Semiconductor Devices

Chapter 3
Introduction to the Quantum Theory of Solids

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Formation of Energy Bands

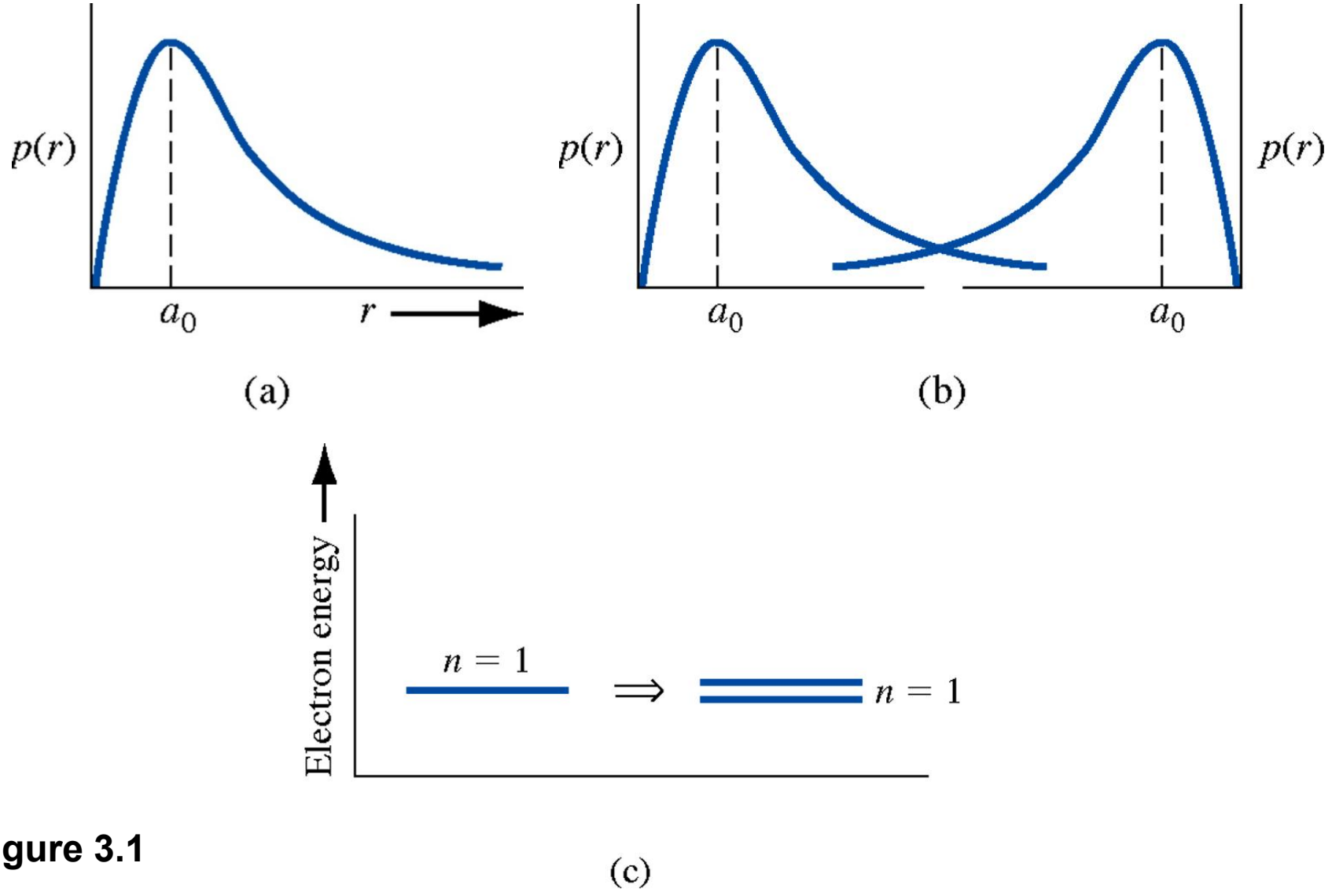
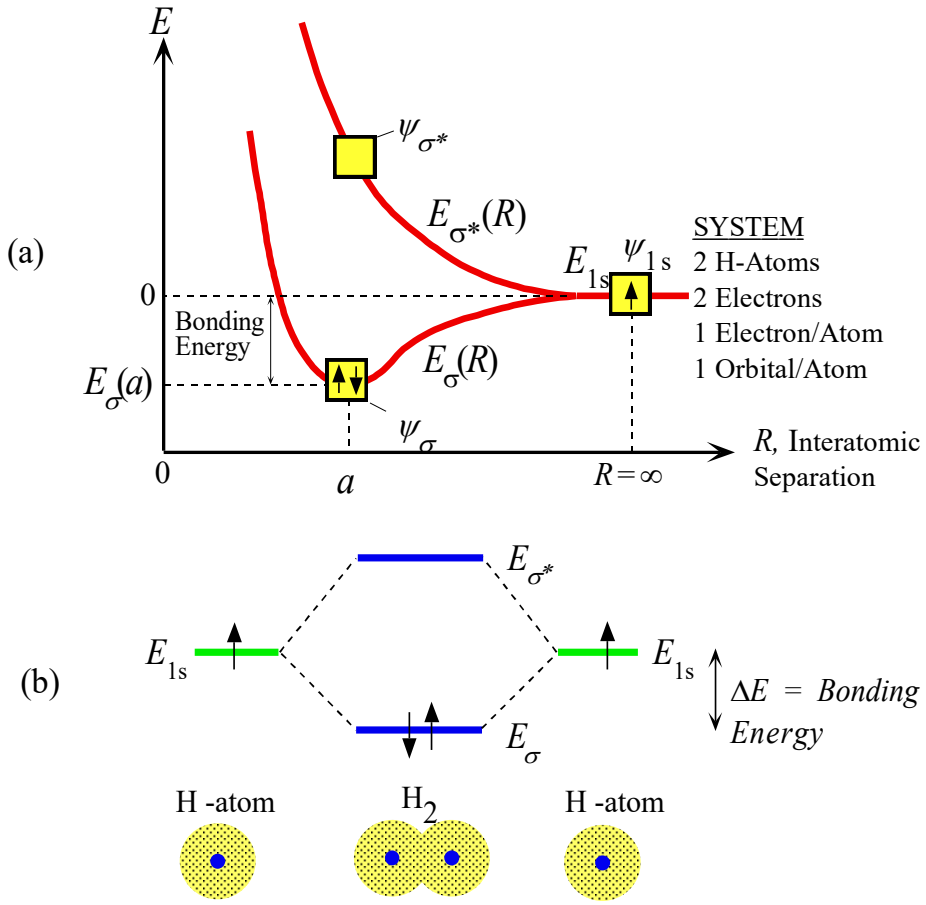


Figure 3.1

Formation of Energy Bands



Formation of Energy Bands

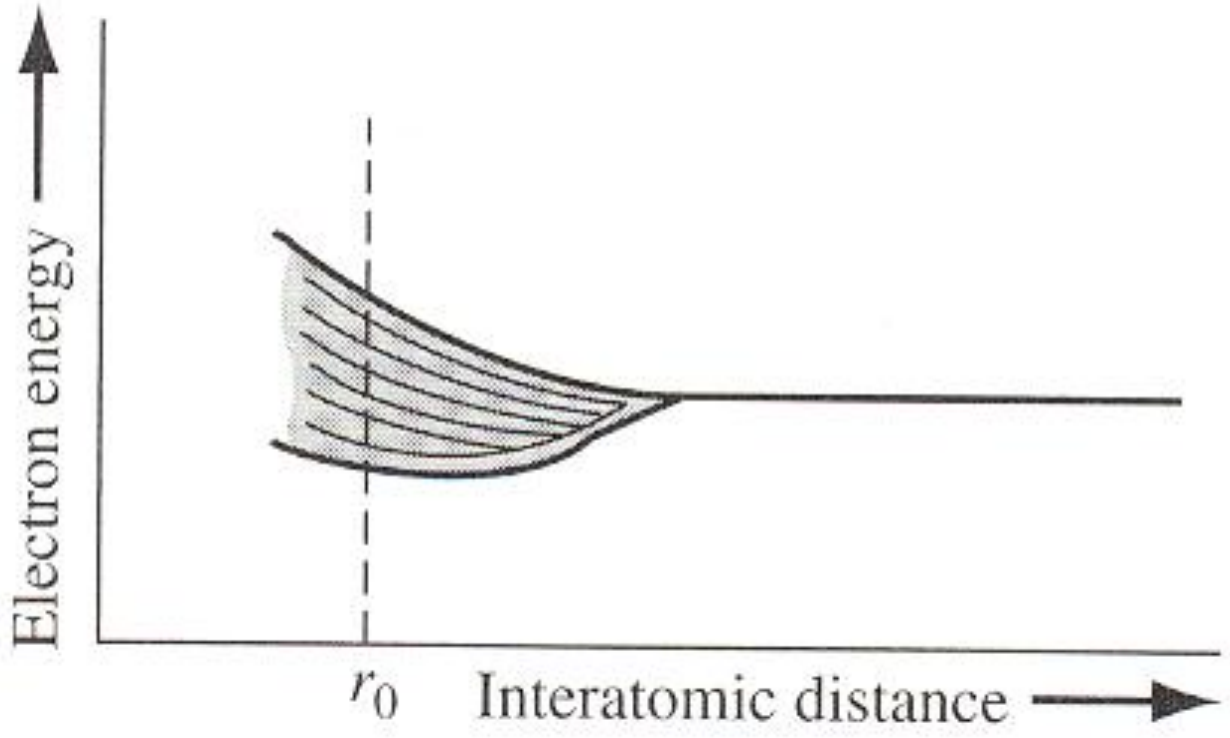


Figure 3.2 | The splitting of an energy state into a band of allowed energies.

Formation of Energy Bands

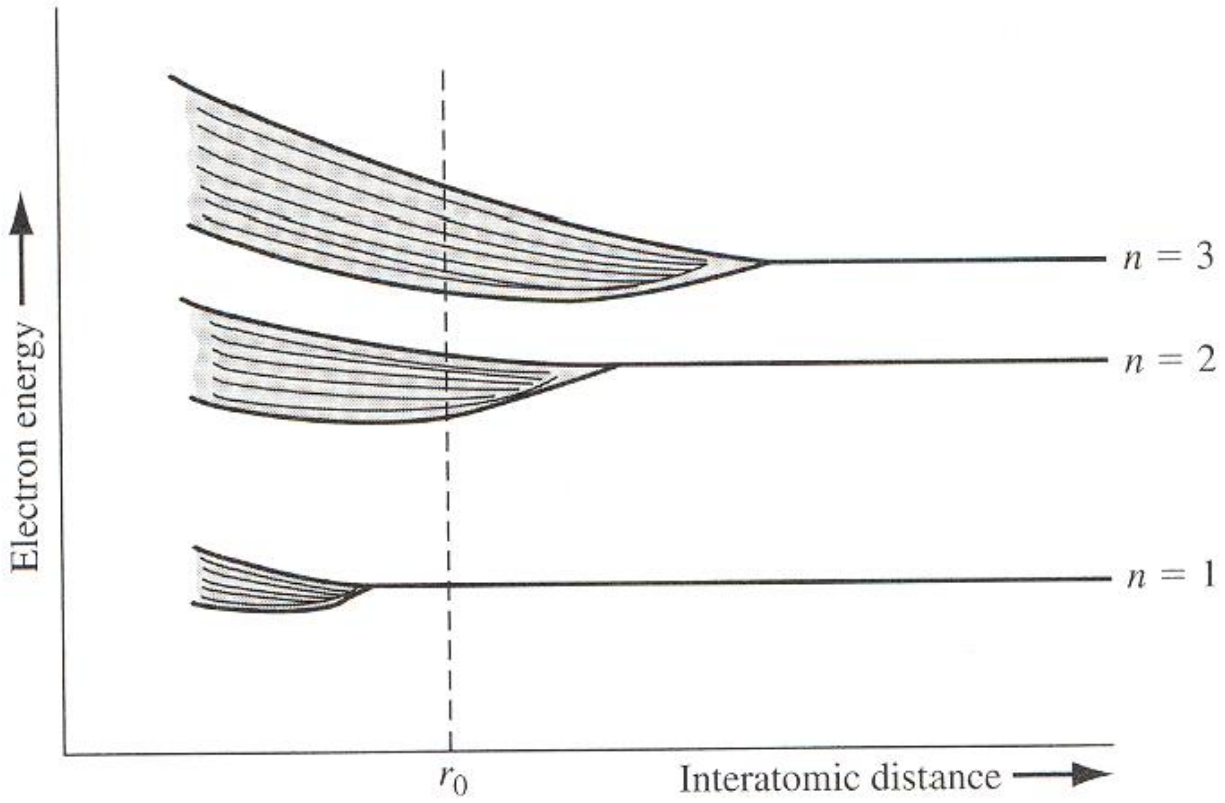


Figure 3.3 | Schematic showing the splitting of three energy states into allowed bands of energies.

