# Density of States and Band Structure

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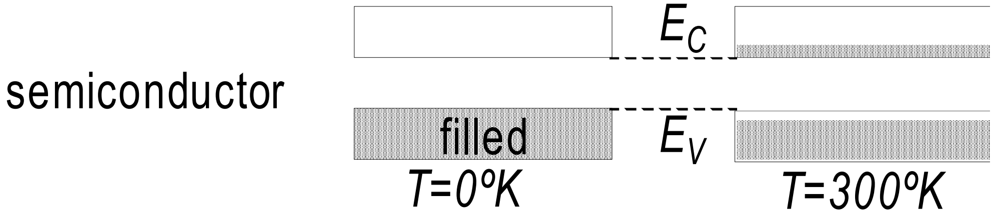
# Band Structure

In insulators, $E_g > 10eV$, empty conduction band

In metals, conduction bands are partly filled or overlaped with valence bands.

In semicondutors, $E_g$ is smaller than that of matals so that electrons can possiblely *jump* to conduction band

In dopped semicondutors. There is an additional donner level(n doped) near the bottom of condution band($E_c$) or an acceptor level(p doped) near the valence band($E_v$)



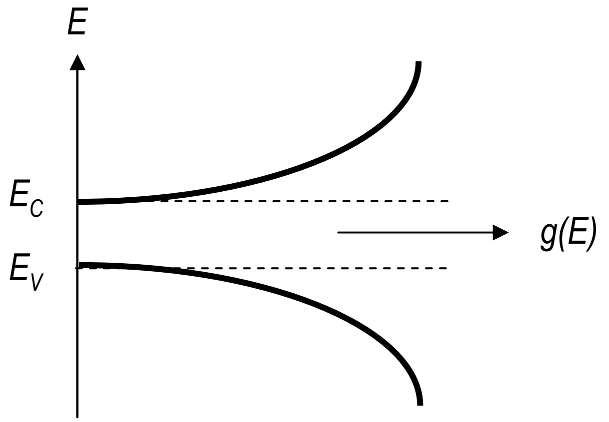
# Carrier concentration

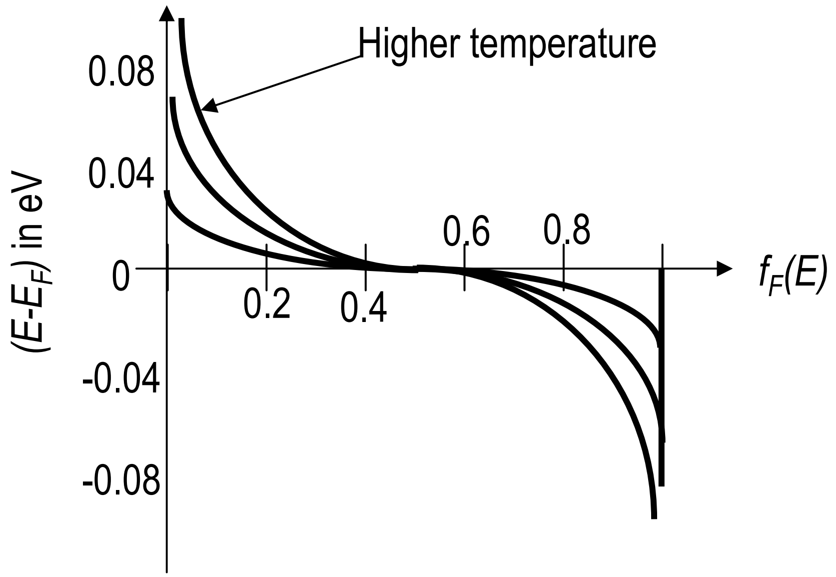
$$n = \int_{E_C}^{\infty} g(E) f_F(E) dE$$

$$\boxed{p = \int_{-\infty}^{E_V} g(E) f_F(E) dE}$$

$$g(E) = 4\pi \left(\frac{2m_n^*}{h^2}\right)^{3/2} E^{1/2}$$

$$f_F(E) = \frac{1}{e^{(E-E_F)/kT}+1}$$





# Density of states

- $g(E)$ is the number of states per volume in a small energy range.

