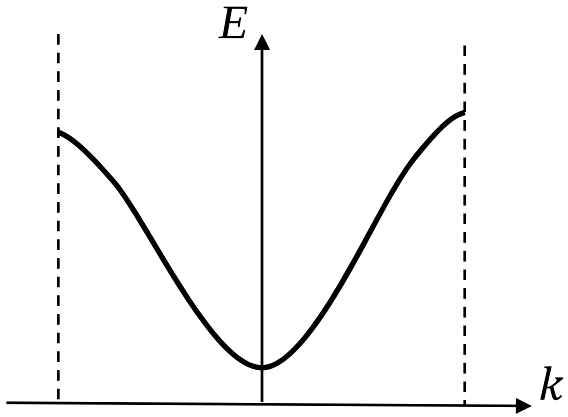
Electron velocity

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

$$E = \frac{\hbar^2 k^2}{m^*}$$

$$v_g = \frac{\hbar k}{m^*}$$

$$m^* = \frac{\hbar^2}{(\partial^2 E/\partial k^2)}$$

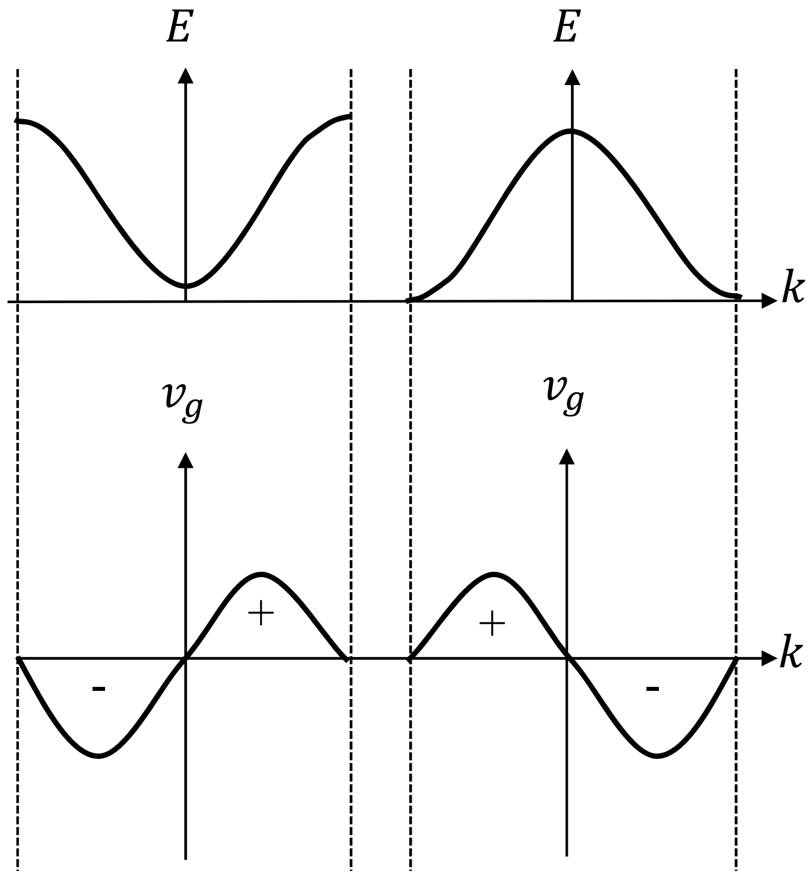


$$\frac{\partial E}{\partial k} = k\frac{\partial^2 E}{\partial k^2}$$

Solution: $E = Ak^2 + B$

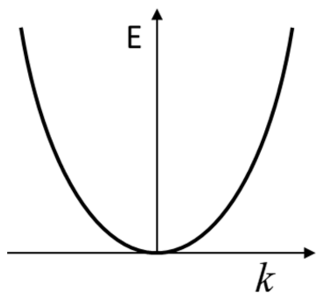
* This is satisfied only for an energy band extremum at $k = 0$

Electron velocity



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

- Velocity is zero at band extrema.
- In free electron system, group velocity goes to infinite or increase as *k* increases.



- In thermal equilibrium, there are equal number of electron-occupied states with positive velocity and negative velocity.
- Therefore, in completely filled band, no net charge transport under an electric field (ex: insulator, no conductivity of valence electrons)