Formation of Energy Bands for Si

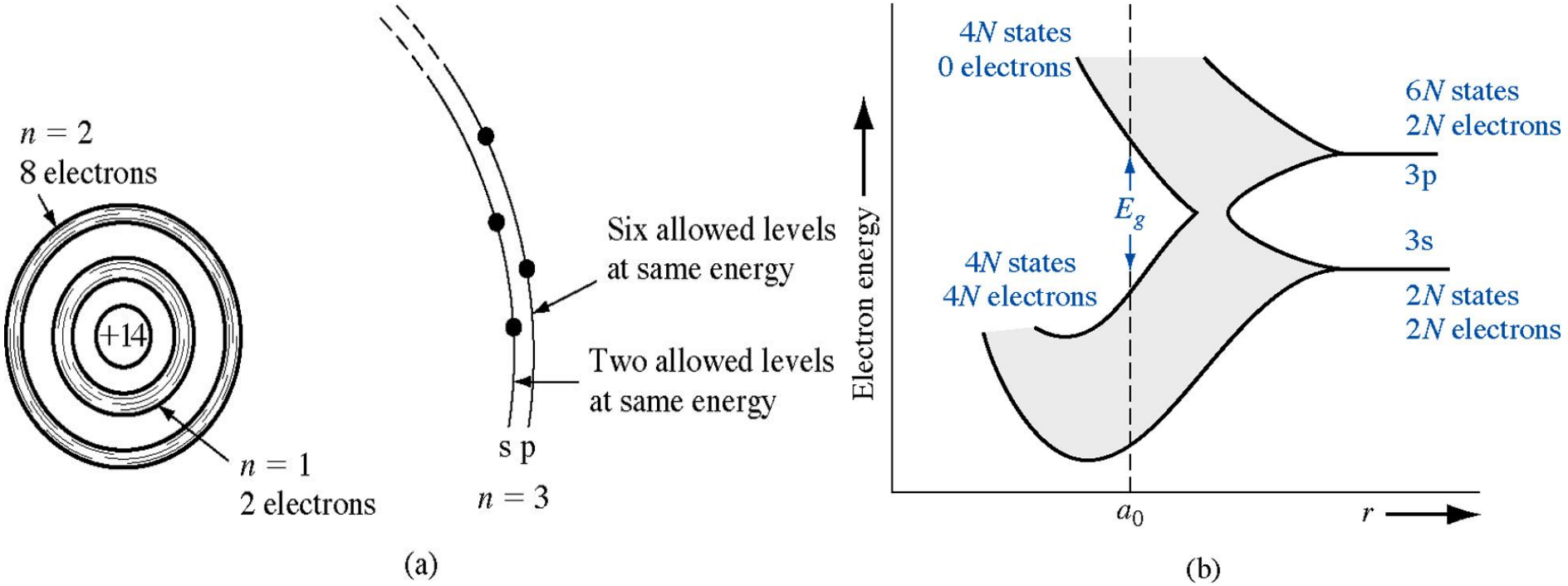
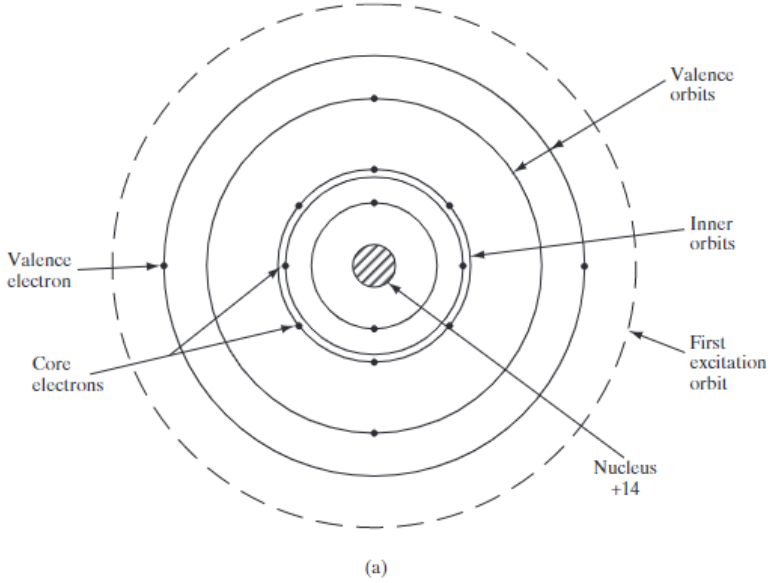
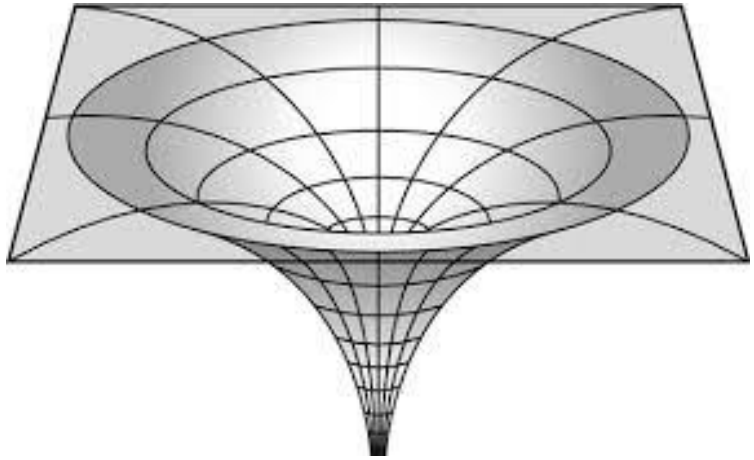
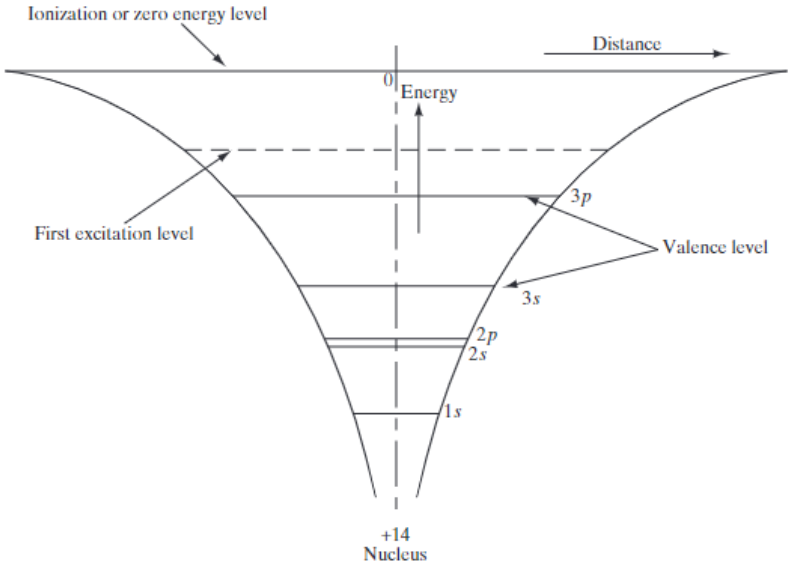


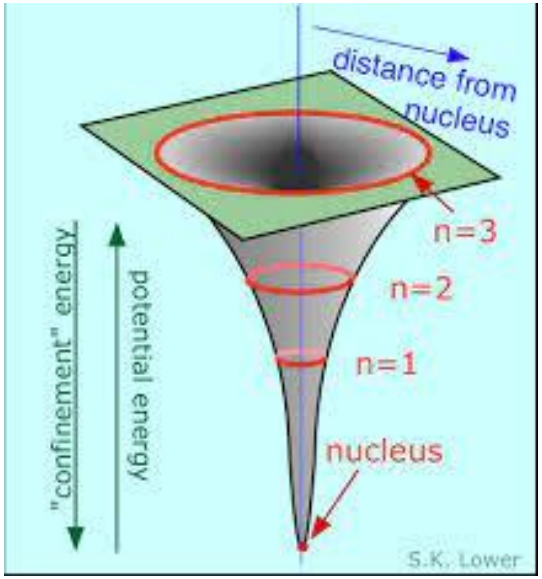
Figure 3.4

Formation of Energy Bands for Si

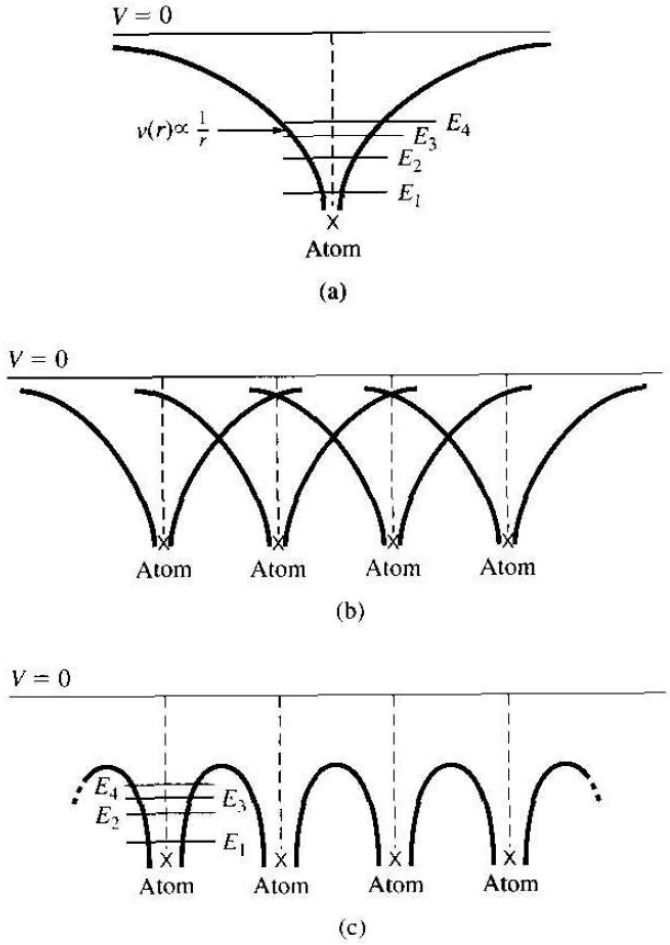








Kronig-Penney model



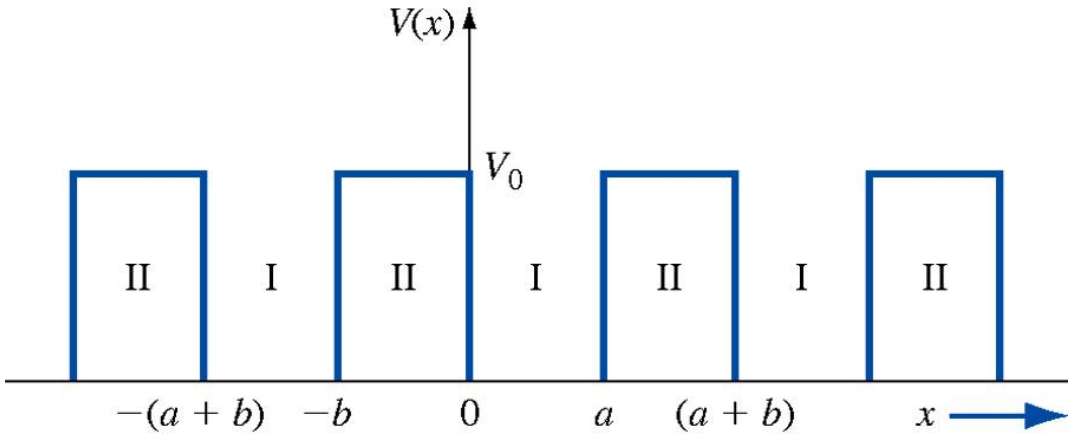


Figure 3.5

Kronig-Penney model
(Schrödinger's wave equation analysis for stepwise potential barrier)