The conduction band is: $$g_C(E)=4\pi\left(\frac{2m_n^*}{h^2}\right)^{3/2}(E-E_C)^{1/2}$$ for $E > E_C$

The valence band is: $$g_V(E)=4\pi\left(\frac{2m_p^*}{h^2}\right)^{3/2}(E_V-E)^{1/2}$$ for $E < E_V$

# Effective density of states

$$n = \int_{E_c}^{\sqcup} g_n(E) f_n(E)\, dE = N_c F_{1/2}(\eta_n)$$

where

$$N_c = 2\left(\frac{m_n k_B T}{2\pi\hbar^2}\right)^{3/2}$$

is called the **effective density of states** for the conduction band

$$\eta_n = (E_F - E_c)/k_B T \qquad F_{1/2}(\eta_n) = \frac{2}{\sqrt{\pi}} \int_0^\infty \frac{x^{1/2}\, dx}{1 + \exp(x - \eta_n)}$$

is the **Fermi integral**. For $\eta_n > 3$,

$$F_{1/2} \approx \exp(\eta_n)$$

For $\eta_n < 3$,

$$F_{1/2} \approx \frac{4\eta_n^{3/2}}{3\sqrt{\pi}}$$

$$N_v = 2\left(\frac{2\pi m_p^* kT}{h^2}\right)^{3/2}$$ For holes

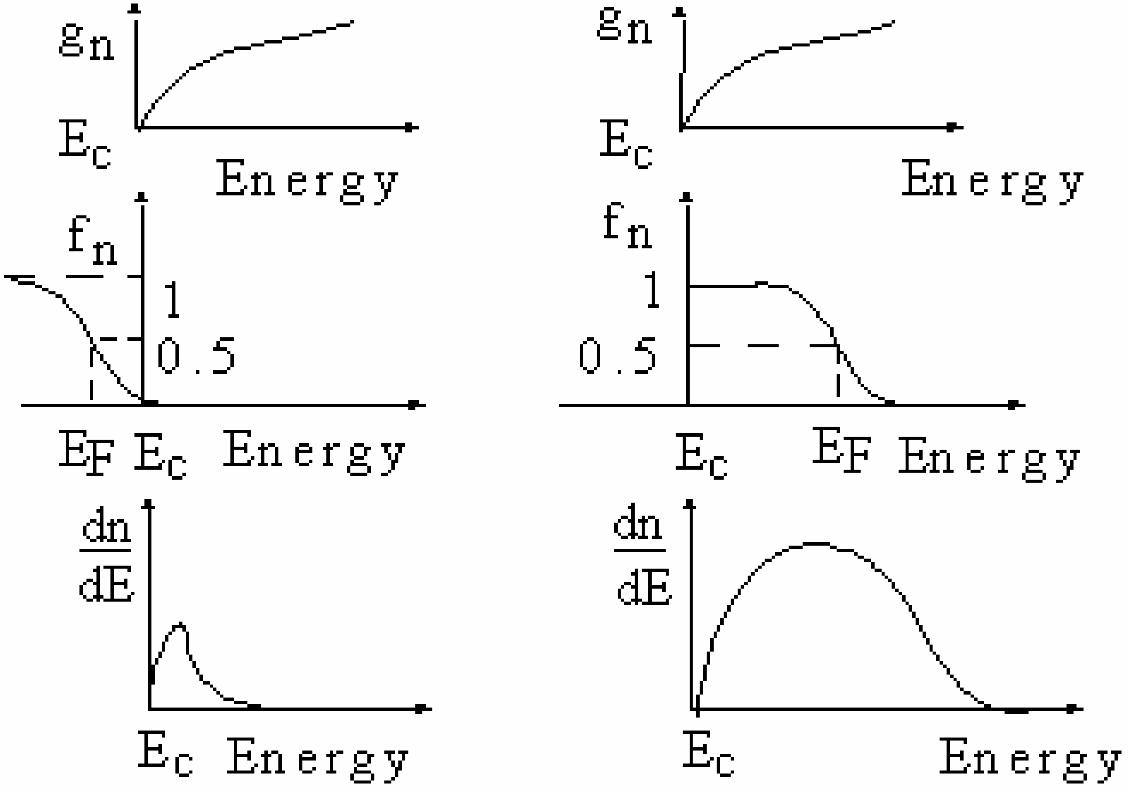
# Fermi Level

- The distribution of electron/holes satisfy Fermi-Dirac distribution

$$f(E) = \frac{1}{1 + e^{(E - E_F)/kT}}$$

- Fermi Level can be defined by the occupation probability of electrons at 0K

# Example:Density of states, distribution function and electron density for degenerate and non-degenerate n-type semiconductor



# Basic Properties of Fermi Level

- Fermi Level is an **intrinsic property** of the material, it is sufficient to describe the carrier occupation function by Fermi Level
- Only the available bands can have electrons/holes even when the occupy function f(E) is not zero.
- Intrinsic carrier density is a strong function of temperature

# Intrinsic semiconductor

**Boltzmann approximation:**

$$n_0 = \frac{\pi}{2}\left(\frac{8m_n^*}{h^2}\right)^{3/2} \int_{E_C}^{\infty} \left(E - E_C\right)^{1/2} e^{-(E-E_F)/kT} dE = N_C e^{-(E_C-E_F)/kT}$$

$$p_0 = \frac{\pi}{2}\left(\frac{8m_p^*}{h^2}\right)^{3/2} \int_{-\infty}^{E_V} \left(E_V - E\right)^{1/2} e^{-(E_F-E)/kT} dE = N_V e^{-(E_F-E_V)/kT}$$

➡ $$n_0 p_0 = N_C N_V e^{-(E_C-E_V)/kT} = N_C N_V e^{-E_g/kT}$$

For intrinsic semiconductor: ***n*$_0$ = *p*$_0$ =*n*$_i$** where ***n*$_i$** is the intrinsic carrier density. and

