Recitation Class for Mid I
Chapter 1-4

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Outline

Overview

Chapter 1 The Crystal Structure of Solids

Chapter 2 INtroduction to Quantum Mechanics

Chapter 3 Introduction to the Quantum Theory of Solids

Chapter 4 The semiconductor in Equilibrium

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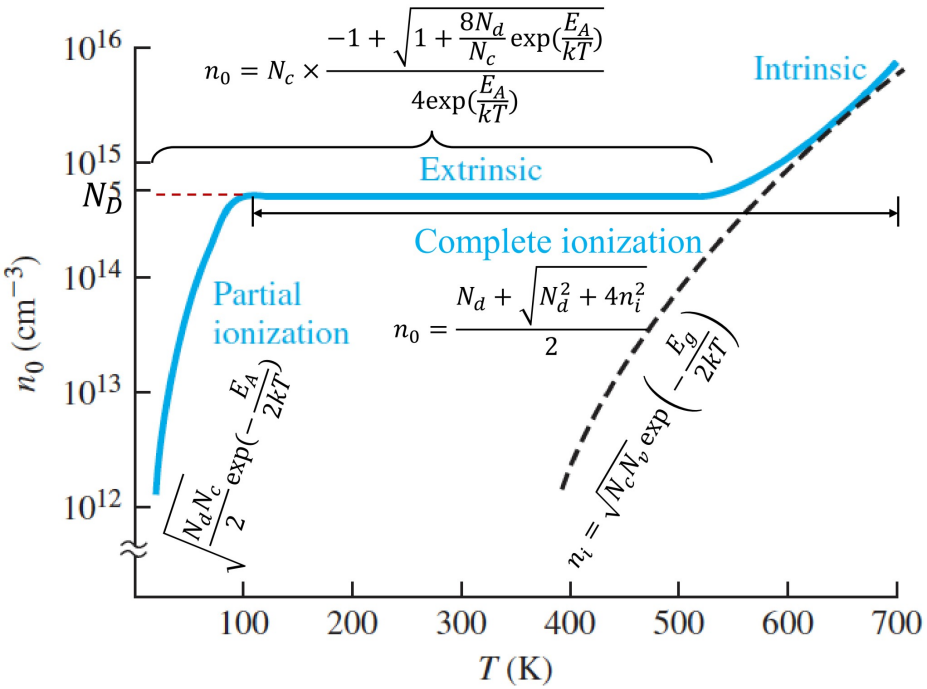
Overview

- **Chapter 5** Carrier Transport Phenomena

$$J = qn\mu_n E_x + qp\mu_p E_x + qD_n \nabla n + qD_p \nabla p$$

- **Chapter 4** The Semiconductor in Equilibrium



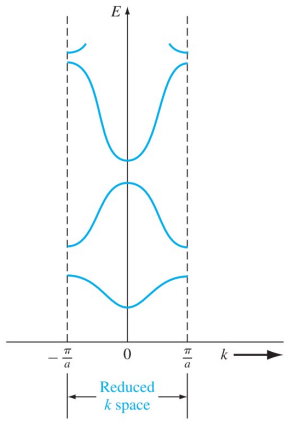
$$n_0 = \int_{E_c}^{\infty} g_c(E) f_F(E)\, \mathrm{d}E = N_c \exp\left(\frac{E_F - E_c}{kT}\right)$$