$$\frac{d^2\psi(x)}{dx^2} + \frac{2m^*E}{\hbar^2}\psi(x) = 0$$

$$\psi(x) = Ae^{+jk_1x} + Be^{-jk_1x}$$

$$k_1 = \sqrt{\frac{2m^*E}{\hbar^2}}$$

$$\frac{d^2\psi(x)}{dx^2} + \frac{2m^*}{\hbar^2}(E - V(x))\psi(x) = 0$$

$$\psi(x) = Ce^{+jk_2x} + De^{-jk_2x}$$

$$k_2 = \sqrt{\frac{2m^*(V_0 - E)}{\hbar^2}}$$

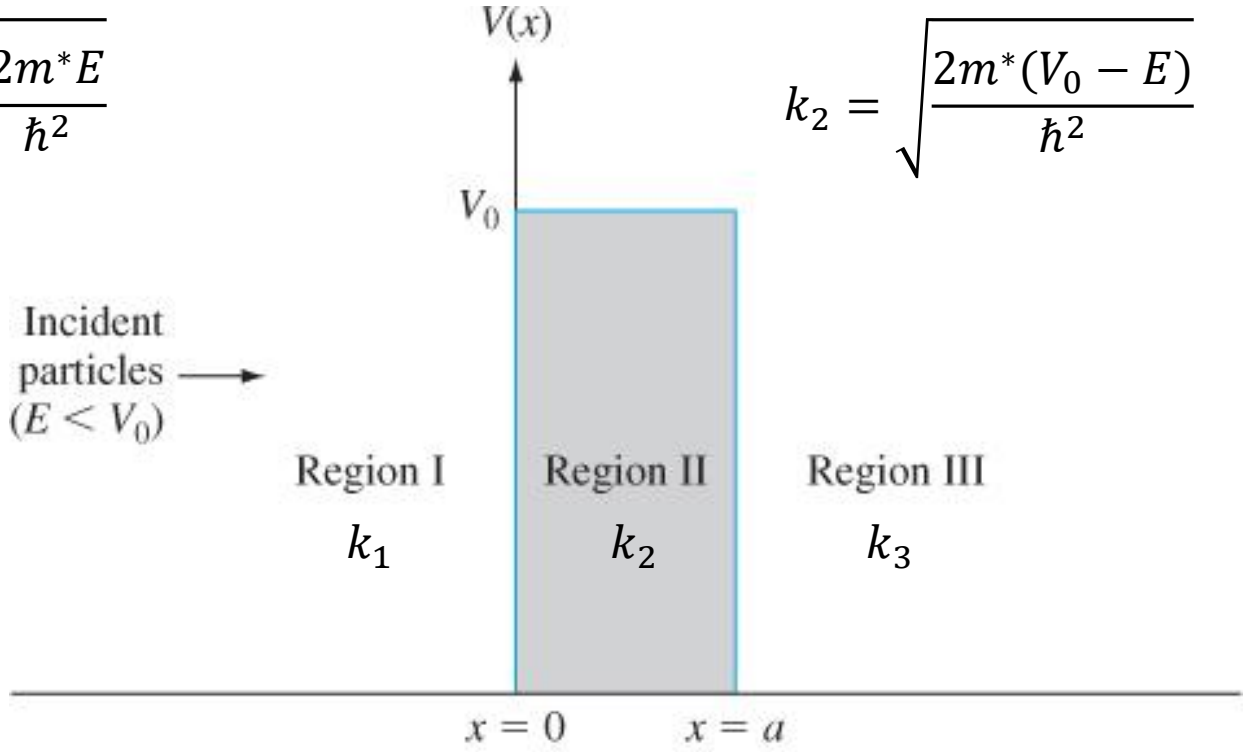
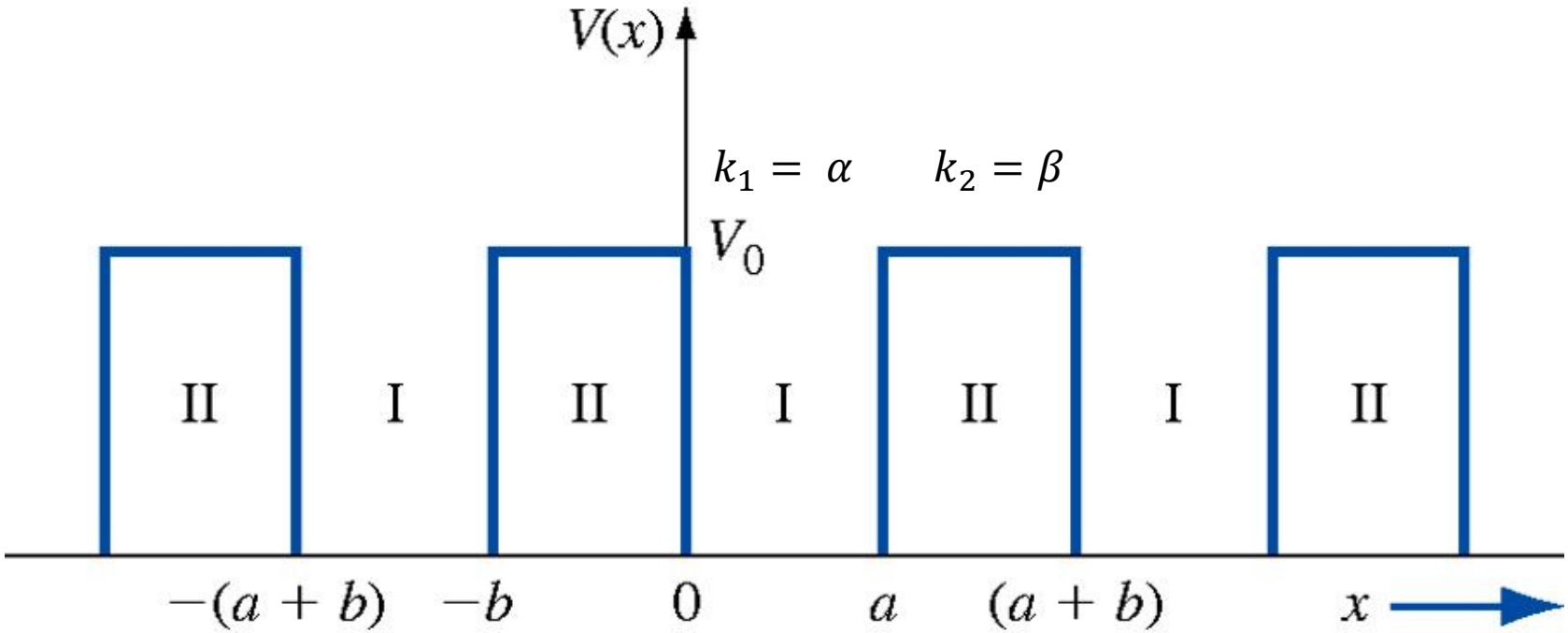


Figure 2.9 | The potential barrier function.

Kronig-Penney model



$$\psi(x) = Ae^{+j\alpha x} + Be^{-j\alpha x}$$

$$\psi(x) = Ce^{+j\beta x} + De^{-j\beta x}$$

Kronig-Penney model

$$P'\frac{\sin \alpha a}{\alpha a} + \cos \alpha a = \cos ka \qquad P' = \frac{m^* V_0 ba}{\hbar^2} \qquad (3.24)$$

Equation(3.24) again gives the relation between the parameter k, total energy E (through the parameter α), and the potential barrier bV_0. We may note that Equation(3.24) is not a solution of Schrodinger's wave equation but gives the conditions for which Schrodinger's wave equation will have a solution.

The k-space Diagram

For Free electron case,

$$P' = 0, \qquad \cos \alpha a = \cos ka \tag{3.25}$$

$$V_0 = 0 \rightarrow P' = \frac{m^* V_0 b a}{\hbar^2} = 0$$

$$\alpha = k \tag{3.26}$$

$$\alpha = \sqrt{\frac{2m^* E}{\hbar^2}} = \sqrt{\frac{2m^* (\frac{1}{2} m^* v^2)}{\hbar^2}} = \frac{p}{\hbar} = k \tag{3.27}$$

$$E = \frac{p^2}{2m^*} = \frac{k^2 \hbar^2}{2m^*} \tag{3.28}$$

The k-space Diagram

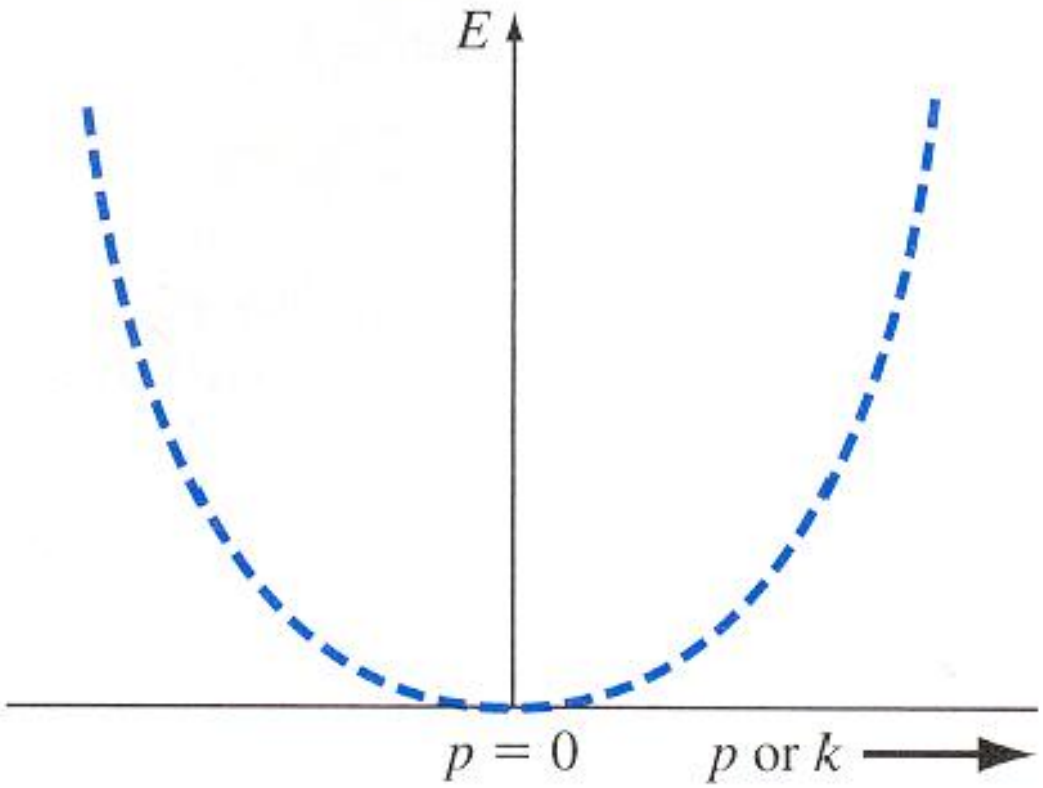


Figure 3.7 | The parabolic E versus k curve for the free electron.

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

The k-space Diagram

For confined electron case,

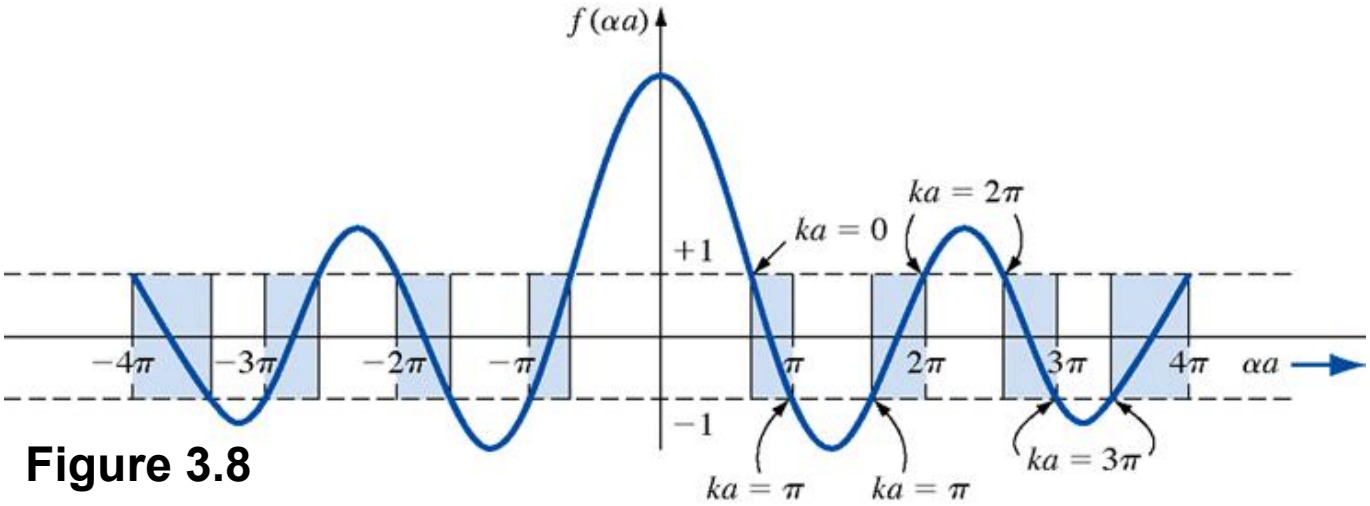


Figure 3.8

$$f(\alpha a) = P' \frac{\sin \alpha a}{\alpha a} + \cos \alpha a = \cos ka$$

$$f(\alpha a) = \cos ka \qquad \text{(3.29)~(3.30)}$$

$$-1 \le f(\alpha a) \le +1 \qquad \alpha = \sqrt{\frac{2m^* E}{\hbar^2}}, \qquad E = \frac{\alpha^2 \hbar^2}{2m^*}$$