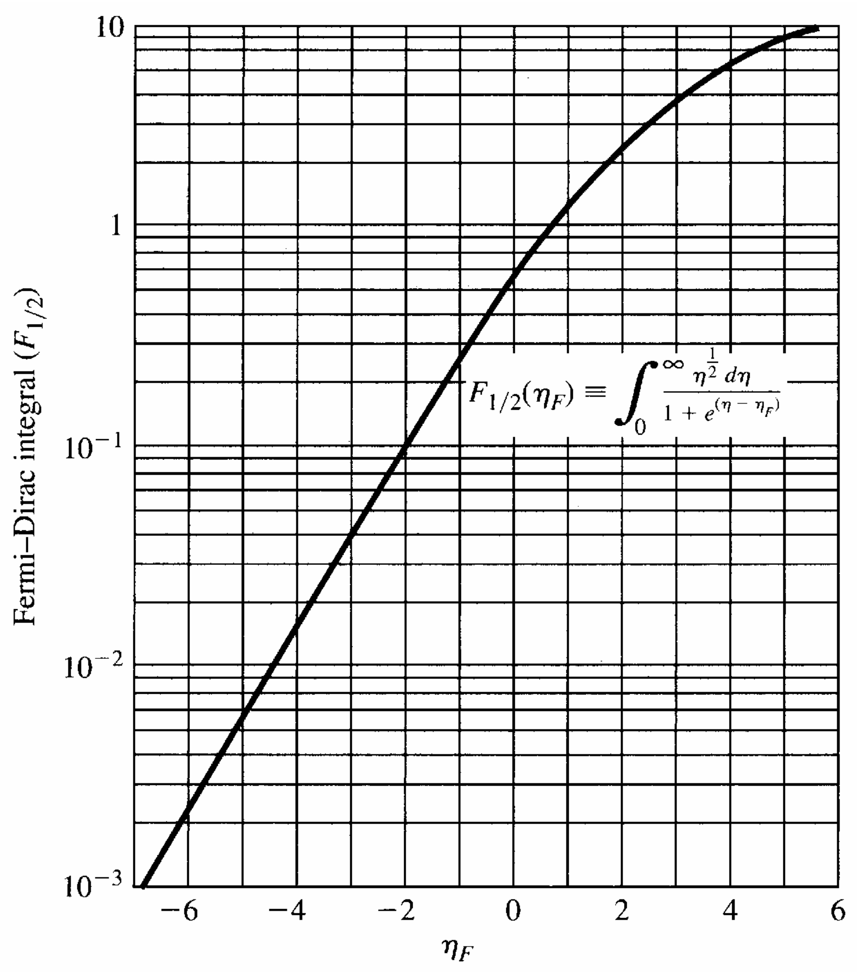
➡ $$\boxed{n_0 p_0 = n_i^2}$$

$$n_i = 2\left(\frac{2\pi kT}{h^2}\right)^{3/2} \left(m_n^* m_p^*\right)^{3/4} e^{-E_g/2kT}$$

Intrinsic Fermi level:

$$E_F = \frac{E_C + E_V}{2} - \frac{3}{4} kT\, ln\left(\frac{m_n^*}{m_p^*}\right) = E_{Fi}$$

# The non-Boltzmann approx. hole Concentration



$$p_0 = \frac{4\pi}{h^3}\left(2m_p^*\right)^{3/2}\int_{-\infty}^{E_V}\frac{\left(E_V - E\right)^{1/2}dE}{1+exp\left(\left(E_F - E\right)/kT\right)}$$