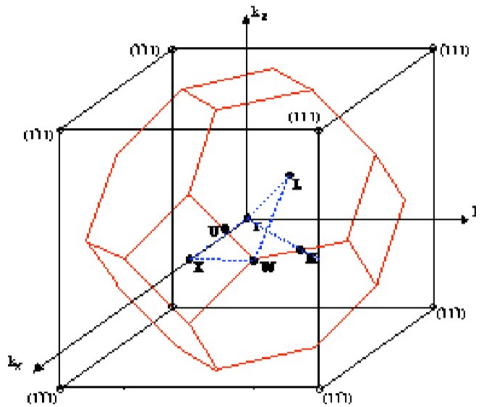
Overview

- **Chapter 3** Introduction to the Quantum Theory of Solids

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

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





Overview

- **Chapter 2** Quantum Mechanics

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

- **Chapter 1** Introduction

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Lattice types

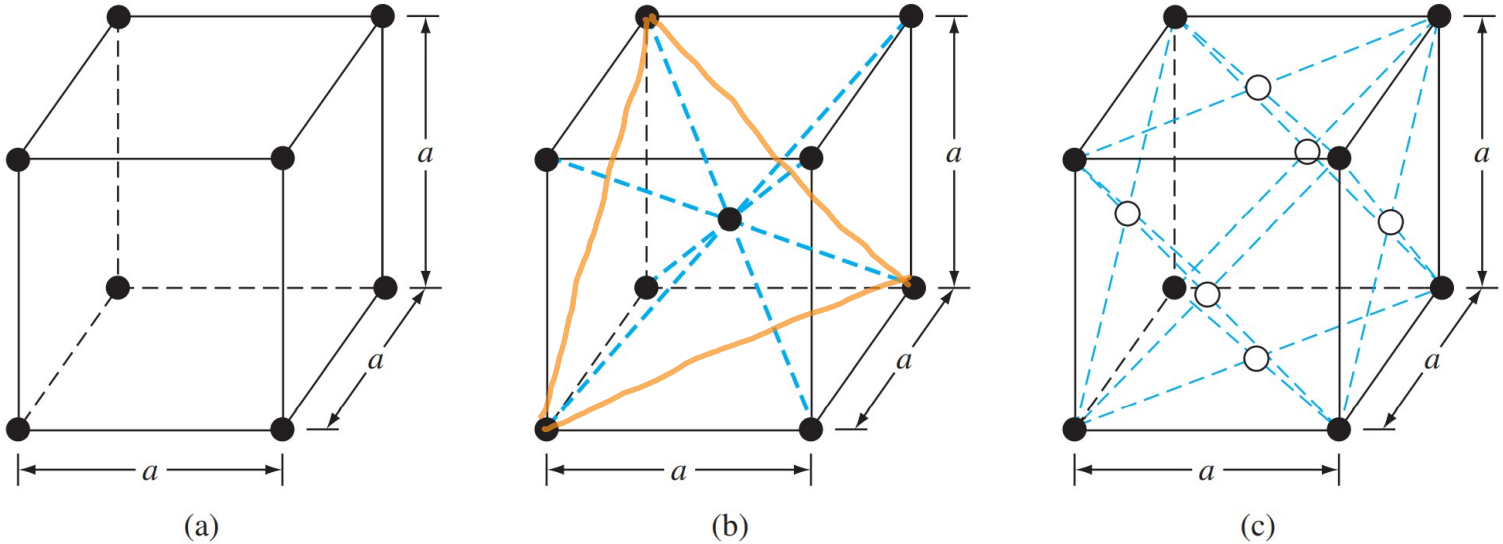


Figure: (a) simple cubic(sc), (b) body-centered cubic(bcc), (c) face-centered cubic(fcc)

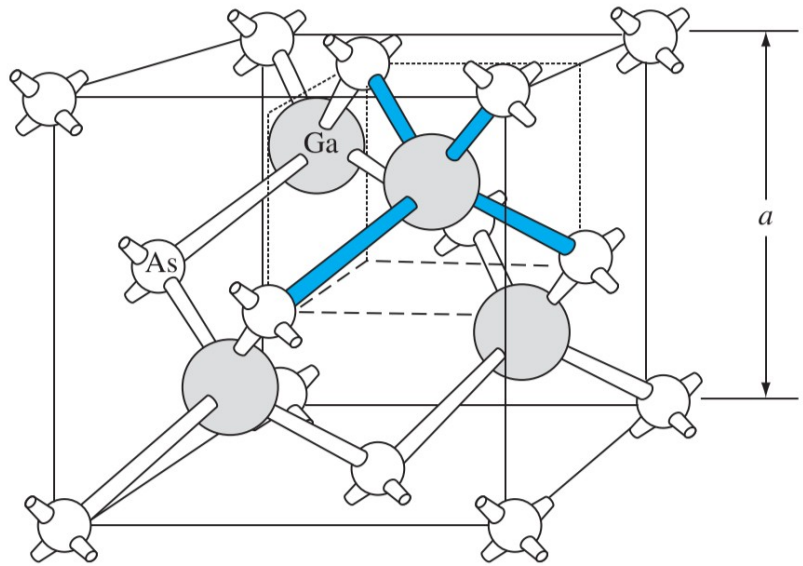
$$\#\text{number of atoms per unit cell}$$

$$\text{Volume Density} = \frac{\#\text{ atoms per unit cell}}{\text{volume of unit cell}}$$

$$\text{Surface Density} = \frac{\#\text{ atoms per lattice plane}}{\text{area of lattice plane}}$$

The diamond structure

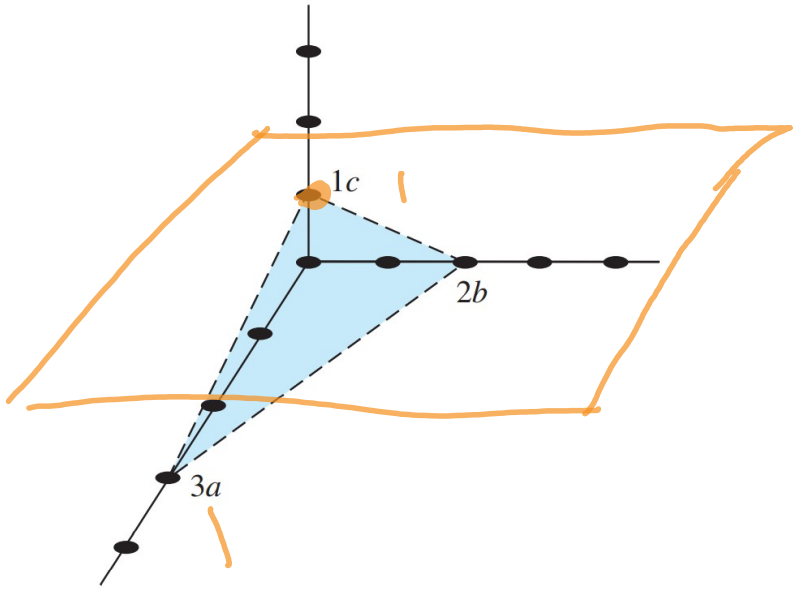
The diamond structure all atoms are of the same species
The zincblende structure two different types of atoms. e.g, GaAs.



