

Lecture #5

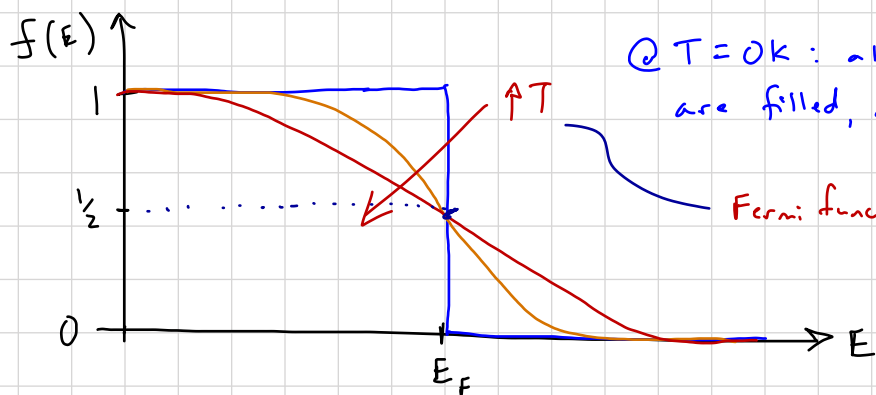
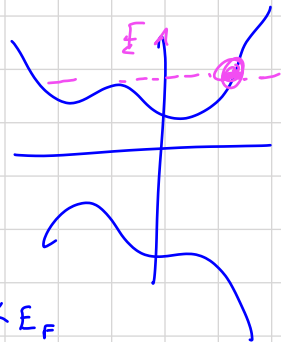
Quantum Theory of Solids (cont.)

→ Where are the e^- ?

- Fermi-Dirac Probability function — see textbook for derivation, which is based on statistics
- Gives the statistical probability of an energy state at energy E being filled by an e^-

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

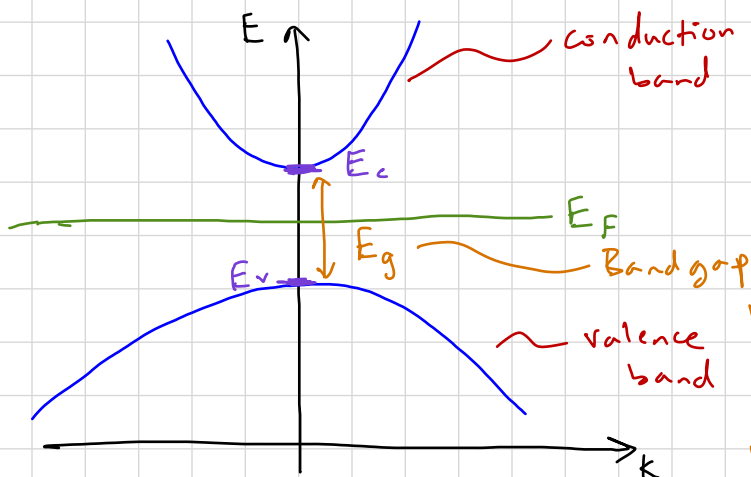
Fermi level
temperature
Boltzmann constant