Let: $\eta = \frac{E_V - E}{kT}$ and $\eta_F = \frac{E_V - E_F}{kT}$

$$p_0 = 4\pi\left(\frac{2m_p^*kT}{h^2}\right)^{3/2}\int_0^\infty\frac{\eta^{1/2}d\eta}{1+exp\left(\eta-\eta_F\right)}$$

Define: $F_{1/2}\left(\eta_F\right) = \int_0^\infty\frac{\eta^{1/2}d\eta}{1+exp\left(\eta-\eta_F\right)}$

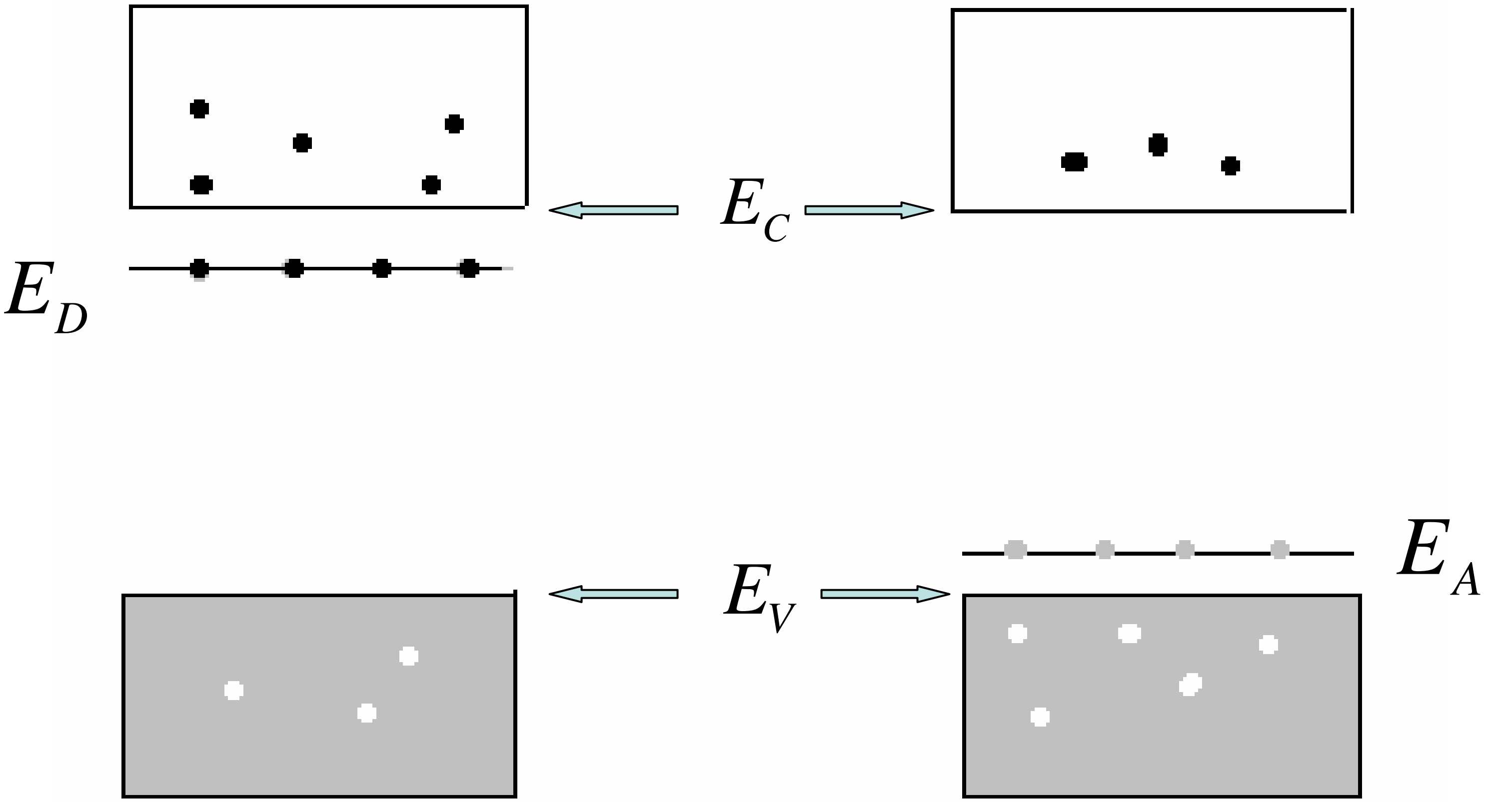
We have: $p_0 = \frac{2}{\sqrt{\pi}}N_V F_{1/2}\left(\eta_F\right)$