Equivalent to two face-centered cubics sliding 1/4 diagonal length along a diagonal.

$$\#\text{ atoms per unit cell} = 8.$$

Crystalline Plane and Miller Index



$$(3, 2, 1) \xrightarrow{\text{Reciprocal}} \left(\frac{1}{3}, \frac{1}{2}, 1\right) \xrightarrow{\text{multiply lcd}} (2, 3, 6)$$

Any parallel plane is entirely equivalent to any other.
The $[hkl]$ direction is perpendicular to the (hkl) plane.

Example: Determine the Miller index of x-y plane.

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Infinite quantum well

$$-\frac{\hbar^2}{2m}\frac{\partial^2\Psi}{\partial x^2} + V(x)\Psi = E\Psi, \quad \begin{cases} V(x) = +\infty, & x \le 0 \text{ or } x \ge a \\ V(x) = 0, & 0 < x < a \end{cases}$$

General solution:

$$\Psi(x) = A\mathrm{e}^{-ikx} + B\mathrm{e}^{ikx}$$

Boundary condition:

$$\Psi(x)|_{x=a,0} = 0$$

$$\int_0^a \Psi(x)\Psi^*(x)\,\mathrm{d}x = 1$$

conclusion:

$$k = \frac{n\pi}{a}, n = 0, \pm1, \pm2, \ldots$$

$$E = \frac{k^2\hbar^2}{2m} = \frac{n^2\pi^2\hbar^2}{2ma^2}$$

Finite quantum well

$$-\frac{\hbar^2}{2m}\frac{\partial^2\Psi}{\partial x^2}+V(x)\Psi=E\Psi,\quad \begin{cases} V(x)=V_0, & x\le 0 \text{ or } x\ge a \\ V(x)=0, & 0<x<a \end{cases}$$

General solution:

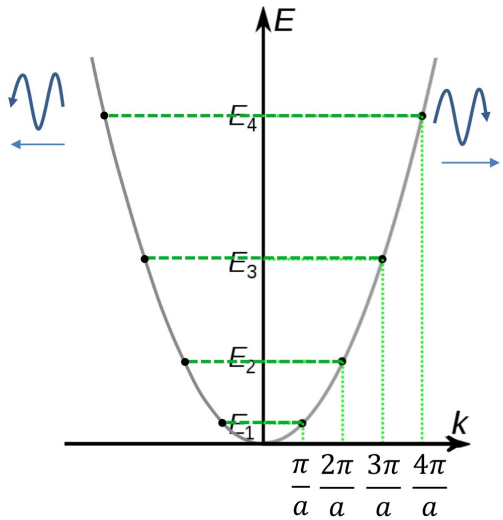
$$\Psi(x)=\begin{cases} Ae^{-ik_1x}+Be^{ik_1x}, & k_1=\sqrt{\frac{2m(E-V_0)}{\hbar^2}}, \quad x\le 0 \text{ or } x\ge a \\ Ce^{-ik_2x}+De^{ik_2x}, & k_2=\sqrt{\frac{2mE}{\hbar^2}}, \quad 0<x<a \end{cases}$$

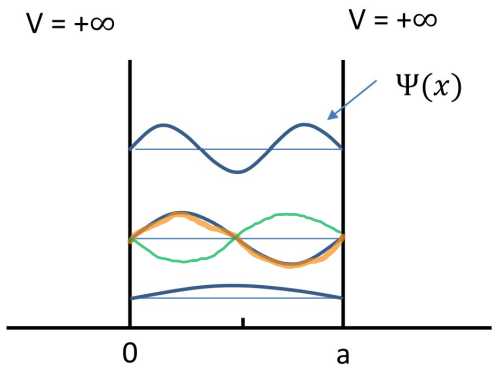
Boundary condition:

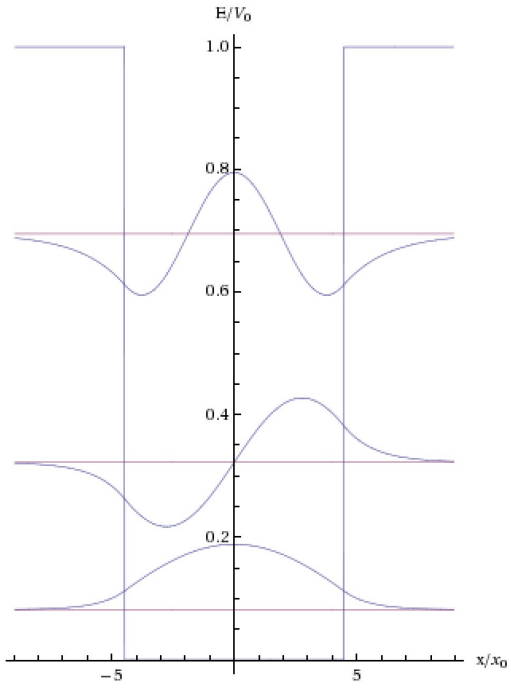
$$\Psi(x)|_{x=0} \text{ continuous}$$
$$\Psi(x)|_{x=a} \text{ continuous}$$
$$\int_{-\infty}^{\infty}\Psi(x)\Psi^*(x)\,dx=1$$

Note: depending on the relationship between E and V_0, $\Psi(x)$ is different.

Energy bands







For same energy level, the k can have two values, Because the wave can move to positive and negative directions.