The k-space Diagram

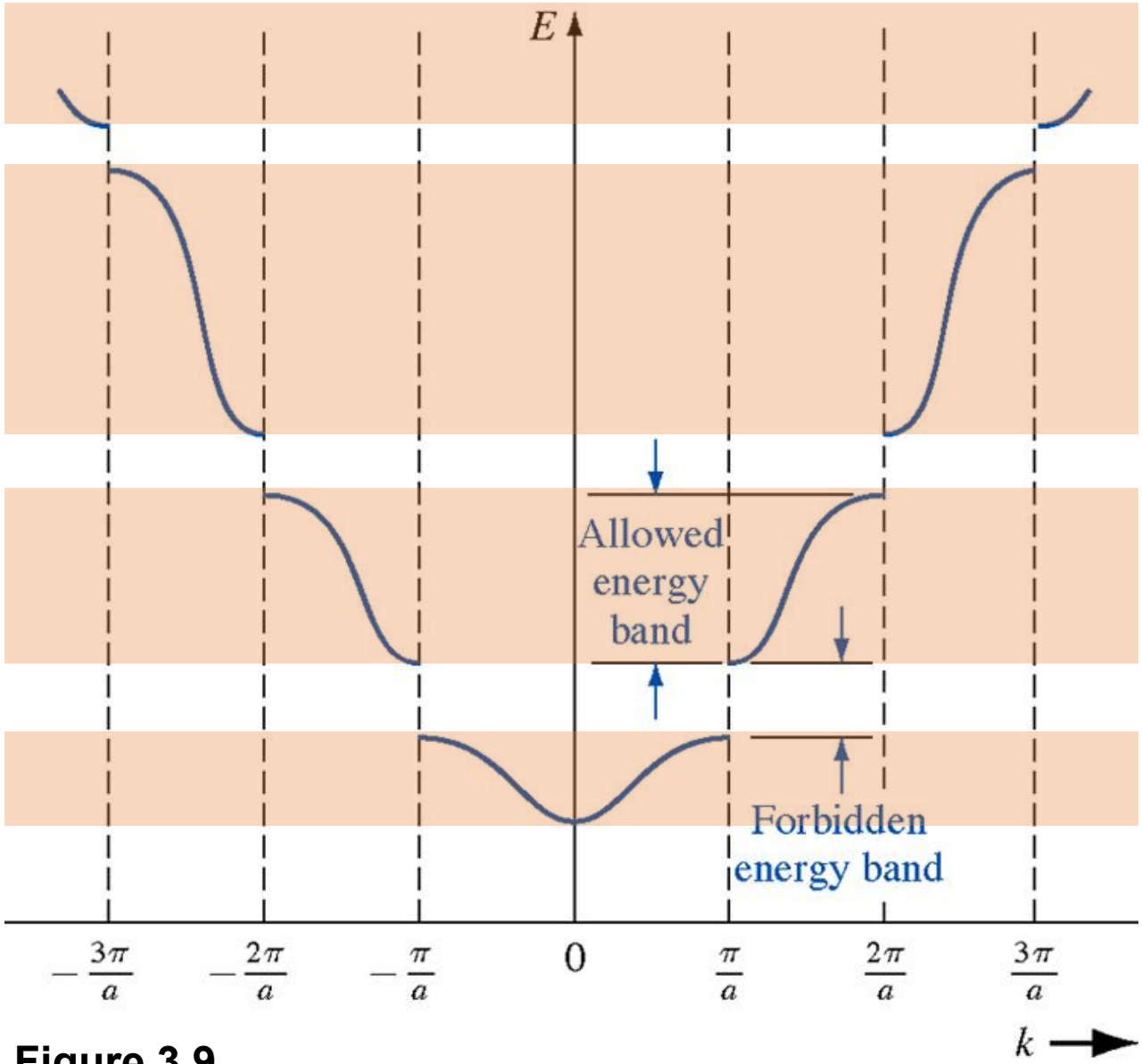


Figure 3.9

The k-space Diagram

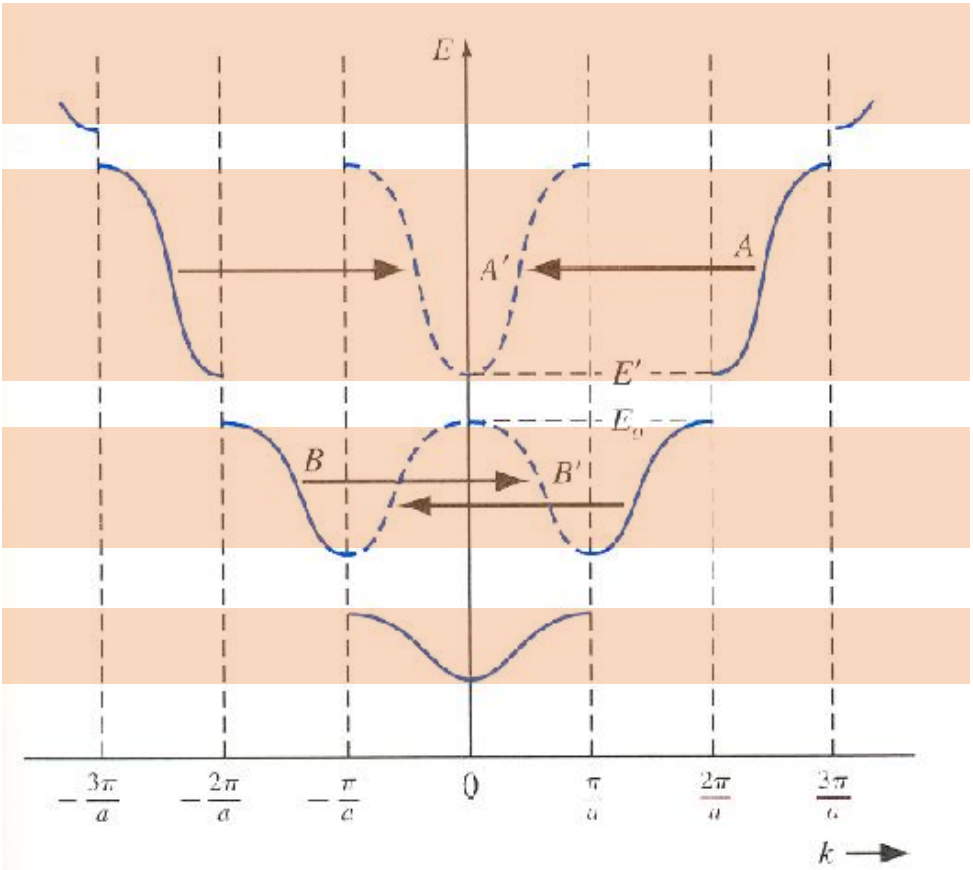
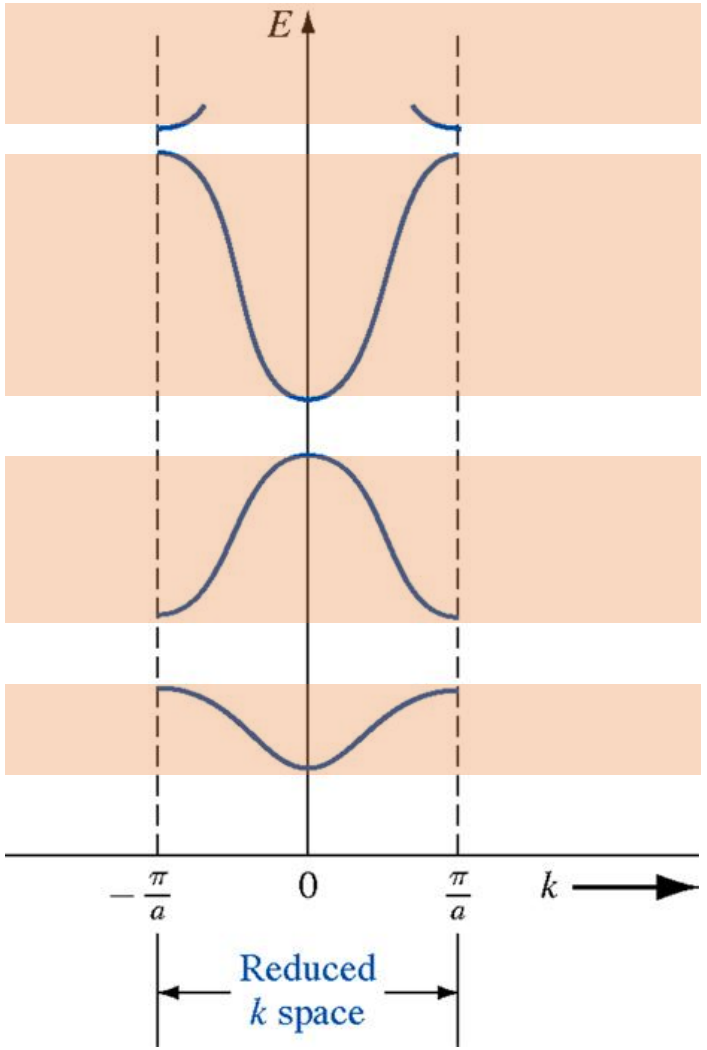
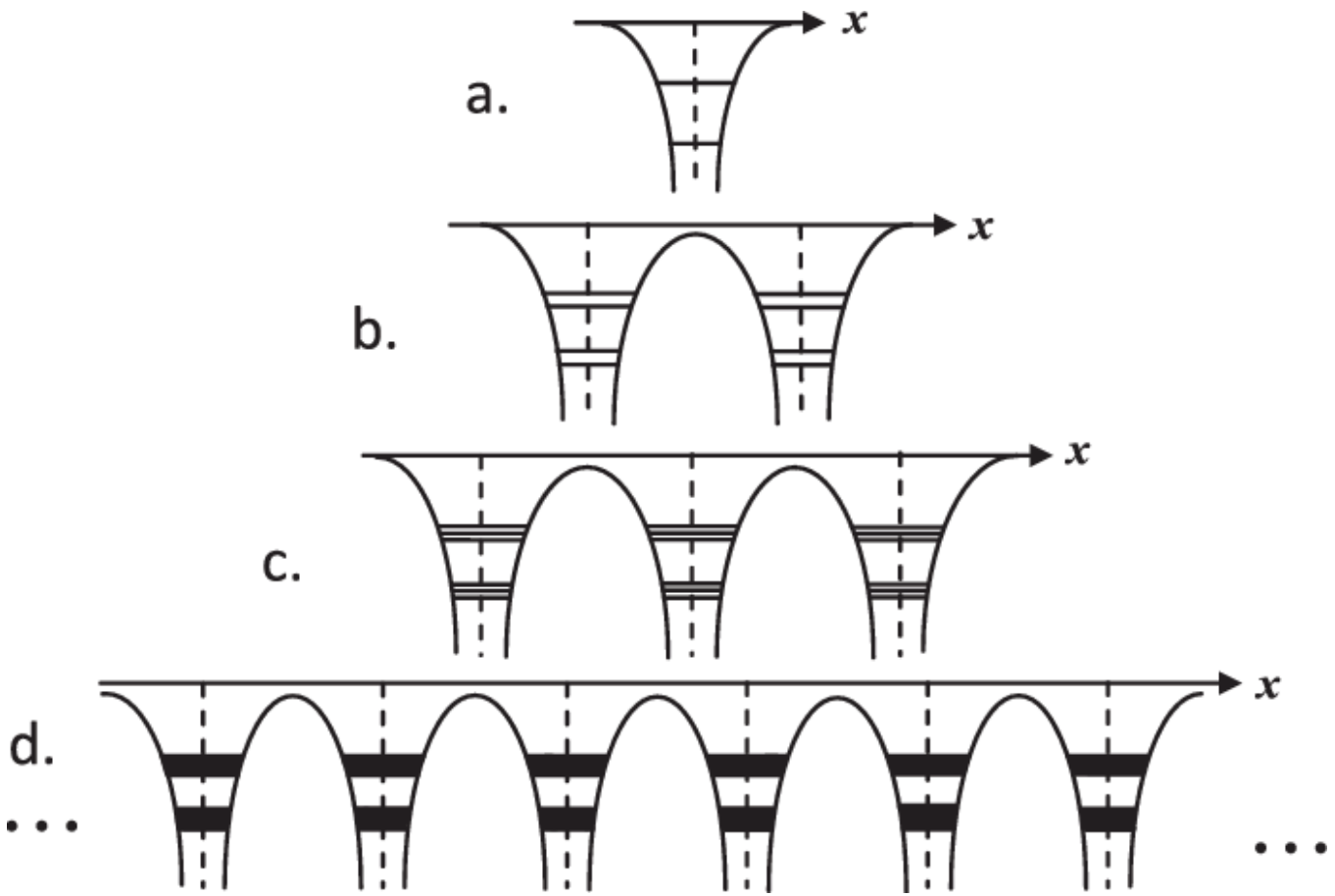


Figure 3.10 | The E versus k diagram showing 2π displacements of several sections of allowed energy bands.