# Why do we need non-Boltzmann model

- The available situation for Boltzmann approximation if that that the Fermi level is far from band edges.
- When highly doped, Fermi Levels are very near band edges.
- Most laser devices are highly doped.
- The 3-D integration is a hard work. That is the challenge of using Fermi-Dirac Model.

# Doping

- N - type
- P - type



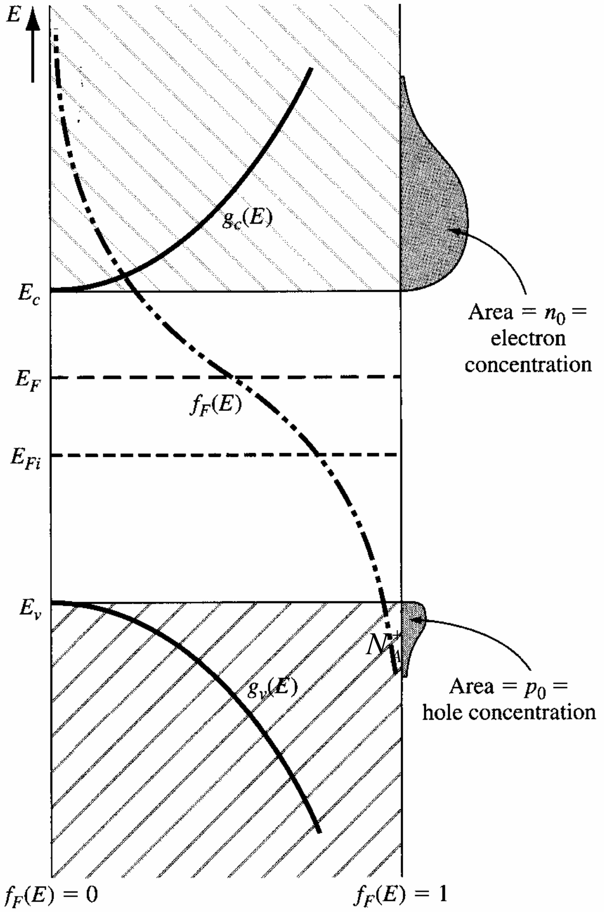
# Doped semiconductor (extrinsic)