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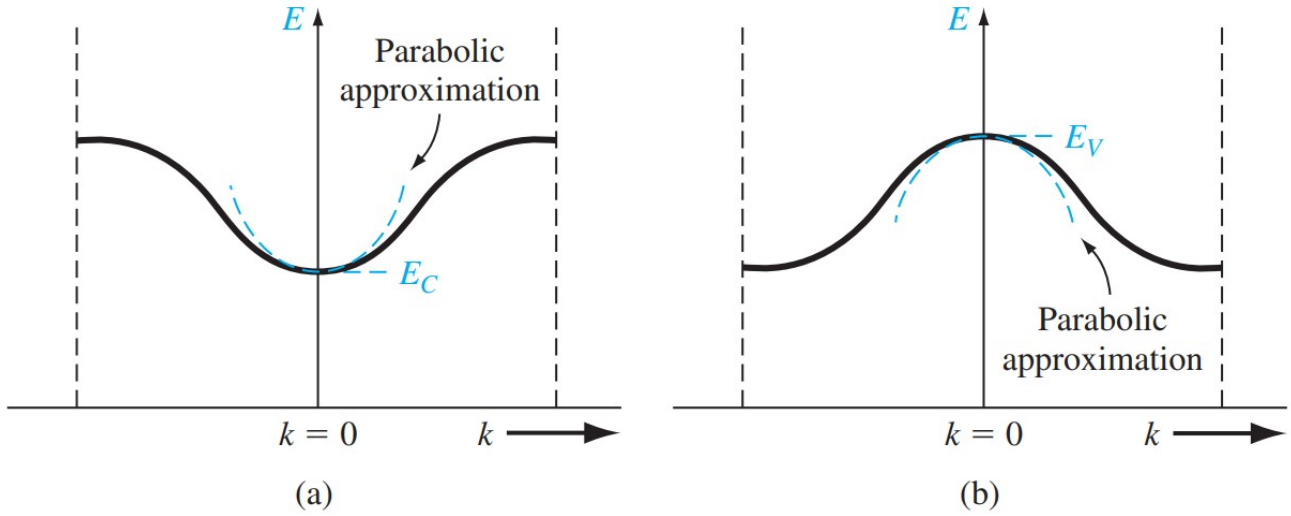
Effective mass



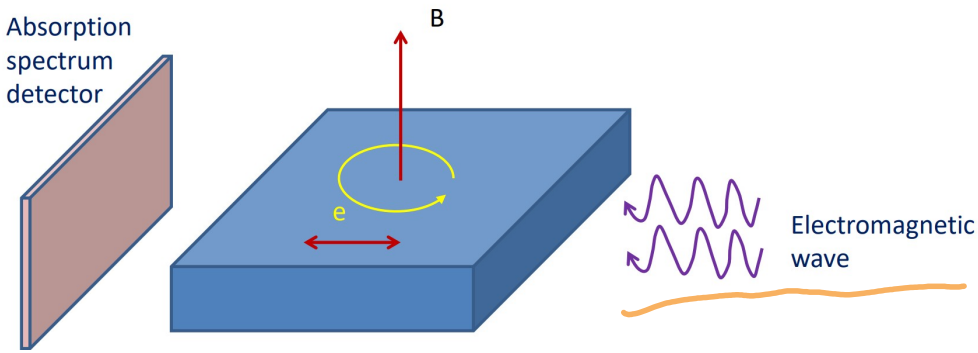
$$\boxed{\frac{1}{\hbar^2}\frac{\mathrm{d}^2E}{\mathrm{d}k^2} = \frac{2C_1}{\hbar^2} = \frac{1}{m^*}}$$

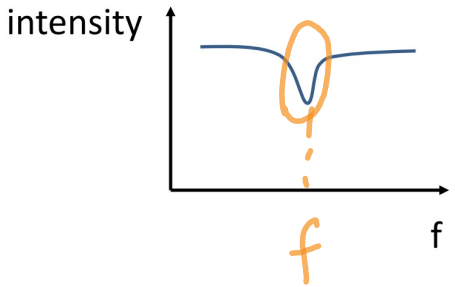
$$E = E(k) = E_c + \frac{\hbar^2}{2m_n^*}(k - k_1)^2$$