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

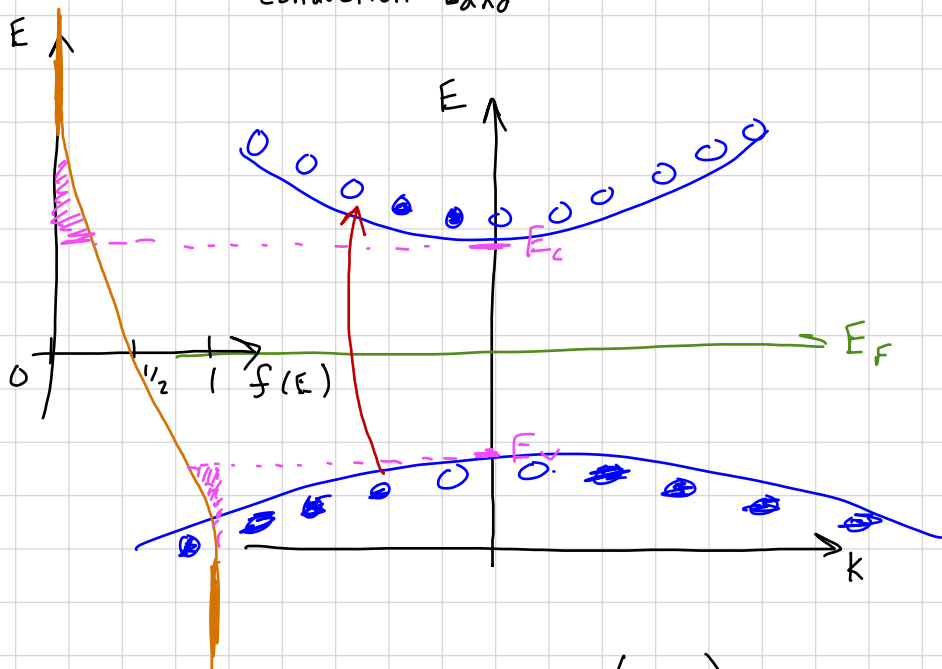
Fermi function spreads out around E_F

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



★ NOTE: The approximate parabolic nature of conduction and valence bands near E_c/E_v allows us to use $E-k$ parabolic expression from free particle!

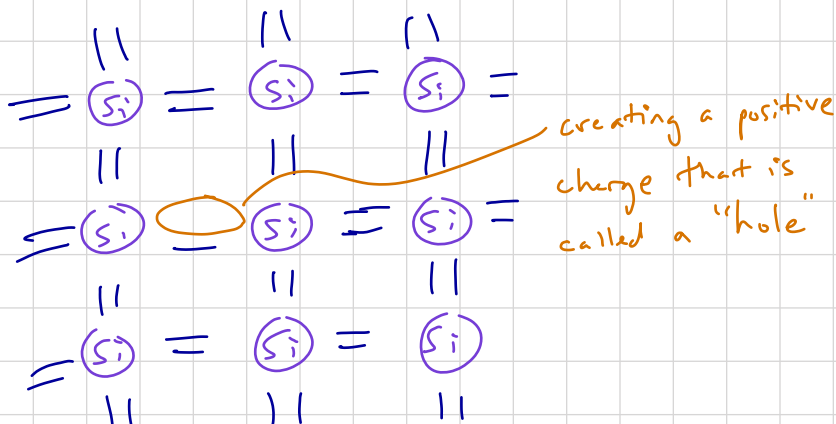
→ Zoom in further to see what happens if e^- have sufficient energy to "jump" into conduction band



★ Density of States (DOS)

→ How many states there are at a given energy

What this looks like in the lattice:



→ For holes, moving $\uparrow E$ is easier, they have positive charge and their own m_h^*

★ See video linked on Piazza for DOS derivation

• Where are the e^- s? (continued)

↳ How many energy states are there at a certain energy? \Rightarrow Density of States (DOS)

Note: There are several different ways to derive the DOS, I will give one different from textbook so you have options:

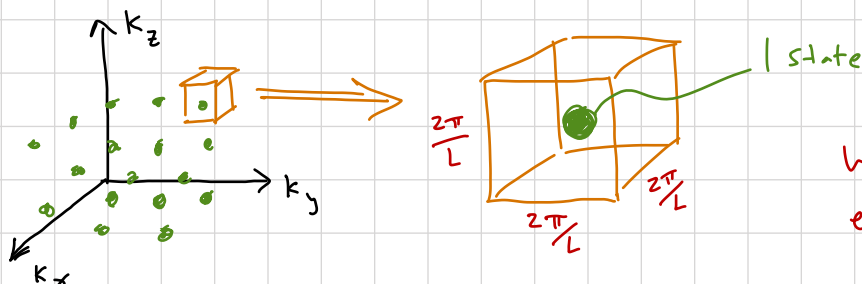
3D-DOS Derivation for Parabolic $E-k$, $E = \frac{\hbar^2 k^2}{2m}$, and crystal that is L in length for x, y, z