Electron velocity

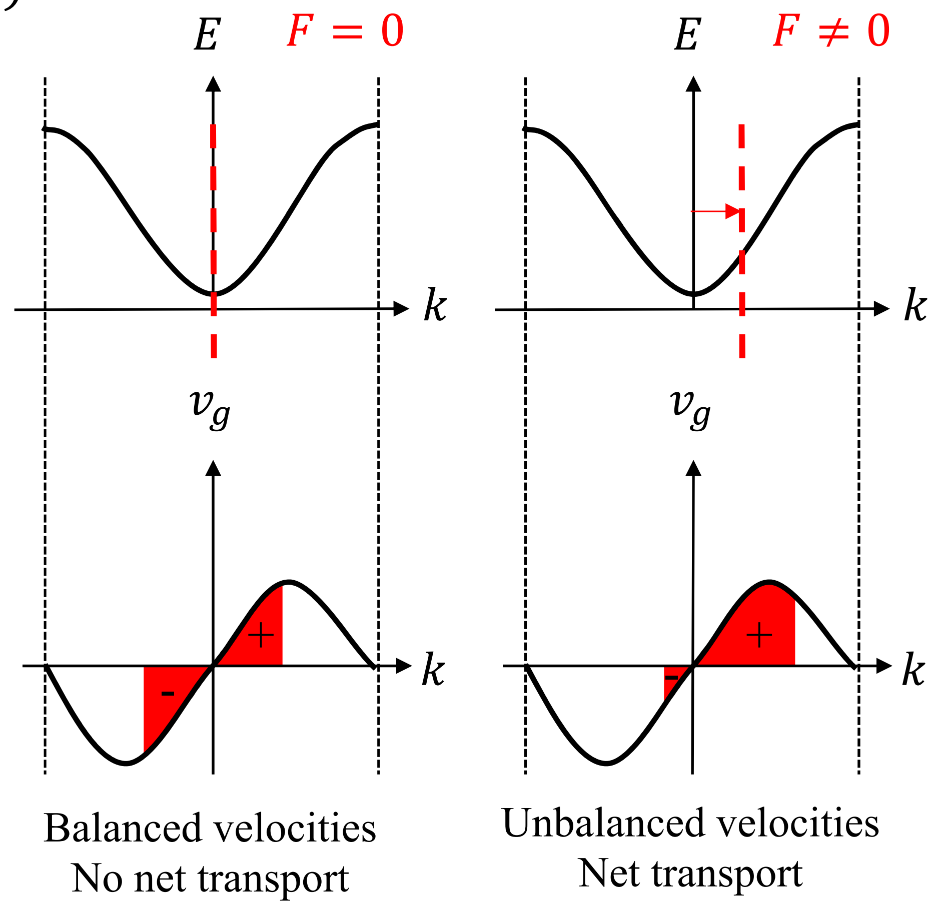
: proportionality factor between force and acceleration

(ex: $F = ma$)

$Fdt = dp = \hbar dk$ (p: momentum)

$$F = \hbar \frac{dk}{dt} \Rightarrow \frac{dk}{dt} = \frac{F}{\hbar}$$

: For positive F, k of all occupied states is shifted toward positive k values. So, there is an unbalance between occupied positive-velocity states and occupied negative-velocity states under electric field, leading to net transport.



Effective mass

In one dimension with periodic potential barriers

$$\frac{dv_g}{dt} = \frac{1}{\hbar}\frac{d}{dt}\left(\frac{dE}{dk}\right) = \frac{1}{\hbar}\frac{d}{dk}\left(\frac{dk}{dt}\frac{dE}{dk}\right)$$

$$\because F = \hbar\frac{dk}{dt}$$

$$F = \left(\frac{\hbar^2}{d^2E/dk^2}\right)\frac{dv_g}{dt} = m^*\frac{dv_g}{dt}$$

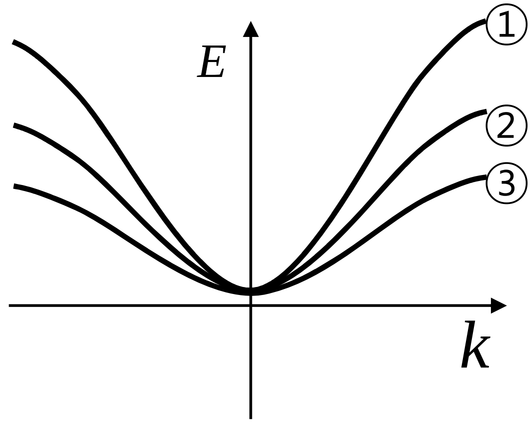
$$\boxed{m^* = \frac{\hbar^2}{(d^2E/dk^2)}}$$ in one dimension

→ The effective mass of an electron is the reciprocal of the curvature of the *E* vs. *k* plot.