$$E = E(k) = E_v - \frac{\hbar^2}{2m_p^*}(k - k_2)^2$$

Effective Mass: experimentally

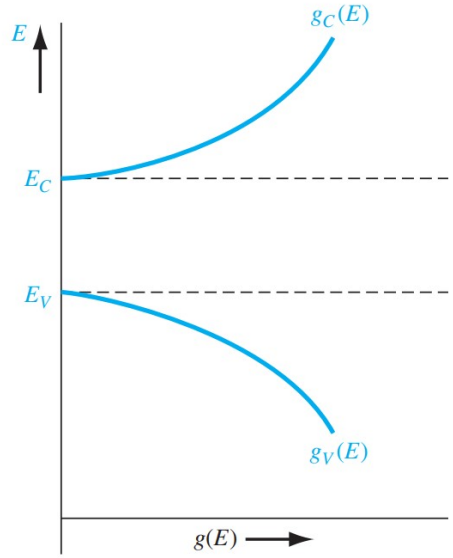
Cyclotron resonance





$$m^* = \frac{eB\lambda}{2\pi c}$$

Density of States Function



$$\int g(E)$$

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

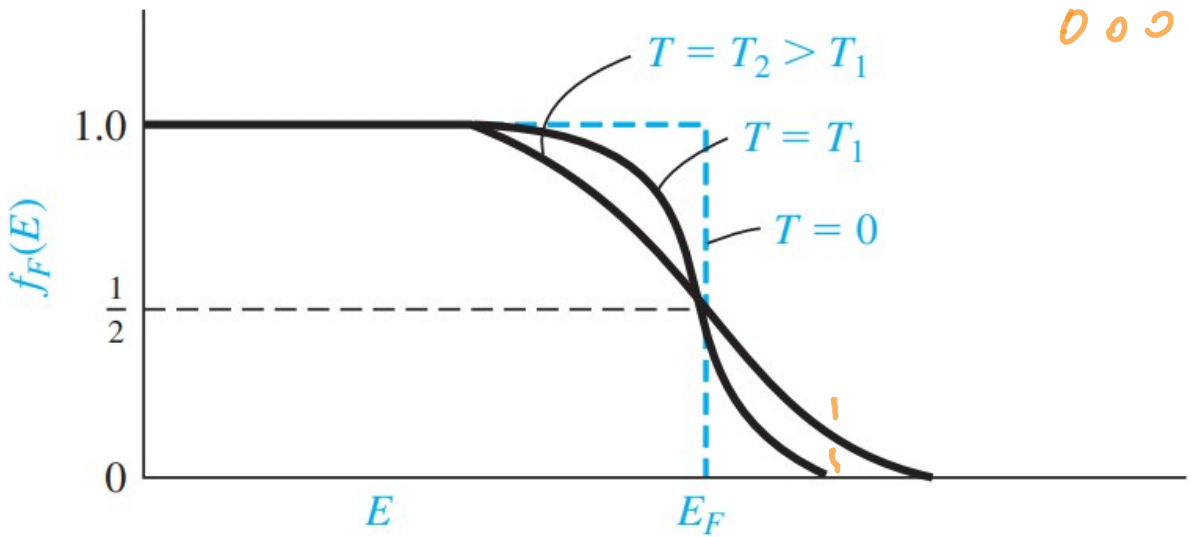
$$g_c(E) = \frac{4\pi(2m_n^*)^{\frac{3}{2}}}{h^3}\sqrt{E - E_c}$$

$$g_v(E) = \frac{4\pi(2m_p^*)^{\frac{3}{2}}}{h^3}\sqrt{E_v - E}$$

Distribution Function

- Fermi-Dirac probability function:

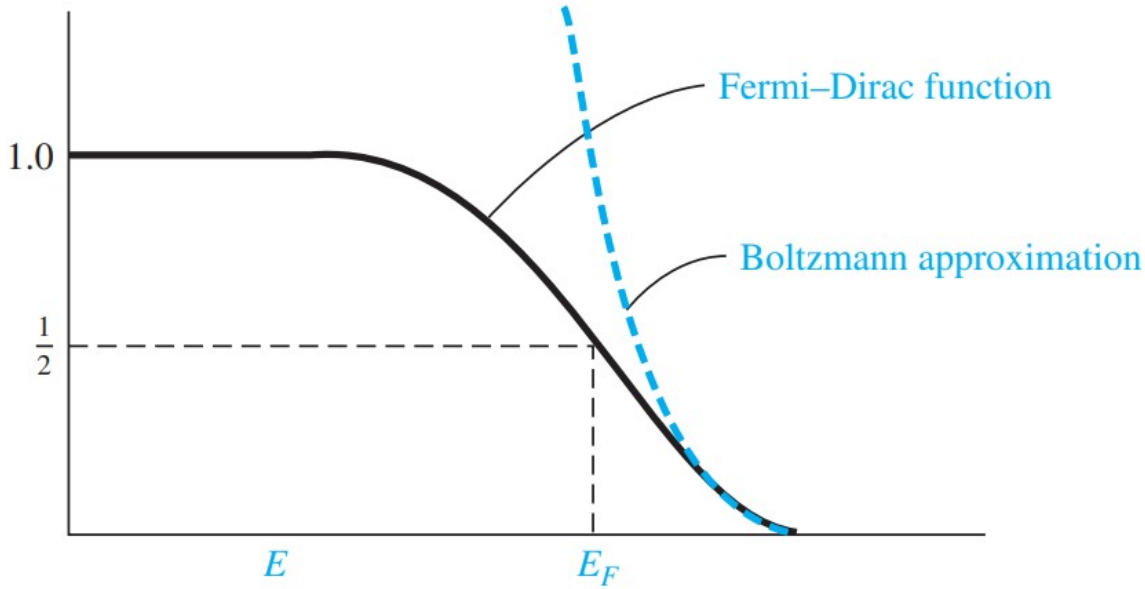
$$f_F(E) = \frac{1}{1 + \exp\left(\frac{E - E_F}{kT}\right)}$$



Distribution Function

- Boltzmann distribution
  When $\exp\left(\frac{E-E_F}{kT}\right) >> 1 \Rightarrow E - E_F > 3kT$

$$f_F(E) \approx exp\left(-\frac{E - E_F}{kT}\right)$$



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n_0 and p_0 Equations

$$n_0 = \int_{E_c}^{\infty} g_c(E) f_F(E)\, \mathrm{d}E$$

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

$$p_0 = \int_{-\infty}^{E_v} g_v(E)\,(1 - f_F(E))\, \mathrm{d}E$$

$$\Rightarrow \quad \boxed{p_0 = N_v \exp\left[\frac{-(E_F - E_v)}{kT}\right], \quad N_v = 2\left(\frac{2\pi m_p^* kT}{h^2}\right)^{3/2}}$$

$$\underline{kT = 0.0259 \text{ only for } T = 300K}$$

Always be careful about the temperature!