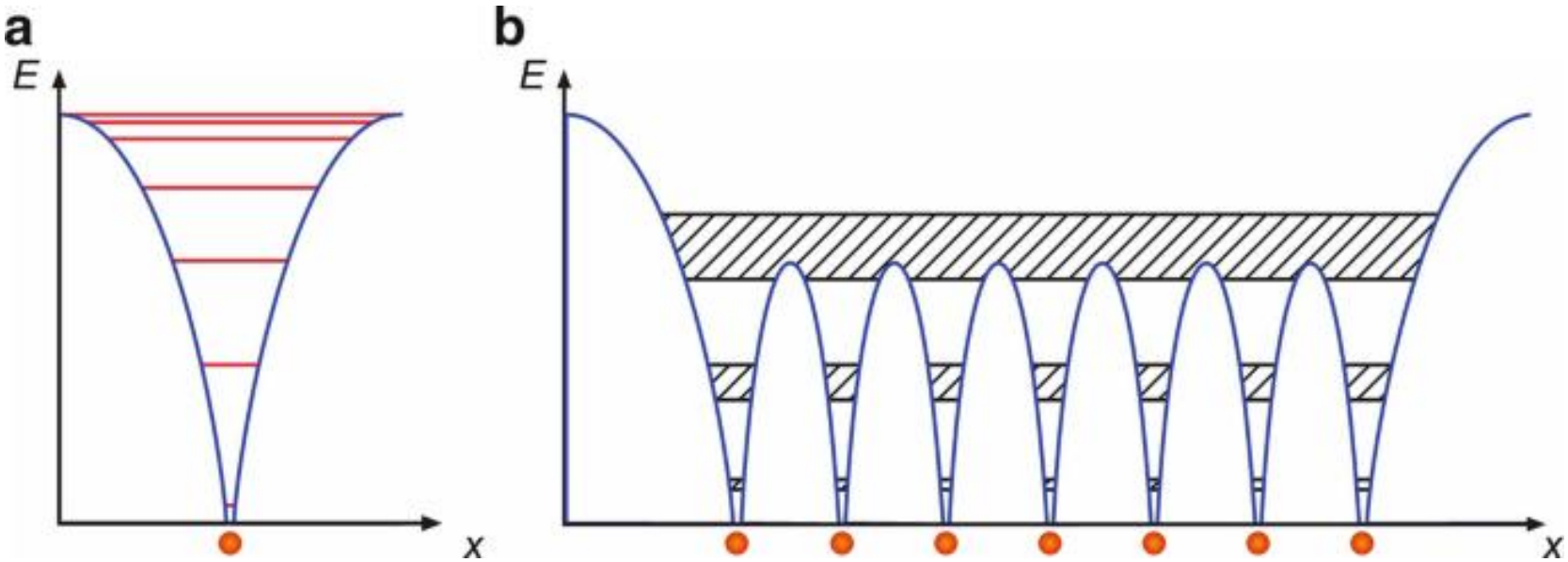


$$\cos ka = \cos(ka + 2n\pi) = \cos(ka - 2n\pi) \tag{3.31}$$

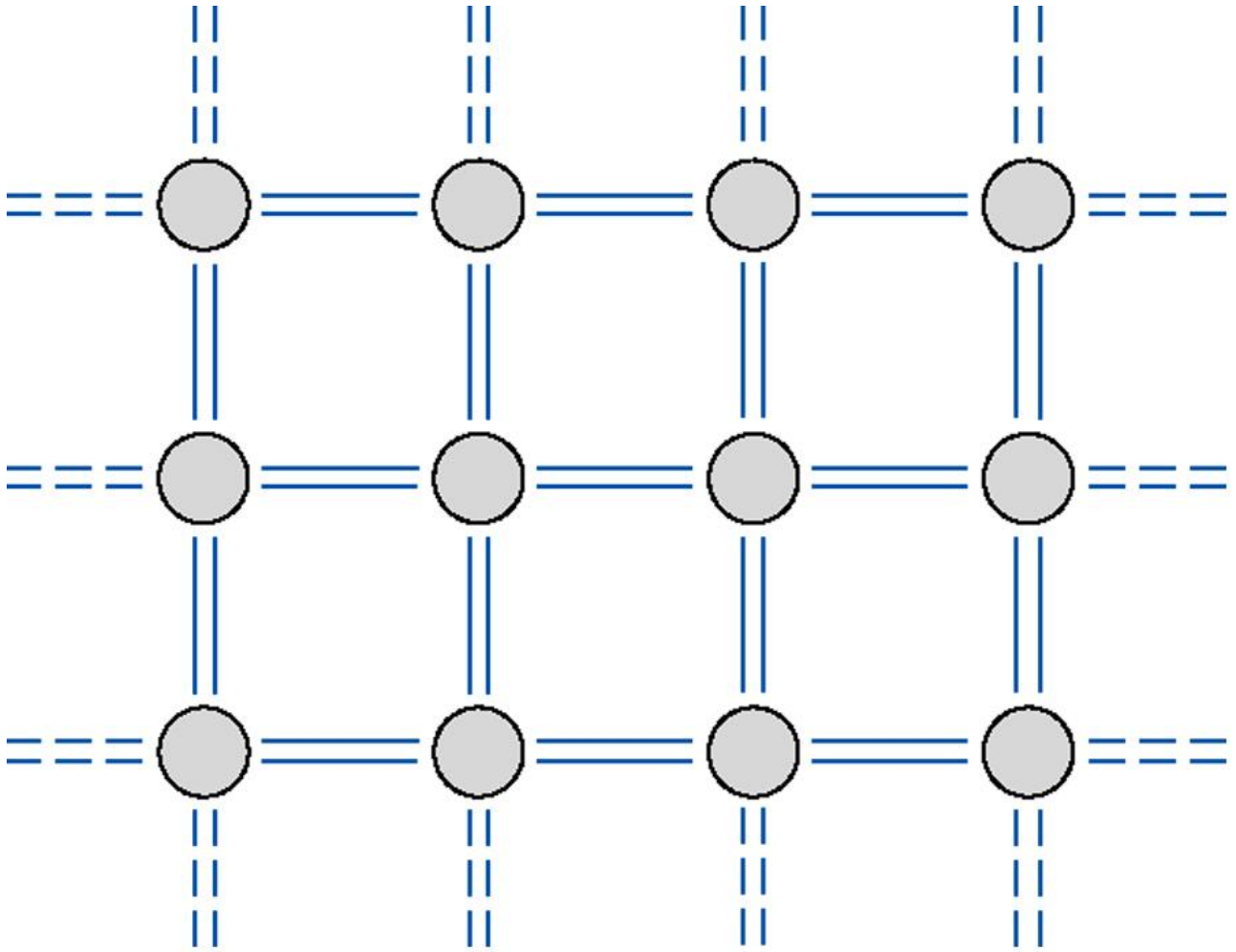
Energy diagram



Energy band diagram



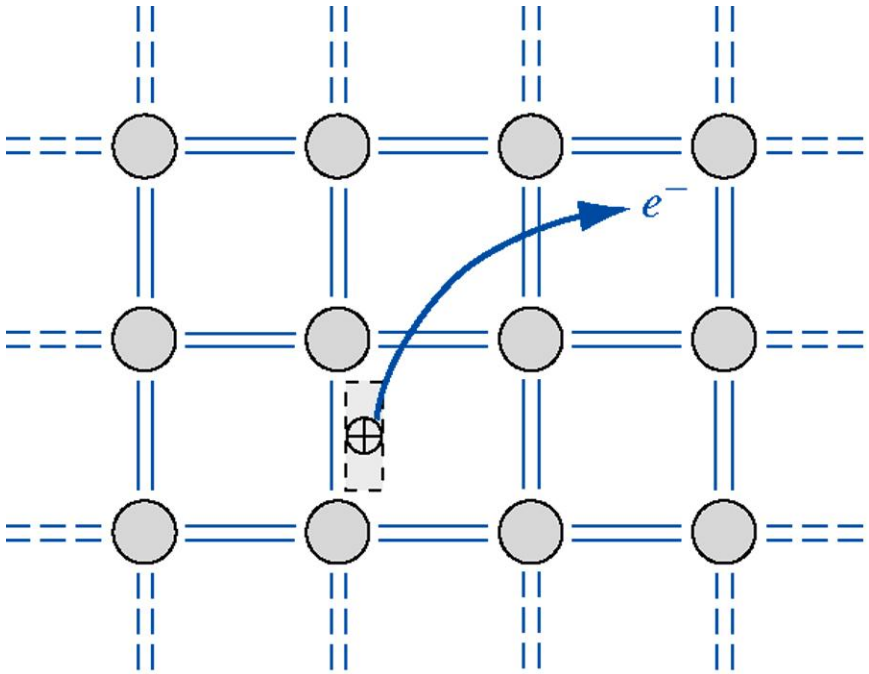
The Energy Band and the Bond Model



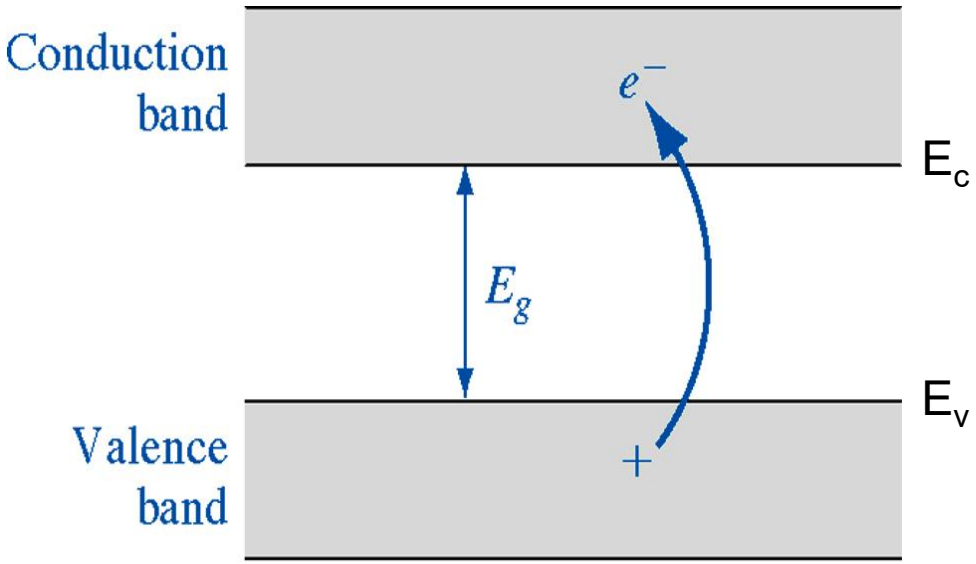
$T = 0$ K

Figure 3.12

The Energy Band and the Bond Model



(a)



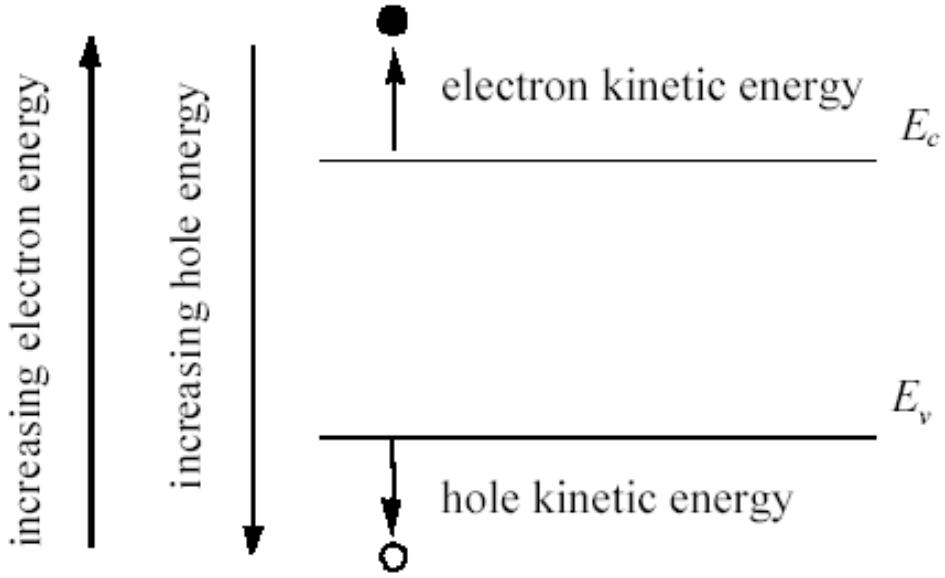
(b)

$T > 0$ K

E_c : The lowest energy level for the electron
E_v : The lowest energy level for the hole

Figure 3.13

Electrons and Holes



- Both electrons and holes tend to seek their lowest energy positions.
- Electrons tend to fall in the energy band diagram.
- Holes float up like bubbles in water.