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

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

\rightarrow 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: $V = L^3$

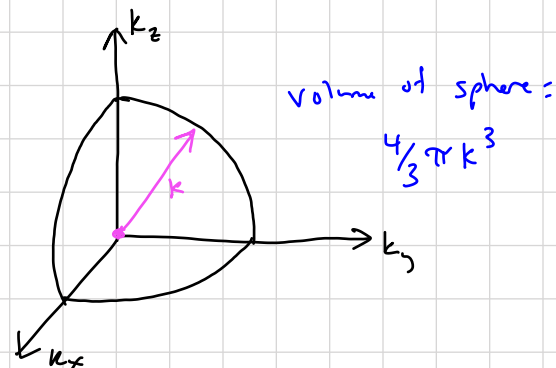
$$\rightarrow \frac{1 \text{ state}}{\left(\frac{2\pi}{L}\right)^3} = \frac{1}{\frac{8\pi^3}{V}} = \frac{V}{8\pi^3} \times 2 = \boxed{\frac{V}{4\pi^3}} \left(\begin{array}{l} \text{allowed energy states} \\ \text{unit volume } k\text{-space} \end{array} \right)$$

e^- spin \uparrow, \downarrow for each state

② Find total # states up to a value k

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

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



③ Convert to total # states up to a 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:

$$DOS_{3D} = g(E) = \frac{1}{V} \frac{d}{dE} N(E) = \frac{m \sqrt{2mE}}{\pi^2 \hbar^3} = g(E) = \frac{4\pi}{h^3} (2m)^{3/2} \sqrt{E}$$

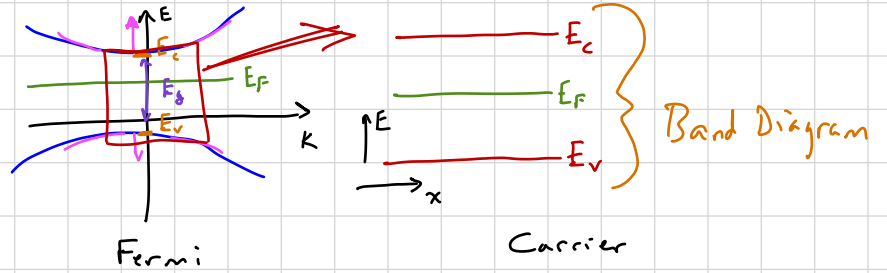
$\hbar = \frac{h}{2\pi}$
(format in book)