$T = 400K$

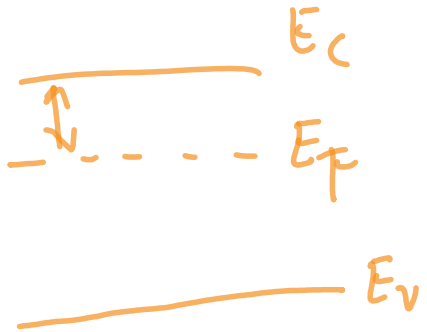
Intrinsic Semiconductor

$$n_0 p_0 = n_i^2 = N_c N_v \exp\left[\frac{-(E_c - E_v)}{kT}\right] = N_c N_v \exp\left[\frac{-E_g}{kT}\right]$$

$$E_{Fi} - E_{midgap} = \frac{1}{2} kT \ln\left(\frac{N_v}{N_c}\right) = \frac{3}{4} kT \ln\left(\frac{m_p^*}{m_n^*}\right)$$

Self-consistency

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



For Si at $300K$:

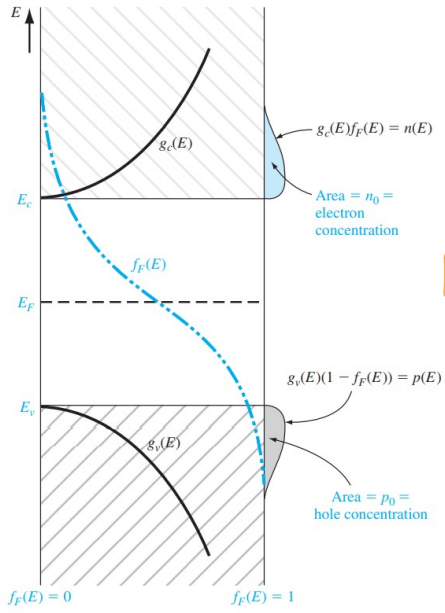
$$n_i = 1.5 \times 10^{10} cm^{-3},$$
$$E_g = 1.12eV,$$
$$N_c = 2.8 \times 10^{19} cm^{-3},$$
$$N_v = 1.04 \times 10^{19} cm^{-3},$$
$$kT = 0.0259eV$$

p_0

$$LHS = 2.25 \times 10^{20} \neq 4.82936 \times 10^{19} = RHS$$

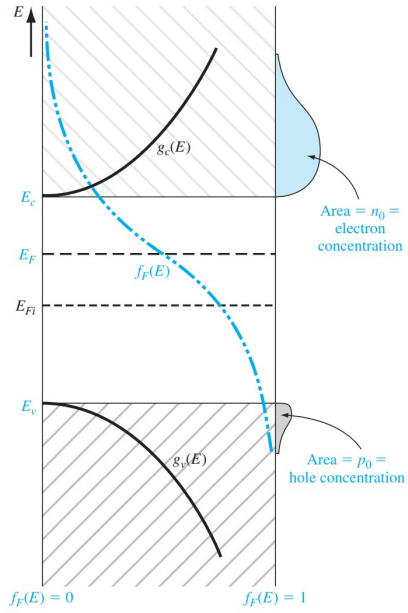
Write down the steps with all equations and constants used!

