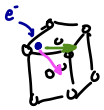
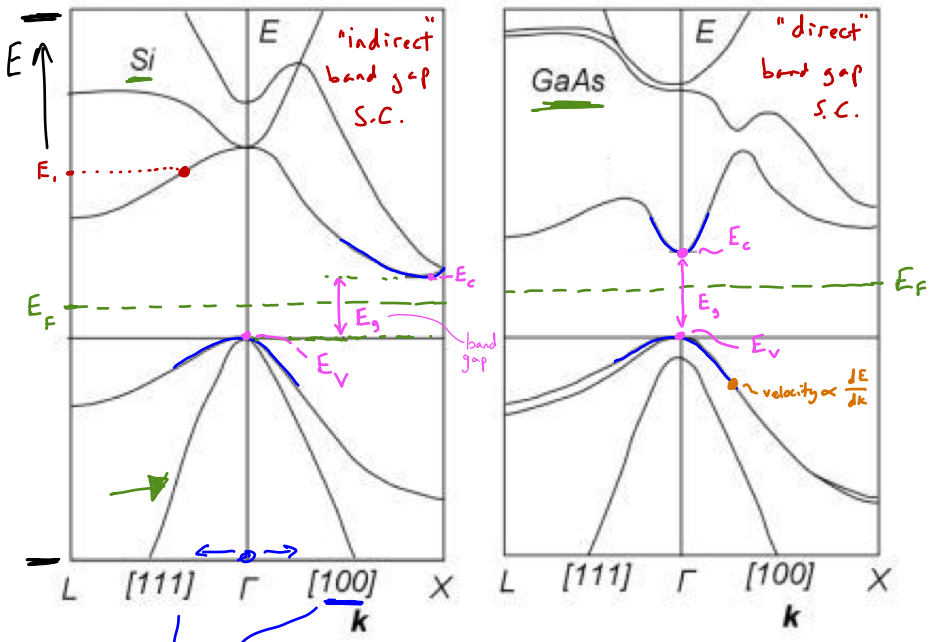
- E-k dispersion relation
  - Thus far, this was developed for 1D (Kronig-Penney model); how does it look in 3D crystal?




These are the +k for each with Γ: k=0 since the -k is just a mirror image of +k

- What properties does an e⁻ have?
  - Effective mass (m*)
    - Consider parabolic E-k relation from free electron: $E = \frac{\hbar^2 k^2}{2m}$

$$\frac{dE}{dk} = \frac{\hbar^2 k}{m} = \frac{\hbar p}{m} \quad (\text{based on } p = \hbar k)$$

relate p to velocity by $v = \frac{p}{m}$: $\frac{1}{\hbar}\frac{dE}{dk} = \frac{p}{m} = v \Rightarrow$ velocity $v = \frac{1}{\hbar}\frac{dE}{dk}$

take 2nd derivative: $\frac{d^2E}{dk^2} = \frac{\hbar^2}{m} \Rightarrow$ effective mass $m^* = \hbar^2\left(\frac{d^2E}{dk^2}\right)^{-1}$

- For a free e⁻, mass is constant; but when bound in a crystal with periodic potential, the e⁻ mass depends on inverse of E-k curvature.

m* ties classical world to quantum: $F = ma = -qE$

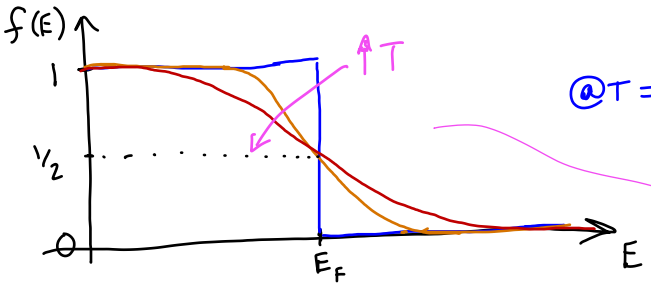
- Where are the e-s?
  - Fermi-Dirac probability function → see textbook for derivation, which is based on statistical dist.
    - Gives the statistical probability of an energy state at energy E being filled by an e-