cf) For free electrons, $m^* = m$

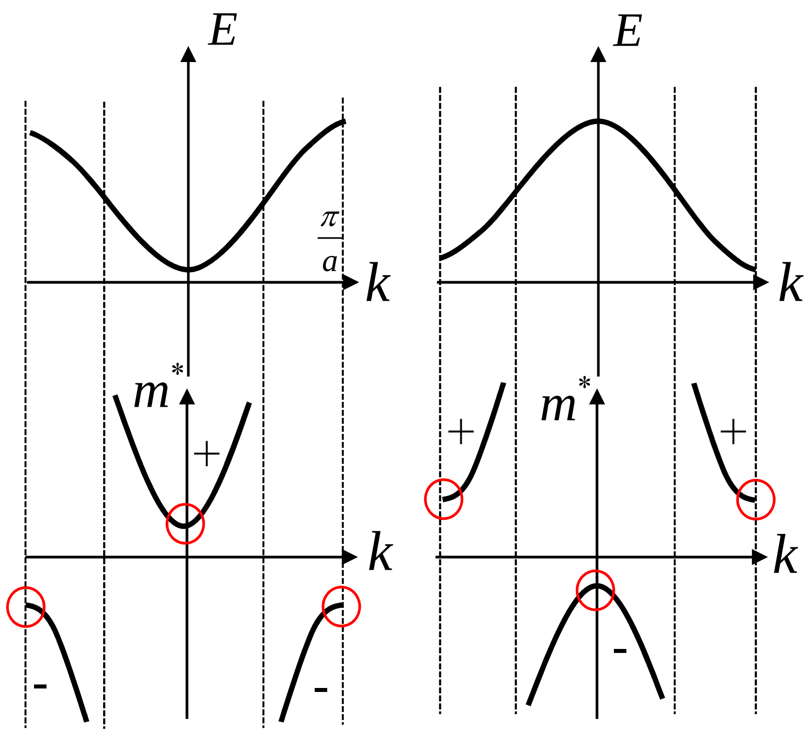
For 3-D, $\frac{d\mathbf{v}_g}{dt} = \frac{1}{\hbar^2}\nabla_k(\mathbf{F}\cdot\nabla_k E(\mathbf{k}))$, $\frac{1}{m_{ij}^*} = \frac{1}{\hbar^2}\frac{\partial^2 E}{\partial k_i \partial k_j}$

Effective mass



$m_1^* < m_2^* < m_3^*$

: Greater the curvature, smaller the effective mass



For a free electron, $m^* = m, v_g = \hbar \frac{k}{m}$

In a crystal, electrons at the extrema have effective mass.

$m^* = (+)$ at the bottom of a band

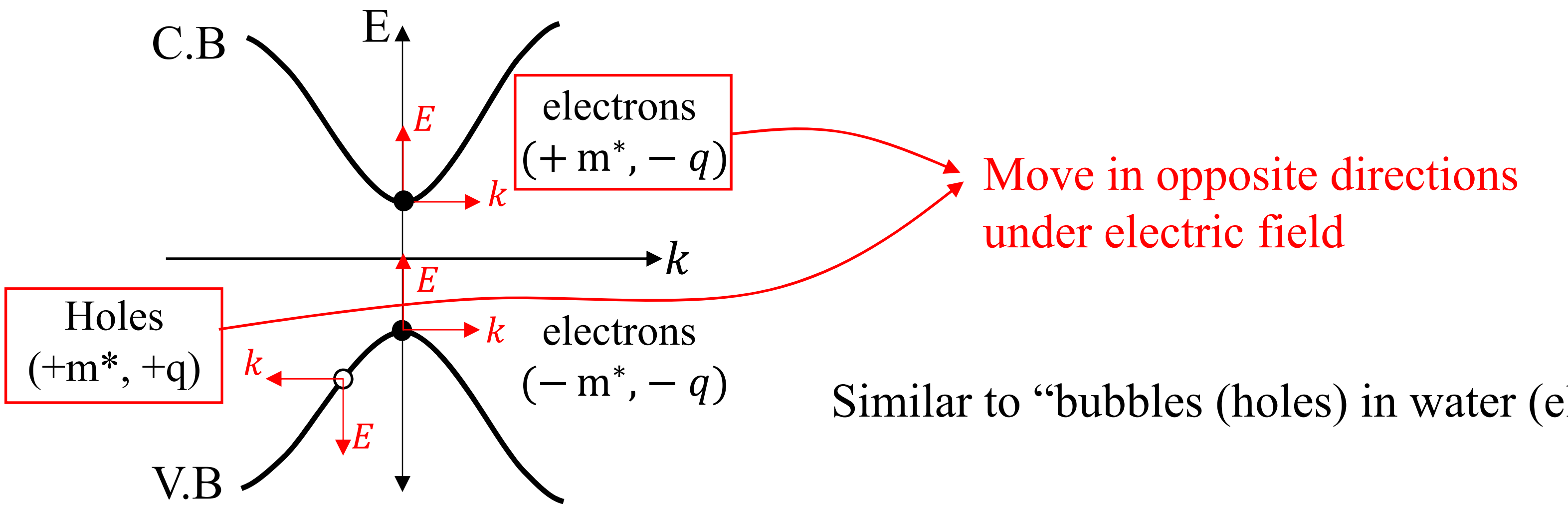
$m^* = (-)$ at the top of a band

A negative mass implies that the induced acceleration is on the opposite direction to the force that caused it (Result of Bragg reflection)

Holes

: missing electrons in a nearly filled band with a positive effective mass and a positive charge.

In a semiconductor or insulator



Similar to "bubbles (holes) in water (electrons)"

: In the presence of an electric field, electrons in the bottom of the conduction band and holes at the top of the valence band move in the opposite directions in real space (same sign mass but different sign charge), whereas electrons and holes both at the top of the valence band move in the same direction (different sign mass cancels different sign charge)