The Extrinsic Semiconductor



$$E_F = \frac{E_c + E_v}{2}$$

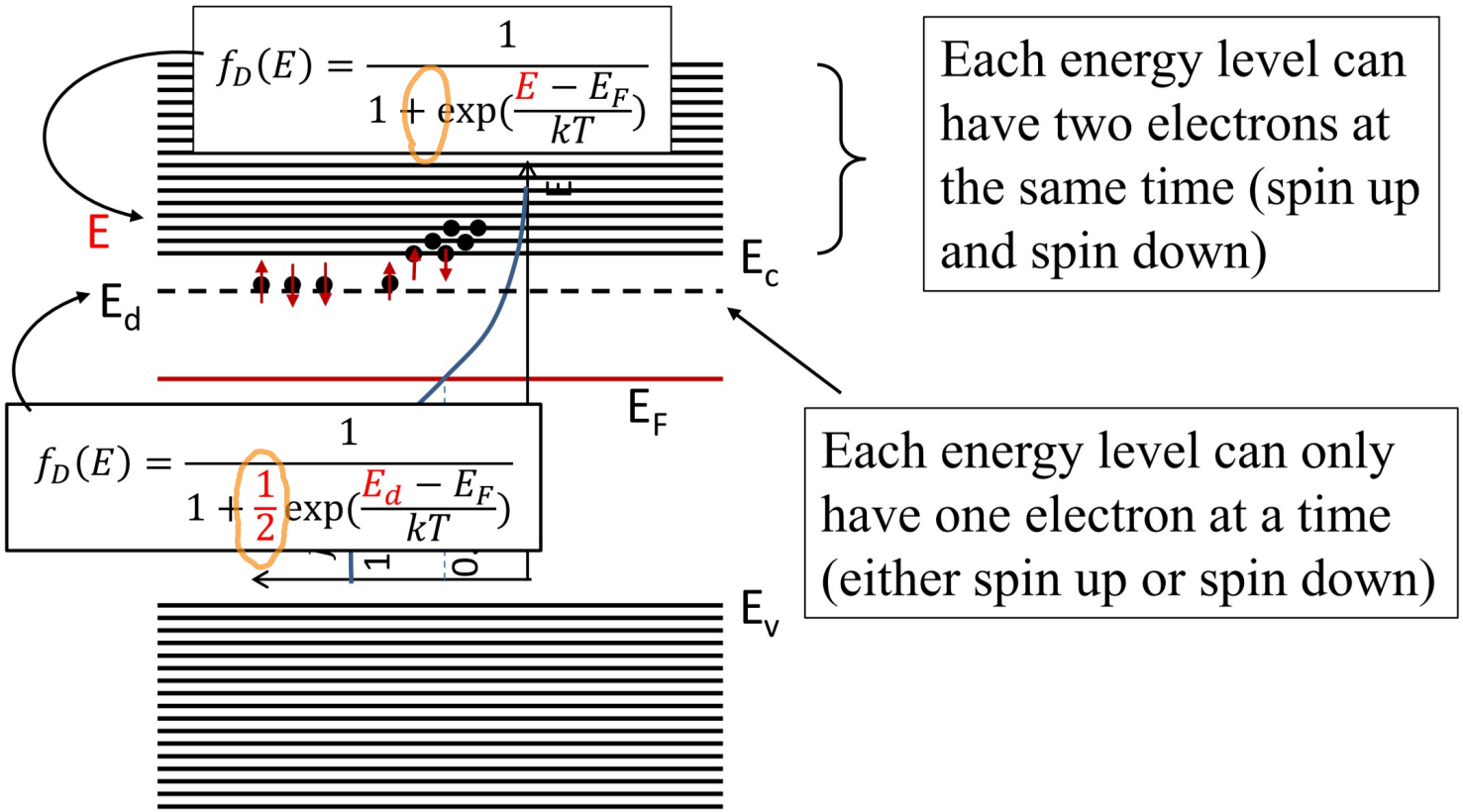
(a) Intrinsic



(b) n-type semiconductor

$$n_0 p_0 = N_c N_v \exp\left(-\frac{E_g}{kT}\right) = n_i^2$$

Statistics of Donors and Acceptors



Statistics of Donors and Acceptors

$$f_d(E) = \frac{1}{1 + \frac{1}{2}\exp\left(\frac{E_d - E_F}{kT}\right)}$$

$$n_d = f_d(E)N_d = N_d - N_d^+$$

where N_d^+ is the concentration of ionized donors.

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

$1/g$ is the degeneracy factor, normally taken as 4 for acceptor level in silicon and gallium arsenide (because of detailed band structure).