$$f(E) = \frac{1}{1 + \exp\left(\frac{E - E_F}{kT}\right)}$$

$E_F$ ≡ Fermi level

T = temperature

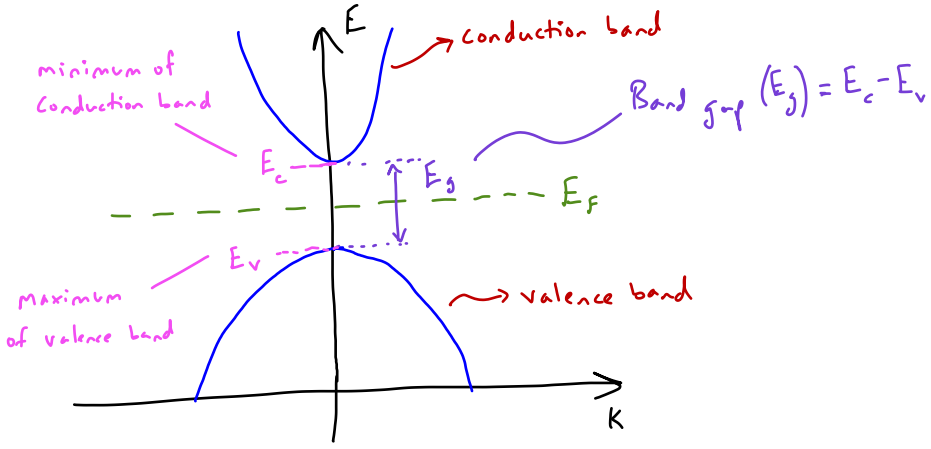
k = Boltzmann constant ($k_B$)



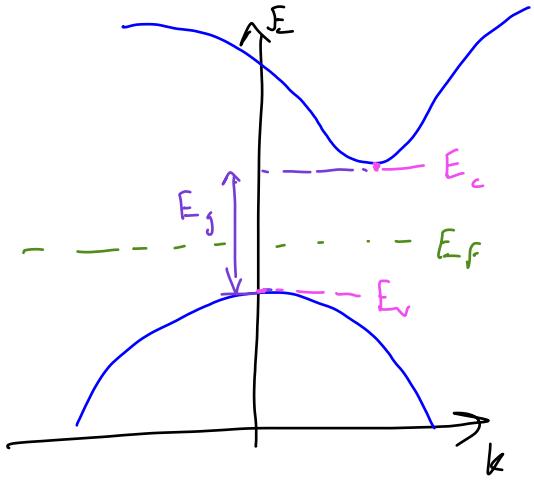

@T = 0K : all energy states at $E < E_F$ are filled, all above $E_F$ are empty

Fermi function spreads out around $E_F$

- Zoomed-in look at E-k near Fermi level ($E_F$):

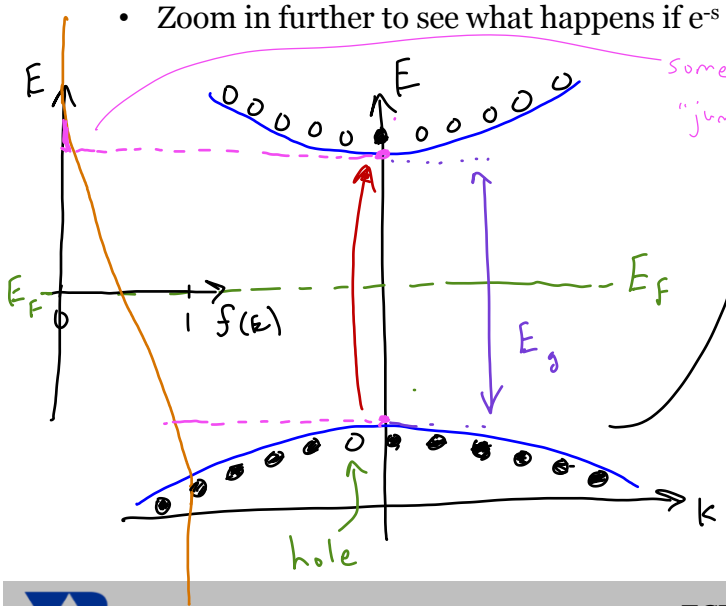



Direct Band gap S.C.