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

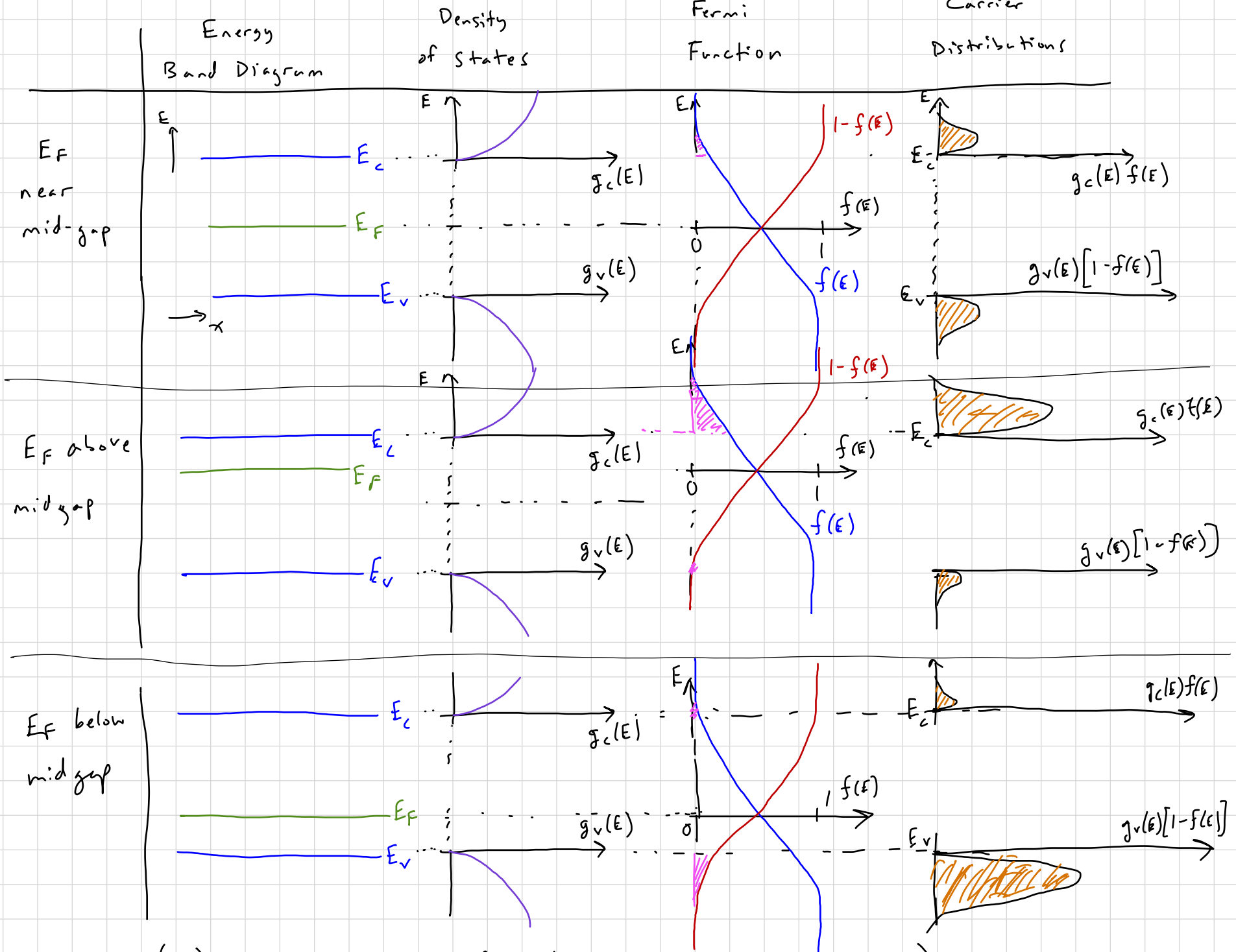
$$\text{Conduction band: } E = E_c + \frac{\hbar^2 k^2}{2m_n^*} \Rightarrow g_c(E) = \frac{4\pi}{h^3} (2m_n^*)^{3/2} \sqrt{E - E_c}$$

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

Semiconductors in Equilibrium (EQ)



- Charge carrier distribution



Equilibrium (EQ) is when no external forces (E-fields, temperature gradients, etc.) are acting on Semiconductor

e^- : $n(E) = g_c(E)f(E)$

h^+ : $p(E) = g_v(E)[1-f(E)]$

Intrinsic semiconductor: (Ideally, semiconductor with NO impurities, E_F is within band gap)

→ Equal concentration of e^- s and h^+ s

$n_i \equiv e^- \text{ conc.}$

$p_i \equiv h^+ \text{ conc.}$

$\Rightarrow n_i = p_i$
just use this
(temperature dependent!)

Thermal EQ carrier conc.

e^- in conduction band

$n_0 = \int g_c(E)f(E)dE$
from E_c to ∞

h^+ in valence band

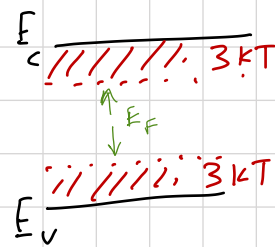
$p_0 = \int g_v(E)[1-f(E)]dE$
from $-\infty$ to E_v

IF E_F isn't too close to E_c or E_v , then we can use

Boltzmann Approx:

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

$$\text{If } E_v + 3kT \leq E_F \leq E_c - 3kT$$



use the approx:

$$n_0 = 2 \left(\frac{2\pi m_n^* kT}{h^2} \right)^{3/2} \exp\left[\frac{-(E_c - E_F)}{kT}\right]$$

$\equiv N_c$, effective density of states in conduction band

DOS effective mass

Then:

Another variation based on E_F shifts:

$$n_0 = n_i \exp\left[\frac{E_F - E_{Fi}}{kT}\right]$$

$$p_0 = n_i \exp\left[\frac{-(E_F - E_{Fi})}{kT}\right]$$

$$\begin{aligned} n_0 &= N_c \exp\left[\frac{-(E_c - E_F)}{kT}\right] & p_0 &= N_v \exp\left[\frac{-(E_F - E_v)}{kT}\right] \\ N_c &= 2 \left(\frac{2\pi m_n^* kT}{h^2} \right)^{3/2} & N_v &= 2 \left(\frac{2\pi m_p^* kT}{h^2} \right)^{3/2} \end{aligned}$$