Concept of the Hole

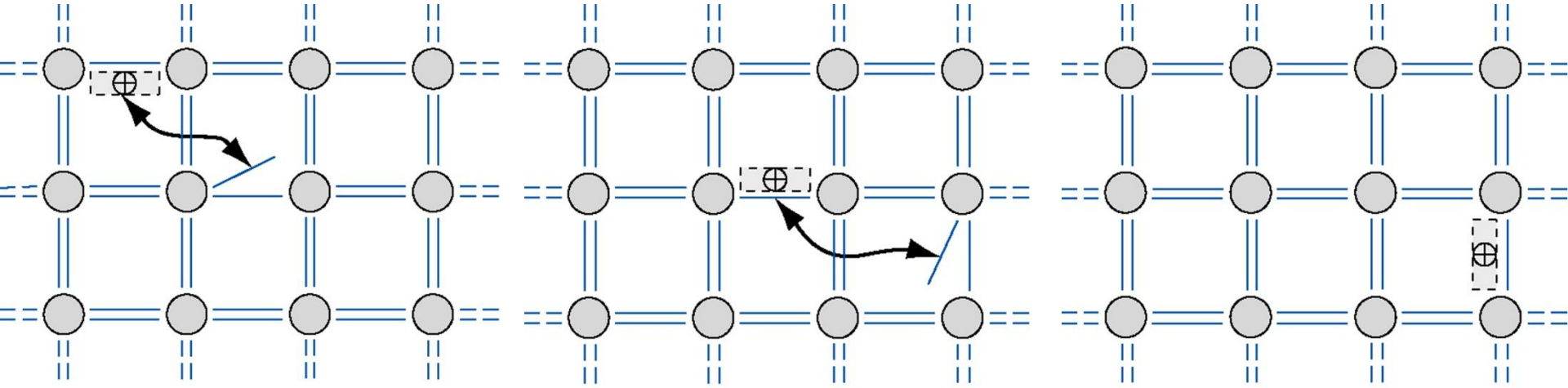


Figure 3.17

Concept of the Hole

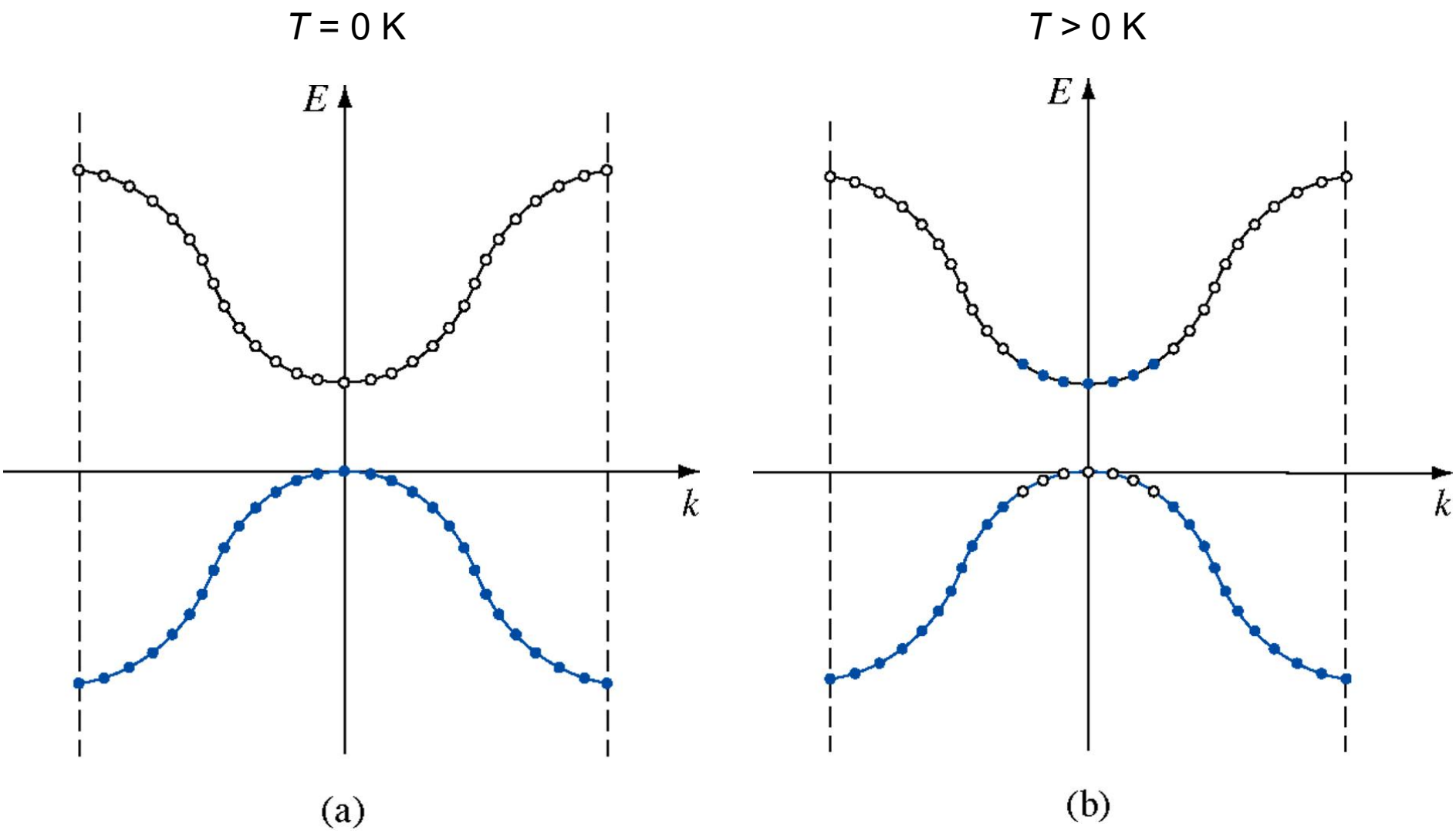
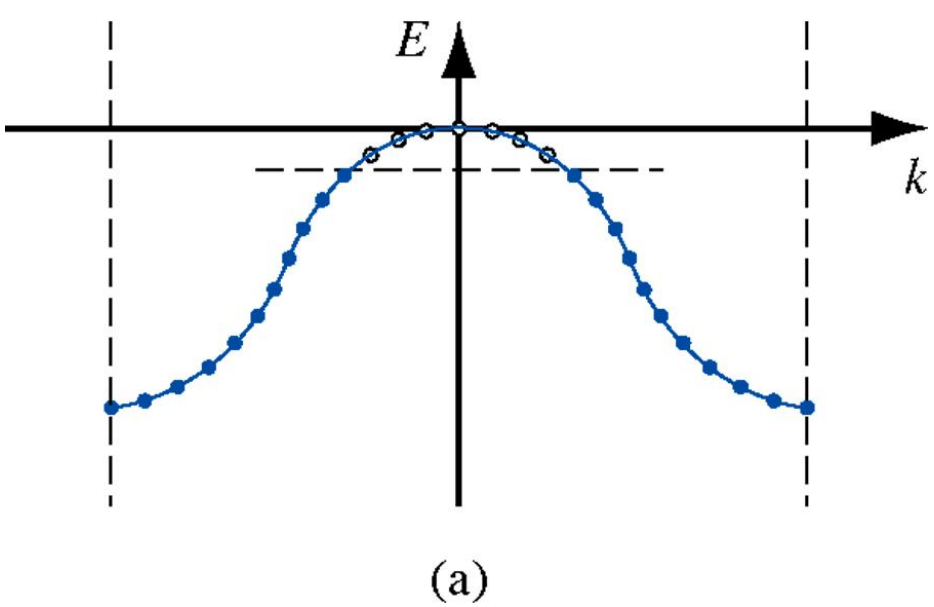


Figure 3.14

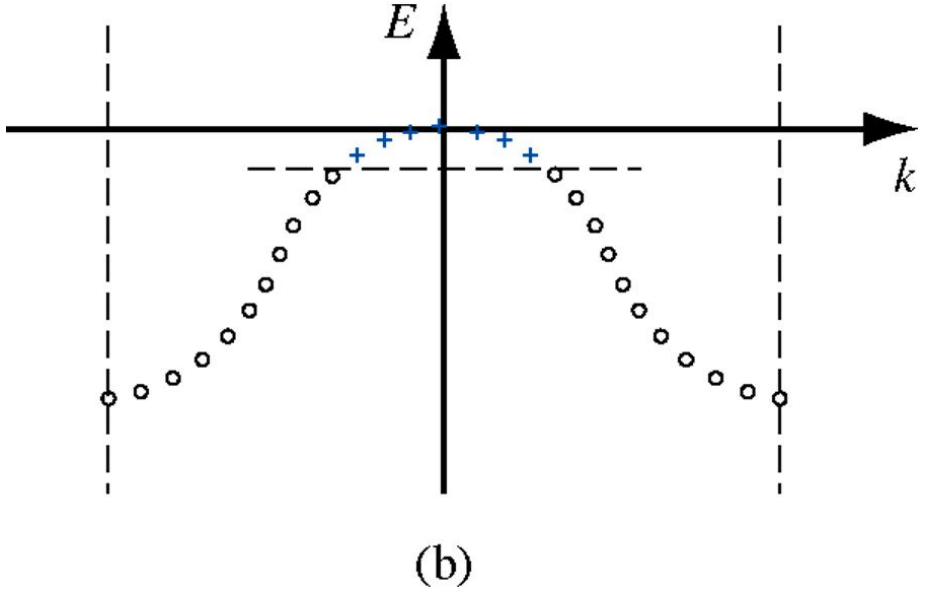
Concept of the Hole

Empty spots for electrons



(a)

Spots of holes



(b)

Extention to three dimensions

2D lattice

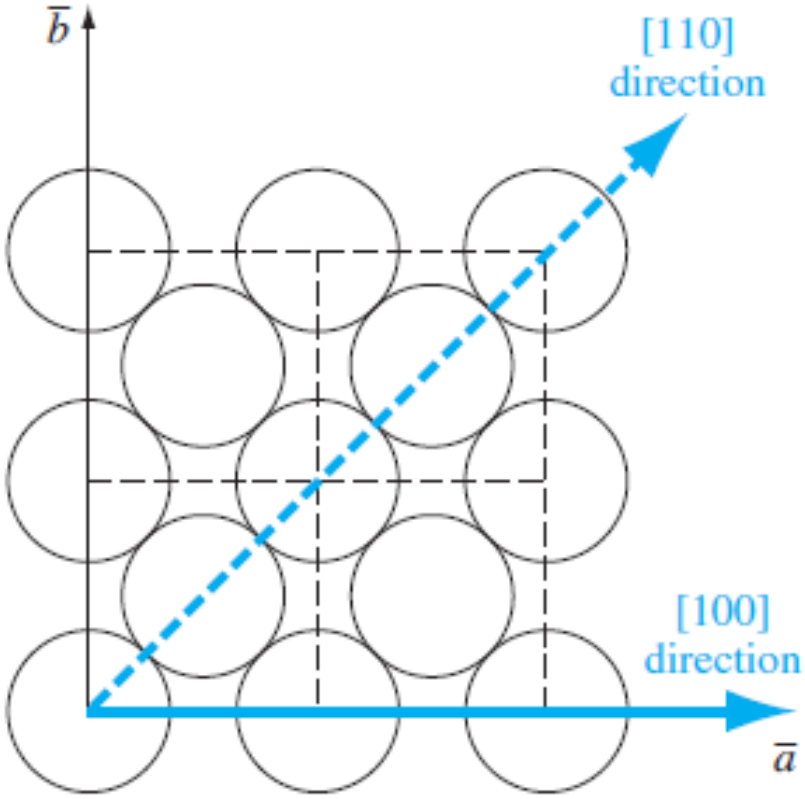
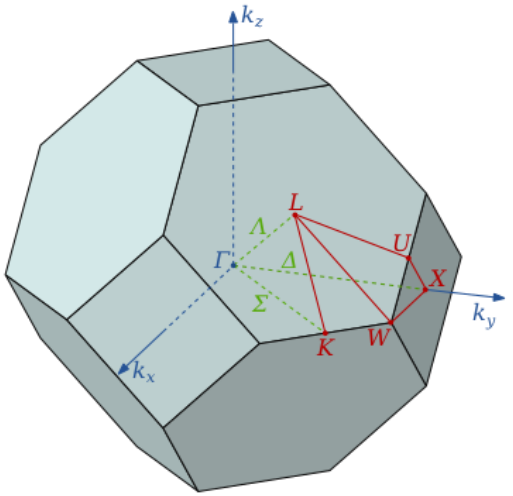
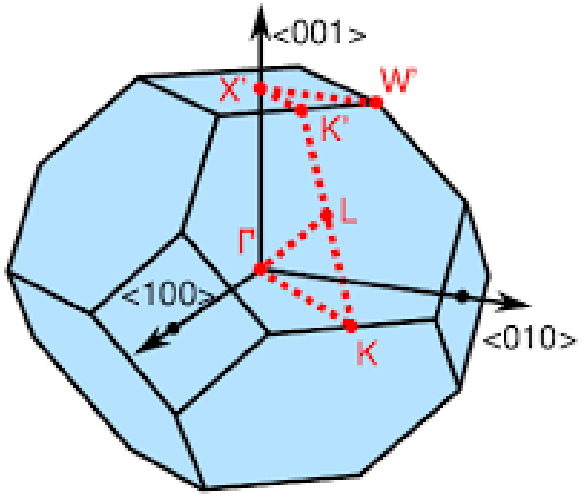


Figure 3.24 | The (100) plane of a face-centered cubic crystal showing the [100] and [110] directions.

3D reciprocal lattice





Energy band structures of GaAs and Si

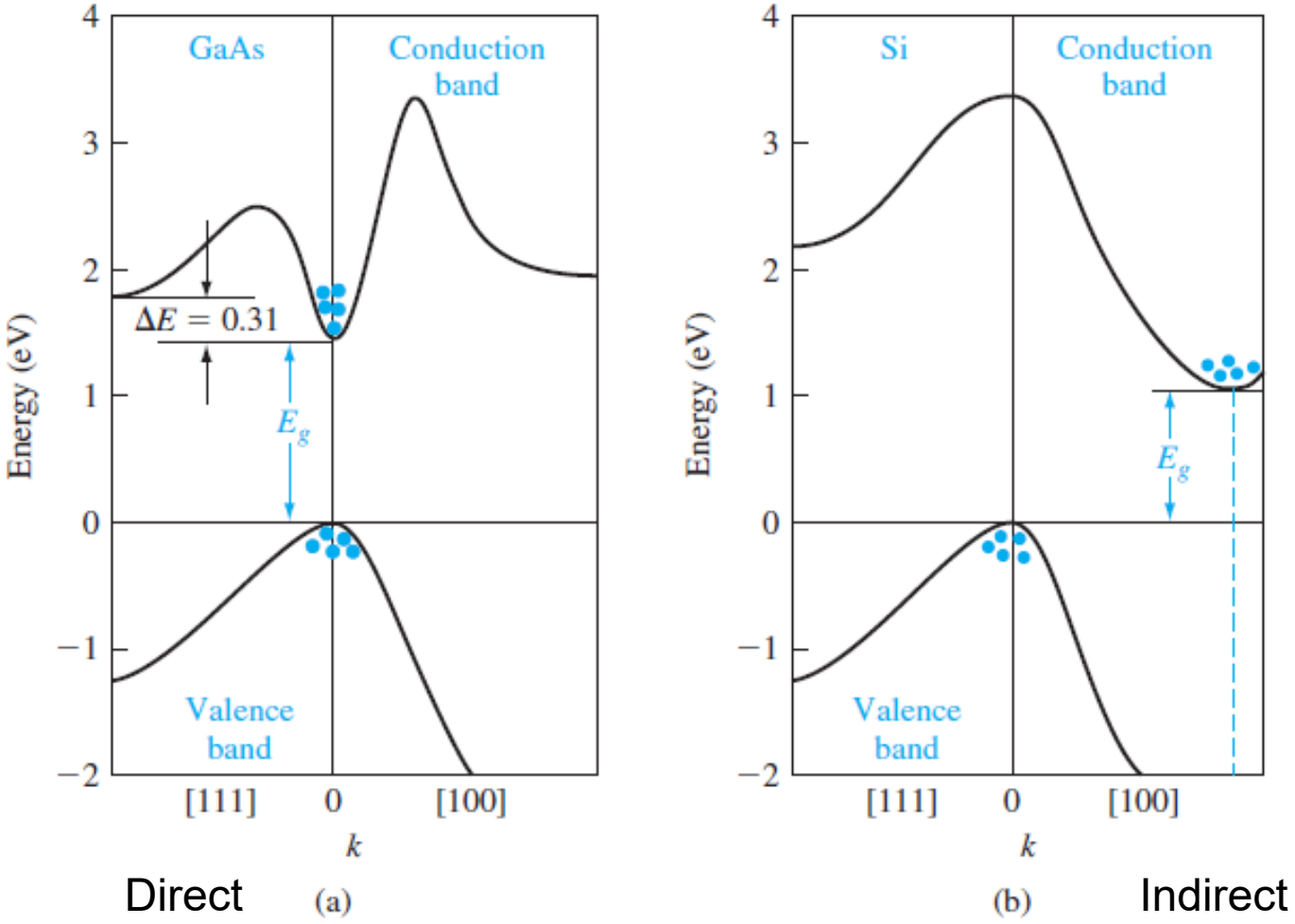
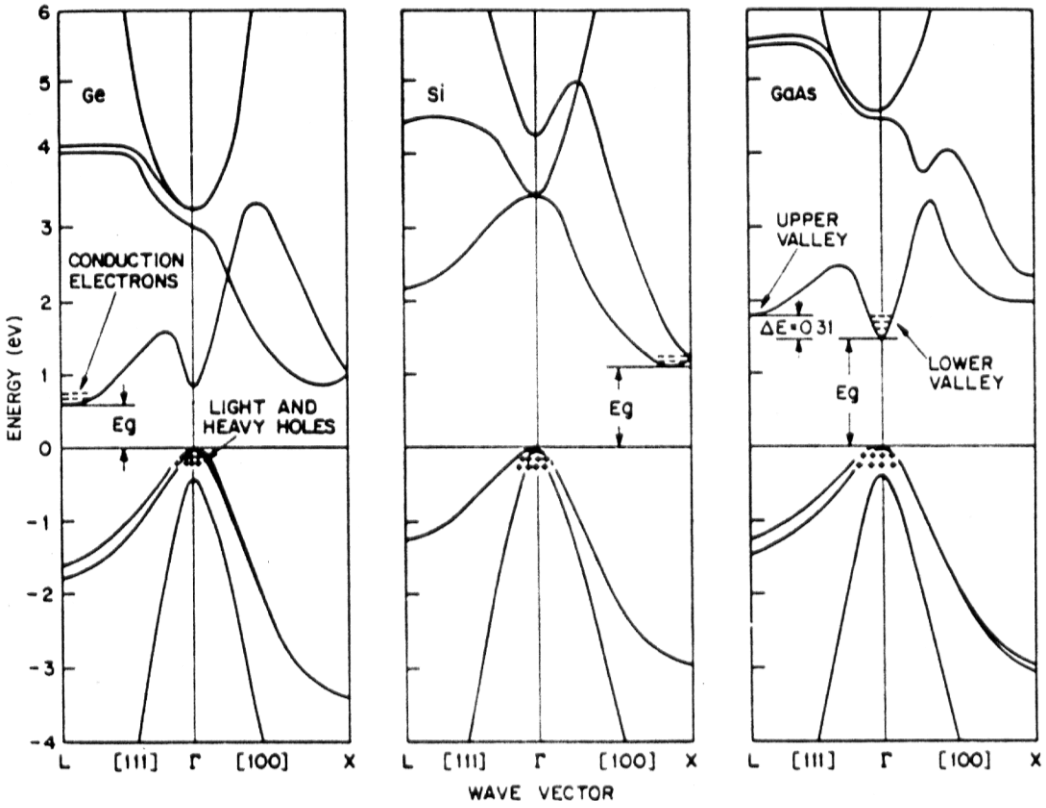