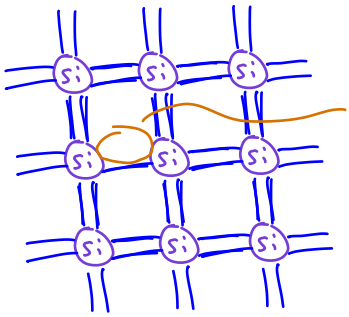

Indirect Band gap S.C.

- Zoom in further to see what happens if e-s have sufficient energy to "jump" into conduction band




some finite probability of sufficient thermal energy to have e- "jump" to $E_c$

what this looks like in the lattice:




created a positive charge that is called a "hole"

→ For HOLES, moving ↑E is easier; they have positive charge and their own $m_h^*$

- Where are the e-s? (cont)
  - Density of States (DOS)
    - How many states are there at a certain energy E?
      - NOTE: There are several different ways to derive the DOS; I will give one different from textbook so you have options:

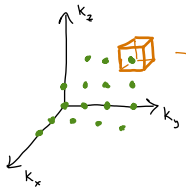
**3D-DOS derivation for parabolic E-k ($E=\frac{\hbar^2k^2}{2m}$) and crystal that is L in length x, y, and z**

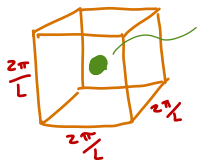
1. Determine the # states per unit volume of k-space

★ From S.E. allowed wave numbers in periodic potential are: $k = \frac{2\pi}{L}n$ ~ integer

⇒ For this class we will always use this!

- so, with $\frac{2\pi}{L}$ periodicity, a box around one state in k-space would be:




where volume of the entire crystal is: $V = L^3$

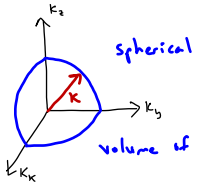
$$\Rightarrow \frac{1\text{ state}}{\left(\frac{2\pi}{L}\right)^3} = \frac{1}{\frac{8\pi^3}{V}} = \frac{V}{8\pi^3} \times 2 = \frac{V}{4\pi^3}\left(\frac{\text{allowed energy states}}{\text{unit volume k-space}}\right)$$

↑ $e^-$ spin ↑ or ↓ for each state

2. Find total # states up to a value k

$$N(k) = \left(\frac{\text{allowed energy states}}{\text{unit volume k-space}}\right)(\text{total volume up to k})$$

$$N(k) = \left(\frac{V}{4\pi^3}\right)\left(\frac{4}{3}\pi k^3\right) = \frac{Vk^3}{3\pi^2}$$




spherical

volume of sphere: $\frac{4}{3}\pi k^3$

3. Convert to total # states up to certain energy E

use this conversion from E-k: $k = \sqrt{\frac{2mE}{\hbar^2}}$

$$N(E) = \frac{V}{3\pi^2}\left(\sqrt{\frac{2mE}{\hbar^2}}\right)^3 = \frac{V}{3\pi^2\hbar^3}(2mE)^{3/2}$$

4. Differentiate w.r.t. energy and divide by volume for DOS per unit volume:

$$DOS_{3D} = g(E) = \frac{1}{V}\frac{d}{dE}N(E) = \frac{m\sqrt{2mE}}{\pi^2\hbar^3} = g(E)$$

using $\hbar = \frac{h}{2\pi}$ gives:

$$g(E) = \frac{4\pi}{h^3}(2m)^{3/2}\sqrt{E}$$

(format in book)

- Applying to conduction & valence bands (approx. parabolic) you get:

Conduction band: $E = E_c + \frac{\hbar^2k^2}{2m_n^*} \rightarrow g_c(E) = \frac{4\pi}{h^3}(2m_n^*)^{3/2}\sqrt{E-E_c}$

valence band: $E = E_v - \frac{\hbar^2k^2}{2m_p^*} \rightarrow g_v(E) = \frac{4\pi}{h^3}(2m_p^*)^{3/2}\sqrt{E_v-E}$