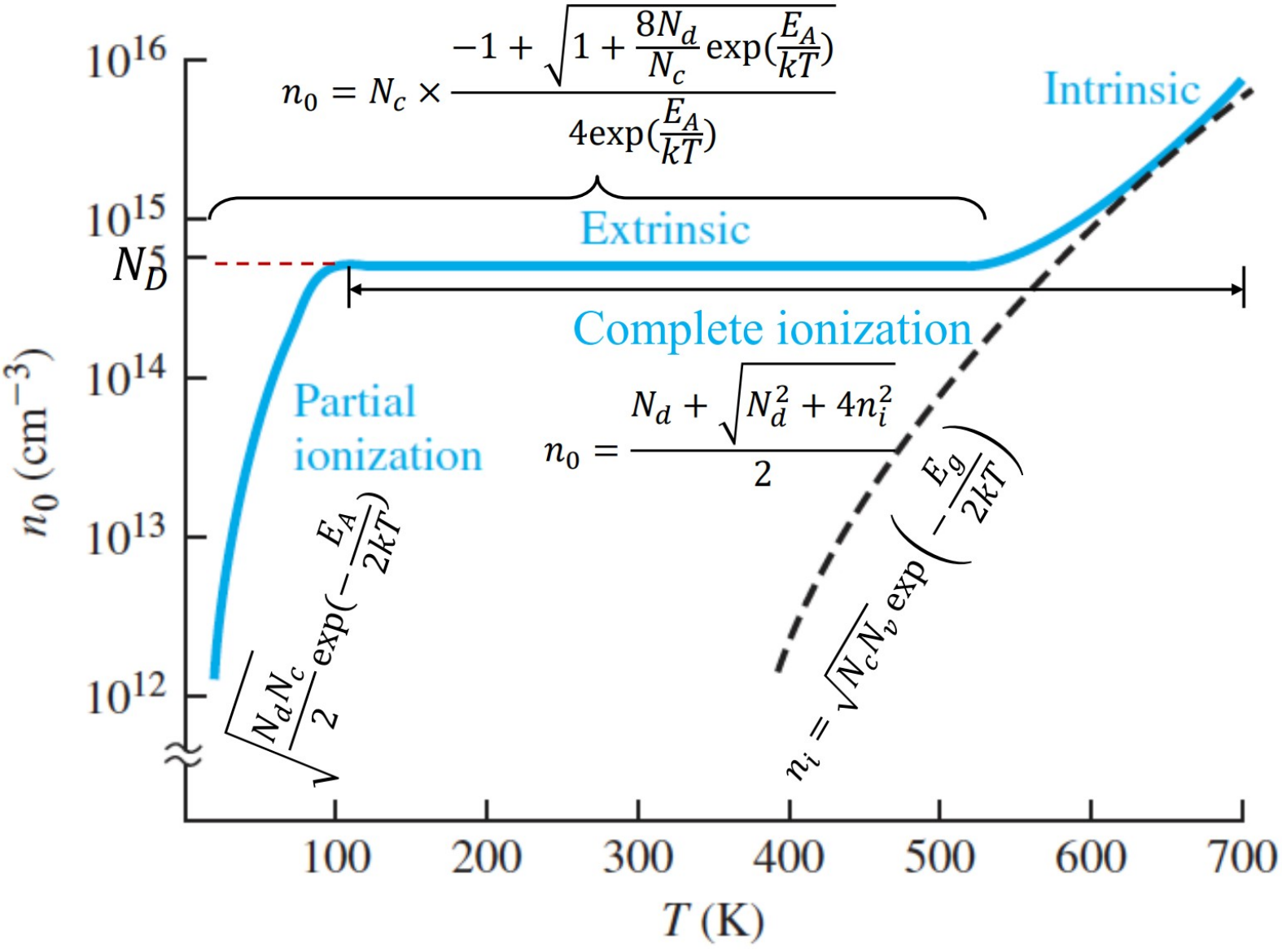
$$p_a = f_a(E)N_a = N_a - N_a^+$$

Statistics of Donors and Acceptors

We calculate the relative number of electrons in the donor state compared with the total number of electrons: (assuming $(E_d - E_F) \gg kT$)

$$\frac{n_d}{n_d + n_0} = \frac{1}{1 + \frac{N_c}{2N_d} \exp\left[\frac{-(E_c - E_d)}{kT}\right]}$$

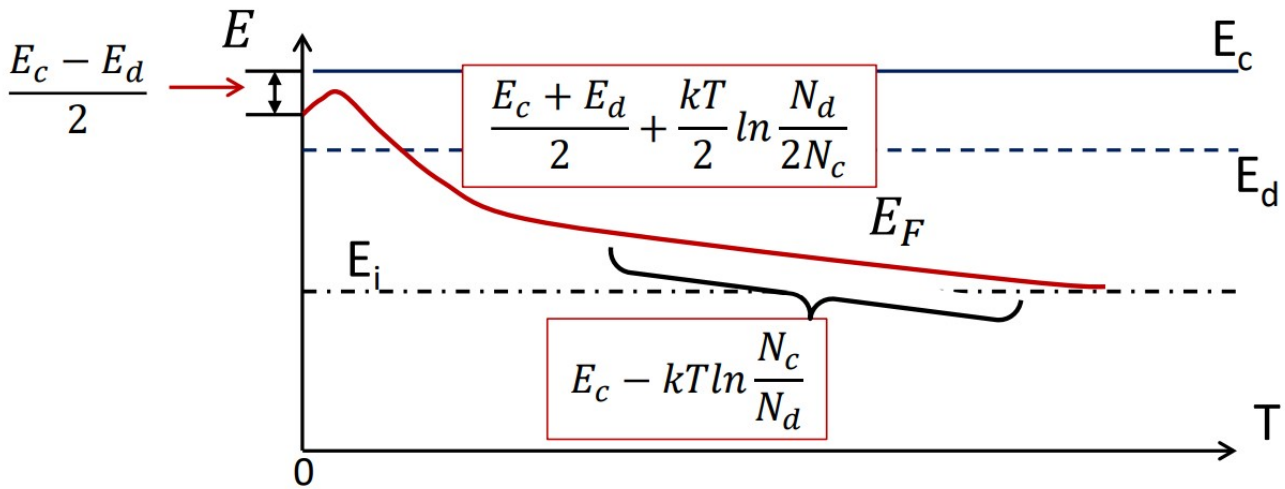
Example: Determine the fraction of total electrons still in the donor states at $T = 300K$. Consider phosphorus doping in silicon, for $T = 300K$, at a concentration of $N_d = 10^{16} cm^{-3}$.
Answer: 0.41%. Very few electrons remains in the donor states (completely ionized).


$n_0 = N_c \times \frac{-1 + \sqrt{1 + \frac{8N_d}{N_c}\exp(\frac{E_A}{kT})}}{4\exp(\frac{E_A}{kT})}$
Intrinsic
Extrinsic
Complete ionization
Partial ionization
$n_0 = \frac{N_d + \sqrt{N_d^2 + 4n_i^2}}{2}$
$\sqrt{\frac{N_d N_c}{2}}\exp(-\frac{E_A}{2kT})$
$n_i = \sqrt{N_c N_v}\exp\left(-\frac{E_g}{2kT}\right)$
10^{16}
10^{15}
N_D
10^{14}
10^{13}
10^{12}
n_0 (cm^{-3})
100
200
300
400
500
600
700
T (K)

Fermi Level Position

$$E_F = E_c + kT \ln \left(\frac{\sqrt{1 + \frac{8N_d}{N_c} \exp\left(\frac{E_A}{kT}\right)} - 1}{4 \exp\left(\frac{E_A}{kT}\right)} \right)$$

$$= \begin{cases} \frac{E_c + E_D}{2} + \frac{kT}{2} \ln \frac{N_d}{2N_c}, & T \text{ small} \\ E_c - kT \ln \frac{N_c}{N_d}, & T \text{ big} \end{cases}$$



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