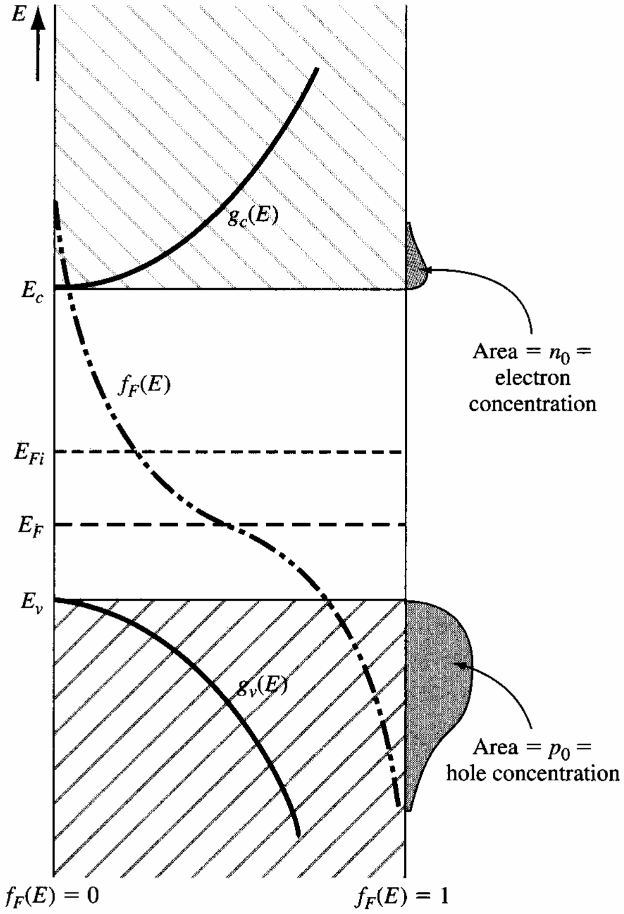
Introducing dopant will shift the Fermi level but the Fermi-Dirac distribution function remains the same. This is the characteristics of thermal equilibrium.

$$\Rightarrow n_0 p_0 = n_i^2$$

Still hold.

where $n_0$ and $p_0$ denote the electron and hole density at thermal equilibrium.