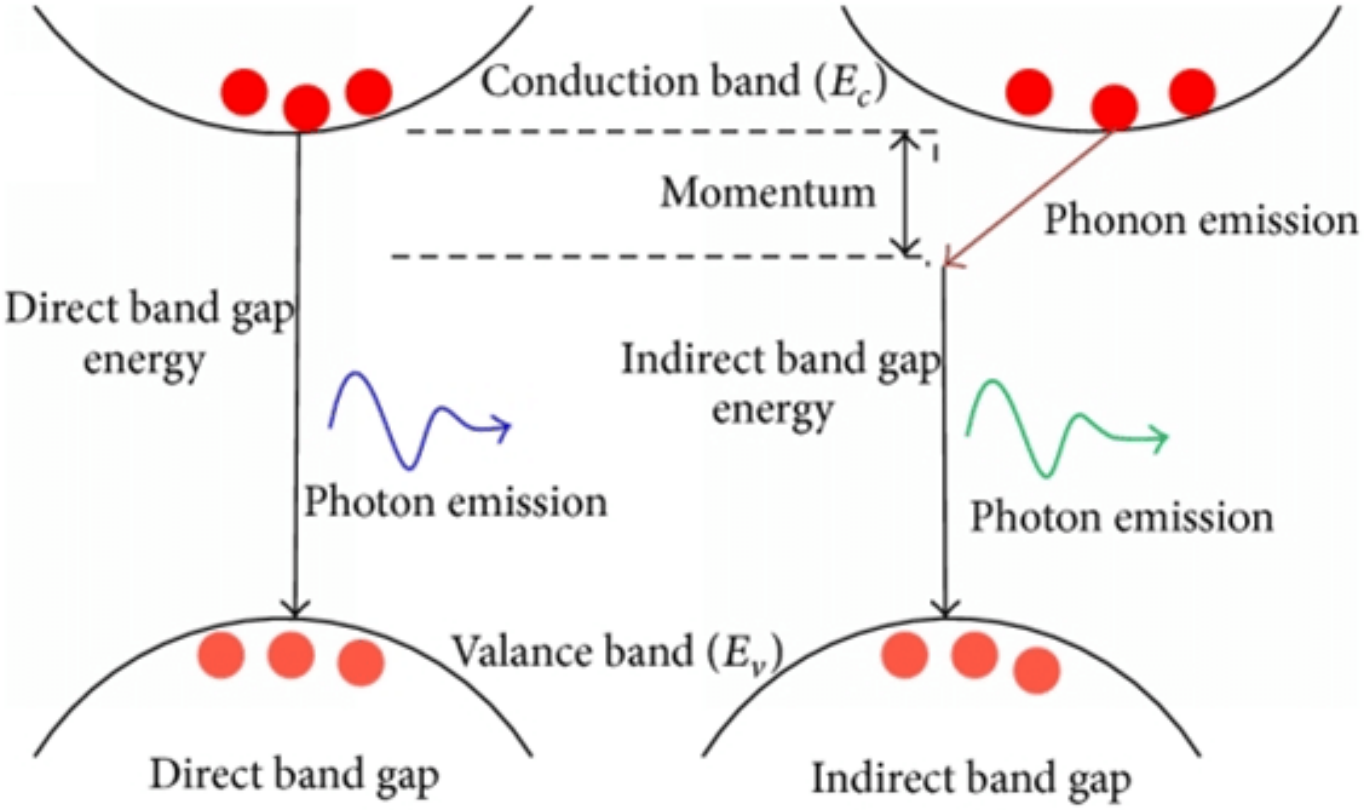
Figure 3.25 | Energy-band structures of (a) GaAs and (b) Si.
(From Sze [12].)

Energy band structures of Si, Ge, and GaAs

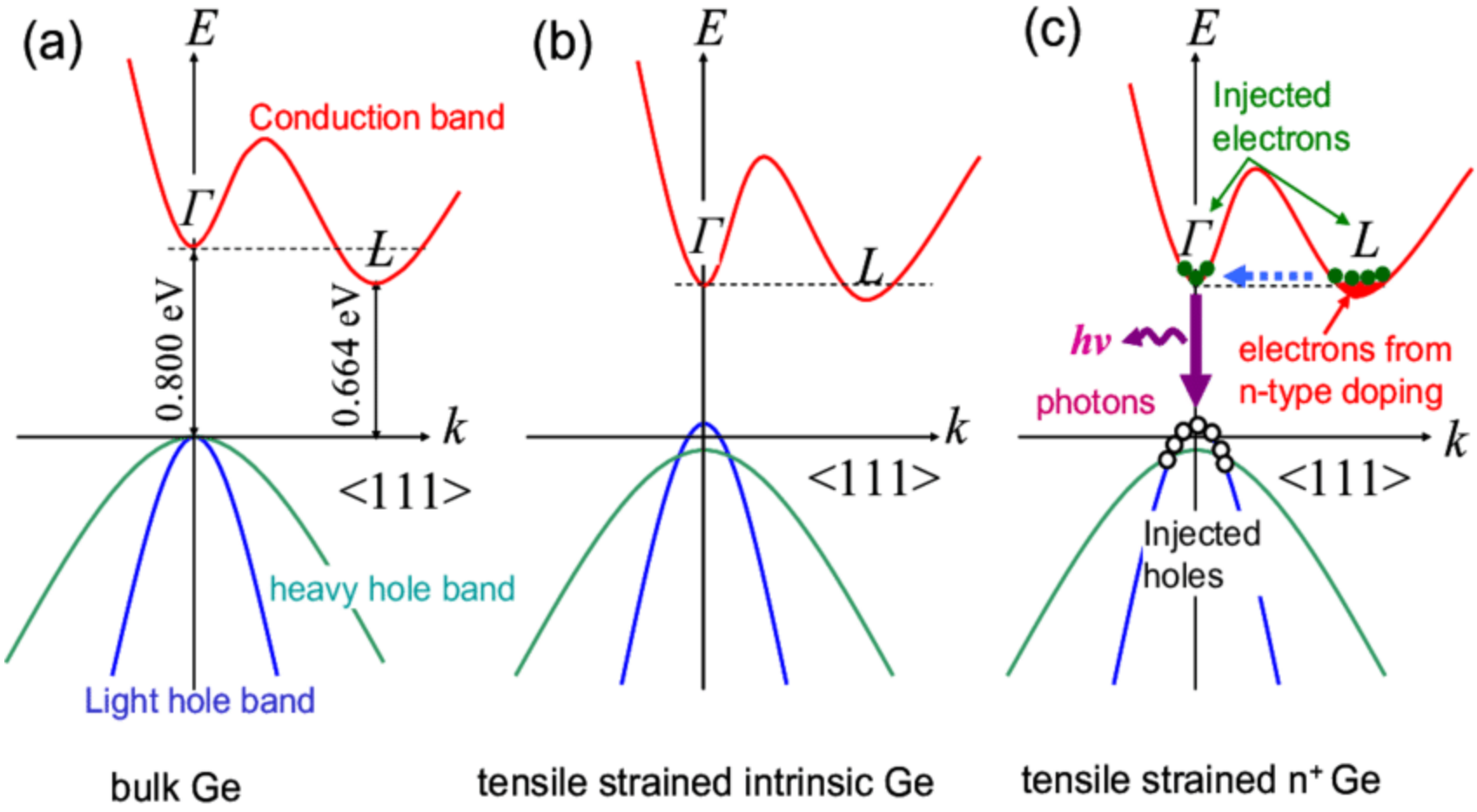


	Si	Ge	GaAs
Bandgap type	Indirect	Indirect	Direct
Bandgap (Eg) @ 300K	1.12 eV	0.66 eV	1.42 eV

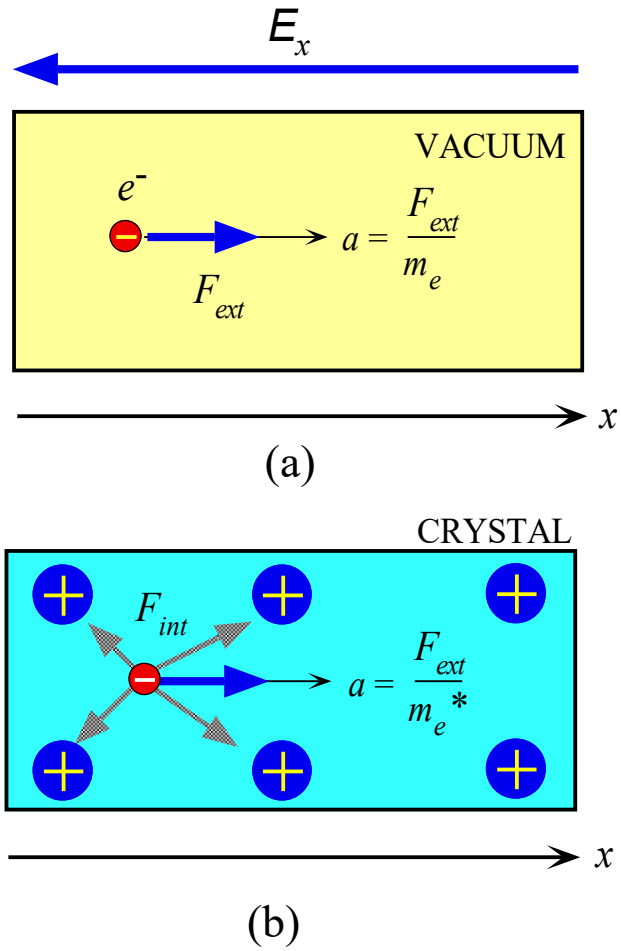
Energy band structures of Direct and Indirect band gap



Stress engineering of Ge



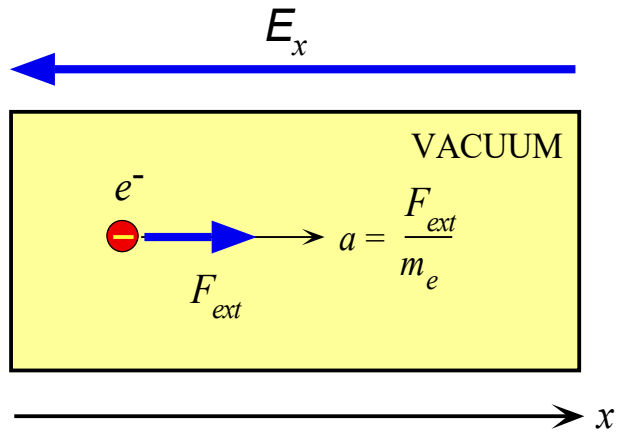
Electron effective mass (m_n^*)