Thermal EQ, $E_v + 3kT \leq E_F \leq E_c - 3kT$

$E_{Fi} \equiv$ midgap energy

NOTE: $N_{c,v} \Big|_{T_B} = N_{c,v} \Big|_{T_A} \left(\frac{T_B}{T_A} \right)^{3/2}$

Apply these n_0, p_0 expressions to the intrinsic S.C. case where: $n_0 = n_i = p_i$ and define the E_F for an intrinsic S.C. as E_{Fi}

NOTE: E_{Fi} at midgap if $g_c(E) = g_v(E)$ (symmetric DOS)

No matter what: $E_g = E_c - E_v$ and:

intrinsic carrier density

$$n_i^2 = N_c N_v \exp\left[\frac{-E_g}{kT}\right]$$

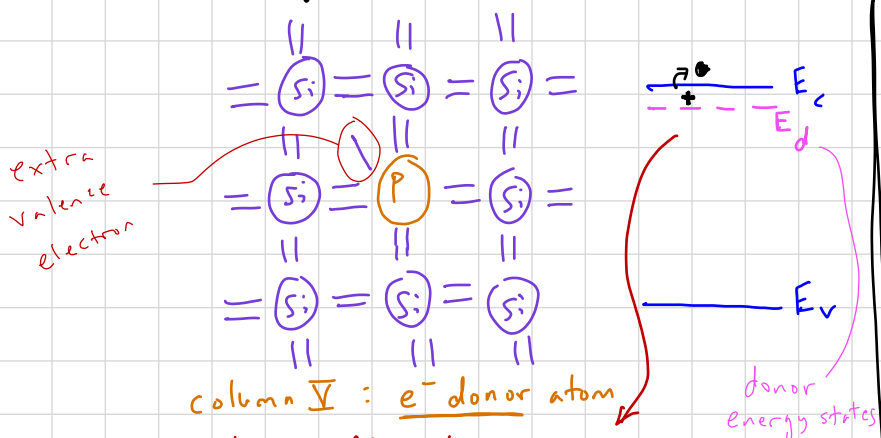
Thermal EQ

\equiv constant, indep. of E_F !

$$n_0 p_0 = n_i^2$$

Dopant atoms and E_F position

When adding an impurity to a S.C. it can contribute to carrier concentration:



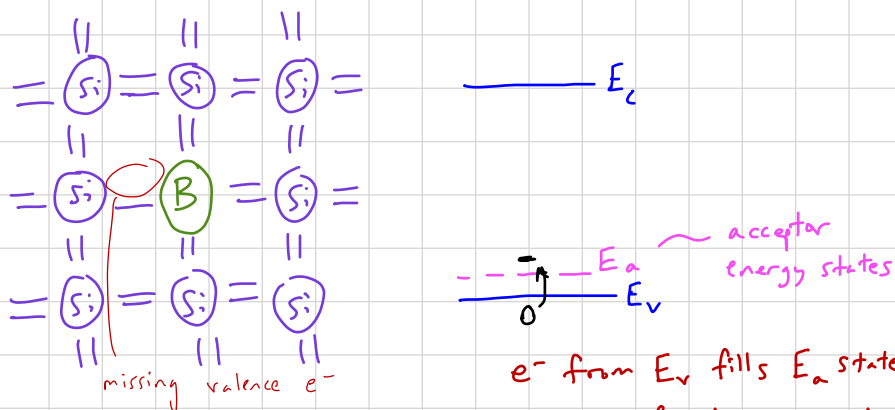
Once e^- has sufficient energy to go to E_c , donor is ionized (+)

★ NOT a h^+ but a fixed + ion

DONOR DOPING: n-type

majority carriers: e^- s

minority carriers: h^+ s



e^- from E_v fills E_a state creating fixed - ion and leaving behind a h^+

ACCEPTOR DOPING: p-type

majority carrier: h^+ s

minority carrier: e^- s