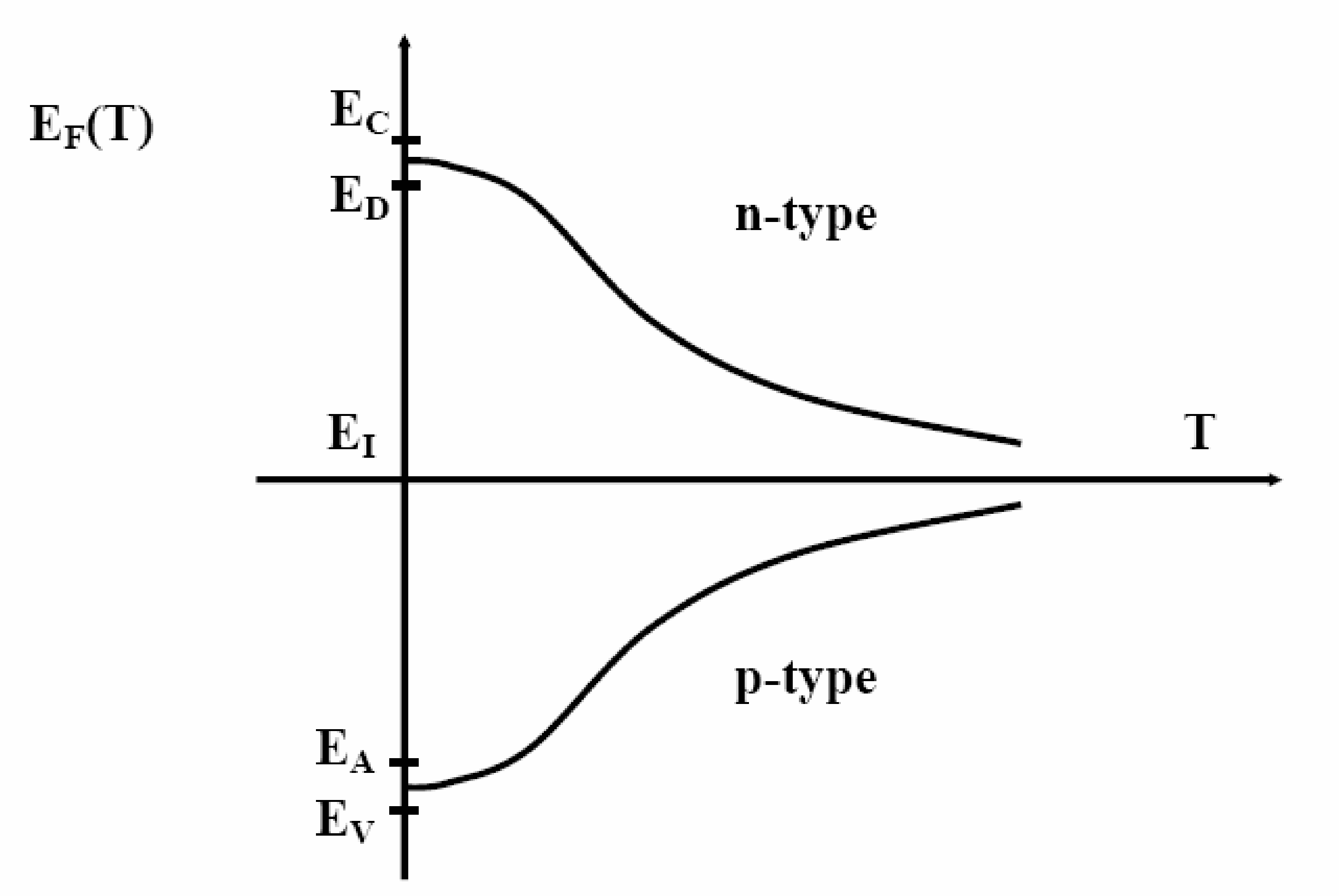
When we introduce dopant, the neutral dopant atom does not change the overall neutrality of the semiconductor.

Assuming 100% ionization of dopants, charge neutrality requires that: $n_0 + N_A^- = p_0 + N_D^+$

where $N_A^-$ and $N_D^+$ are ionized acceptor and donor concentrations, respectively.

$$\Rightarrow n_0 + N_A^- = \frac{n_i^2}{n_0} + N_D^+$$

# Temperature dependence



http://touch.caltech.edu/courses/EE40%20Web%20Files/Thermoelectric%20Notes.pdf

# Steady state vs. Equilibrium State

- Equilibrium refers to a condition of no external excitation except for temperature, and no net motion of charge.
- Steady state refers to a nonequilibrium condition in which all processes are constant and are balanced by opposing process.

# Quasi-Fermi level

For convenient, we introduce the concept of quasi-Fermi levels $E_{Fn}, E_{Fp}$ such that:

$$\begin{cases} n = n_0 + \Delta n = n_i \exp\left(\dfrac{E_{Fn} - E_{Fi}}{kT}\right) \\ p = p_0 + \Delta p = n_i \exp\left(\dfrac{E_{Fi} - E_{Fp}}{kT}\right) \end{cases}$$

Since

$$\begin{cases} n_0 = n_i \exp\left(\dfrac{E_F - E_{Fi}}{kT}\right) \\ p_0 = n_i \exp\left(\dfrac{E_{Fi} - E_F}{kT}\right) \end{cases}$$

Obviously, when the excess carrier concentration is small compare to the equilibrium carrier concentration, the quasi-Fermi level must be very close to the Fermi level. Otherwise it will be far from Fermi Level

For device operation, we often use a low-level injection condition, meaning that while the minority carrier concentration is changed, the majority carrier concentration remain un-affected. Thus the quasi-Fermi level of the majority carrier is the same as the Fermi level.

# References

- *Ben G. Streetman, Sanjay Banerjee* Solid state electronic devices, Fifth edition, Chapter 3,4,5
- *Chuang* Optielectronics,Chapter 2
- http://nina.ecse.rpi.edu/shur/SDM1/Notes/Noteshtm/07Concentr/Index.htm
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