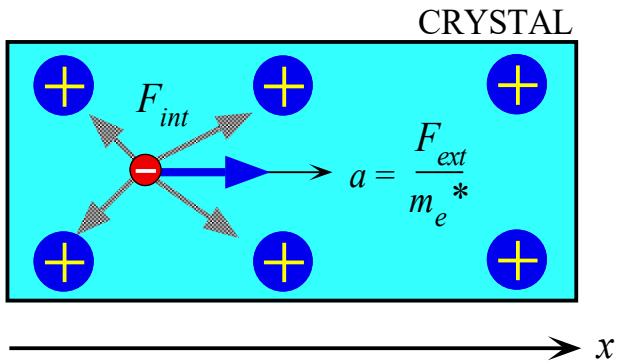
$$F_{ext} = m_e a$$

$$F_{total} = F_{ext} - F_{int} = m_e^* a$$

Electron effective mass (m_n^*)



(a)

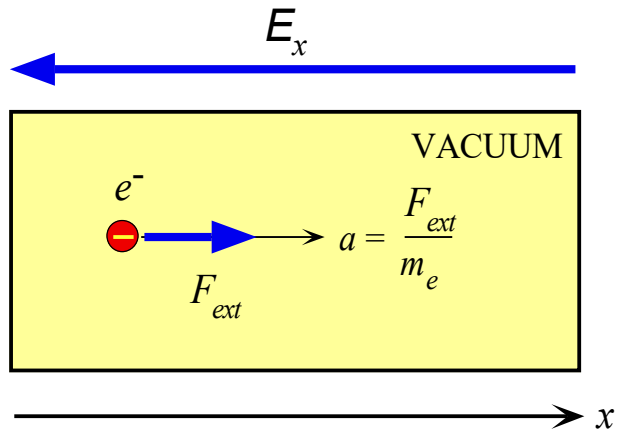


(b)

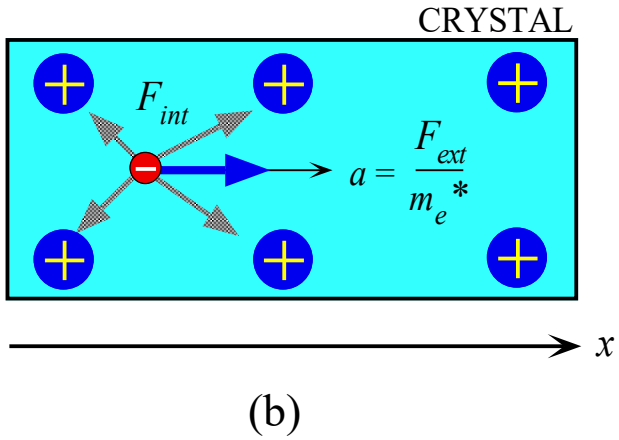
$$E = \frac{p^2}{2m^*} = \frac{k^2\hbar^2}{2m^*}$$

$$\rightarrow \quad \frac{dE}{dk} = \frac{\hbar^2 k}{m^*} = \frac{\hbar p}{m^*} \qquad (p = \hbar k)$$

Electron effective mass (m_n^*)



(a)



(b)

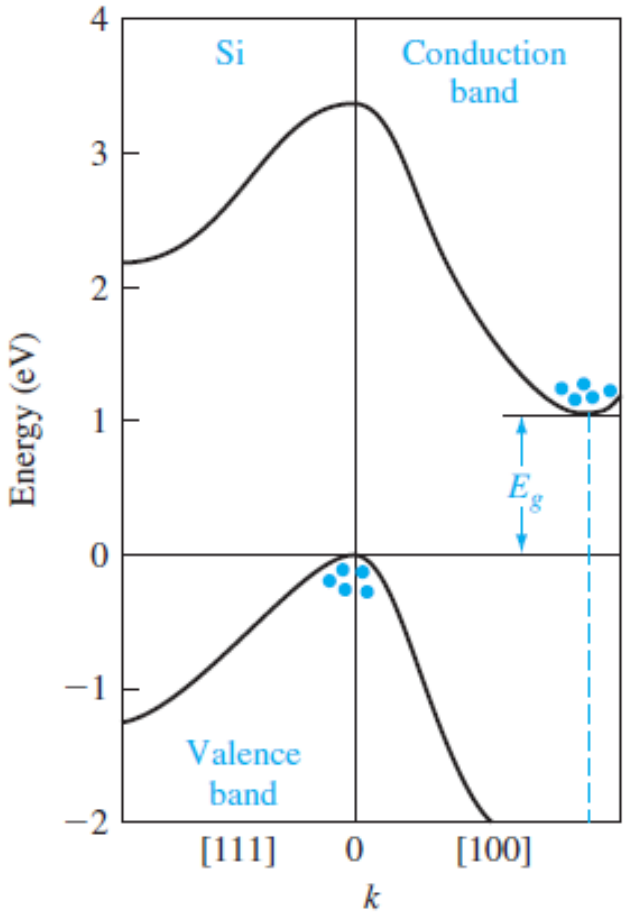
$$E = \frac{p^2}{2m^*} = \frac{k^2\hbar^2}{2m^*}$$

$$\rightarrow \quad \frac{dE}{dk} = \frac{\hbar^2 k}{m^*} = \frac{\hbar p}{m^*} \qquad (p = \hbar k)$$

$$\rightarrow \quad \frac{d^2E}{dk^2} = \frac{\hbar^2}{m^*} \qquad \frac{1}{\hbar^2}\frac{d^2E}{dk^2} = \frac{1}{m^*}$$

$$m^* = \left(\frac{1}{\hbar^2}\frac{d^2E}{dk^2}\right)^{-1}$$

Electron effective mass (m_n^*)



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

$$\rightarrow \quad \frac{dE}{dk} = \frac{\hbar^2 k}{m^*}$$

1st derivatives = 기울기

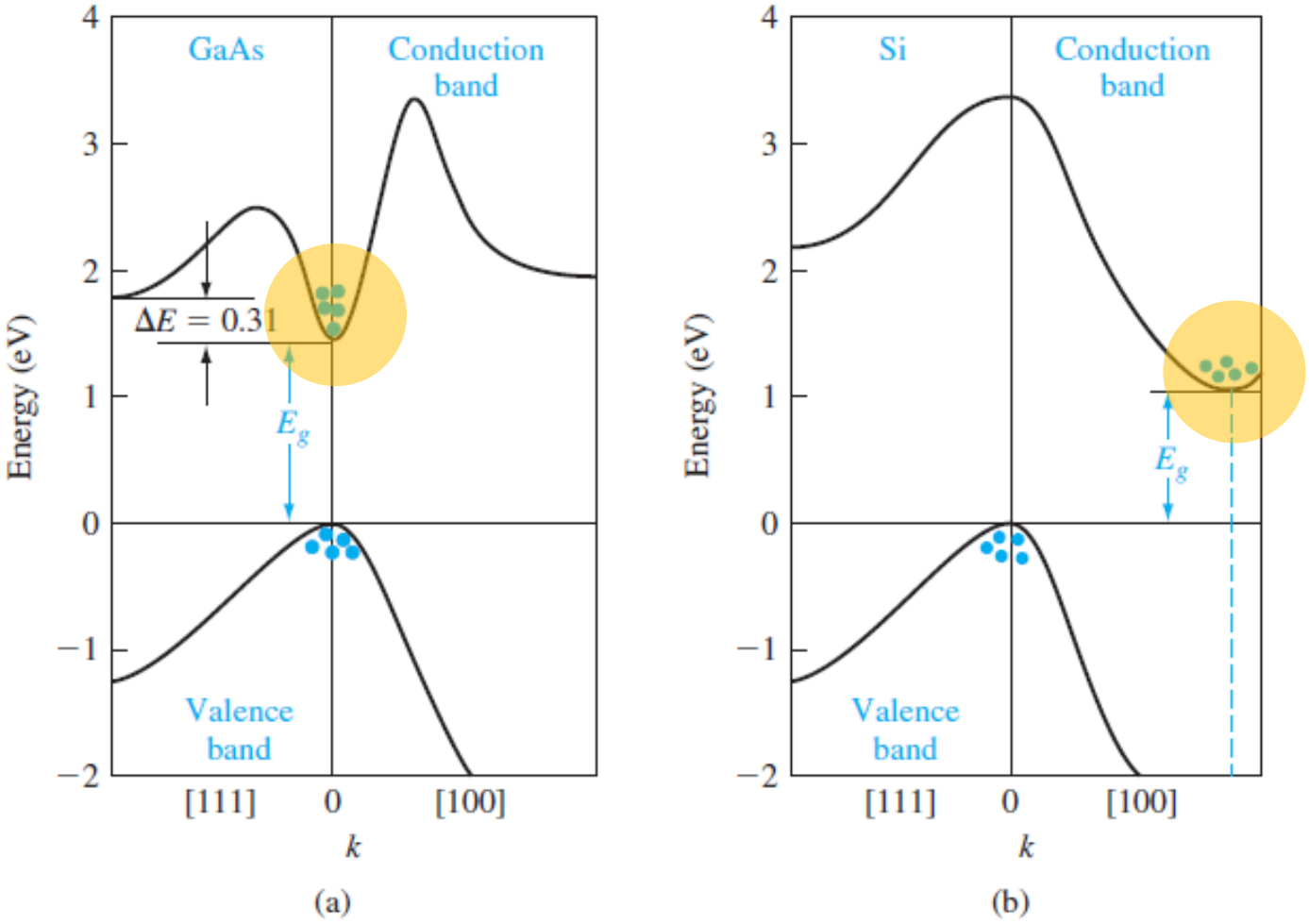
$$\rightarrow \quad \frac{d^2E}{dk^2} = \frac{\hbar^2}{m^*} \qquad \frac{1}{\hbar^2}\frac{d^2E}{dk^2} = \frac{1}{m^*}$$

2nd derivatives = 곡률

$$m^* = \left(\frac{1}{\hbar^2}\frac{d^2E}{dk^2}\right)^{-1}$$

곡률의 역수

Electron effective mass (m_n^*)



$$m^* = \left(\frac{1}{\hbar^2}\frac{d^2E}{dk^2}\right)^{-1}$$

$$m^*_{\text{GaAs}} < m^*_{\text{Si}}$$

Metals, Insulators, and Semiconductors

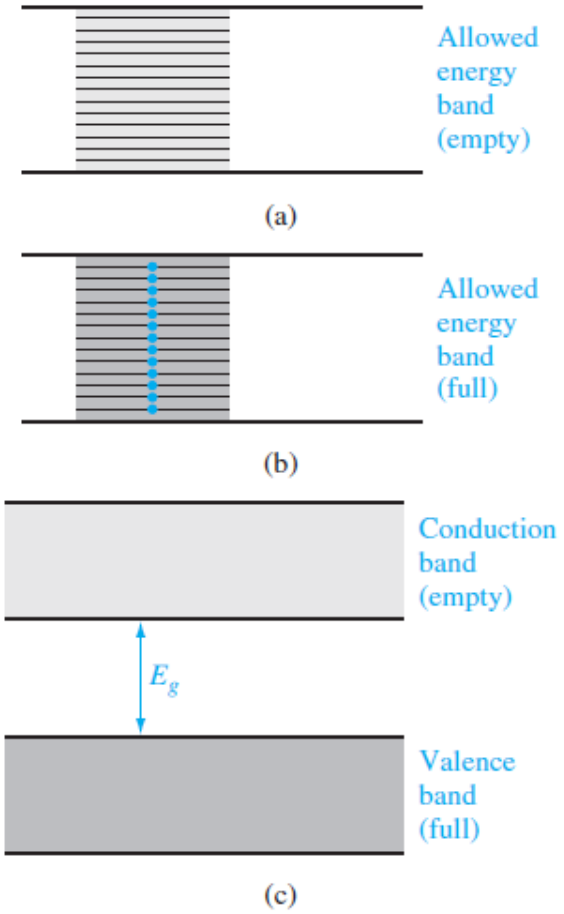


Figure 3.19 | Allowed energy bands showing (a) an empty band, (b) a completely full band, and (c) the bandgap energy between the two allowed bands.

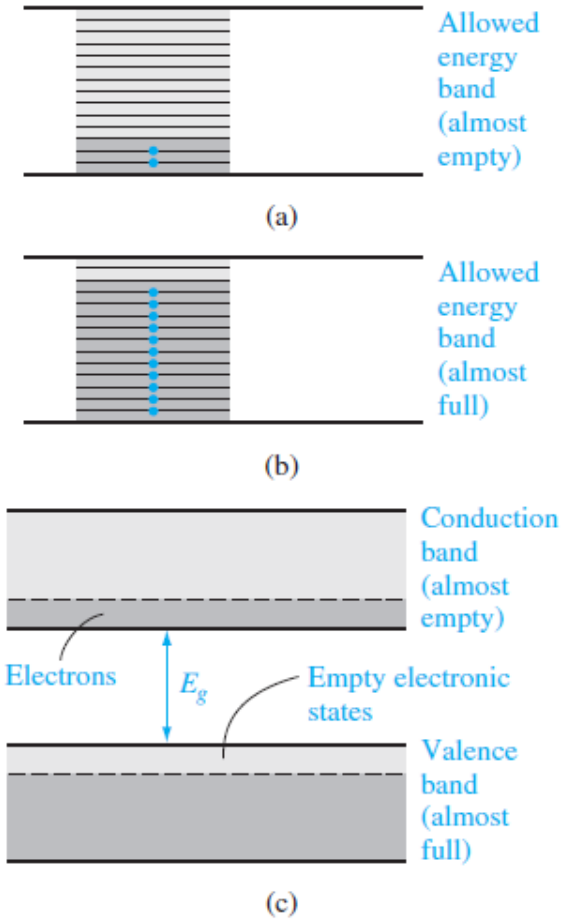


Figure 3.20 | Allowed energy bands showing (a) an almost empty band, (b) an almost full band, and (c) the bandgap energy between the two allowed bands.

Metals, Insulators, and Semiconductors

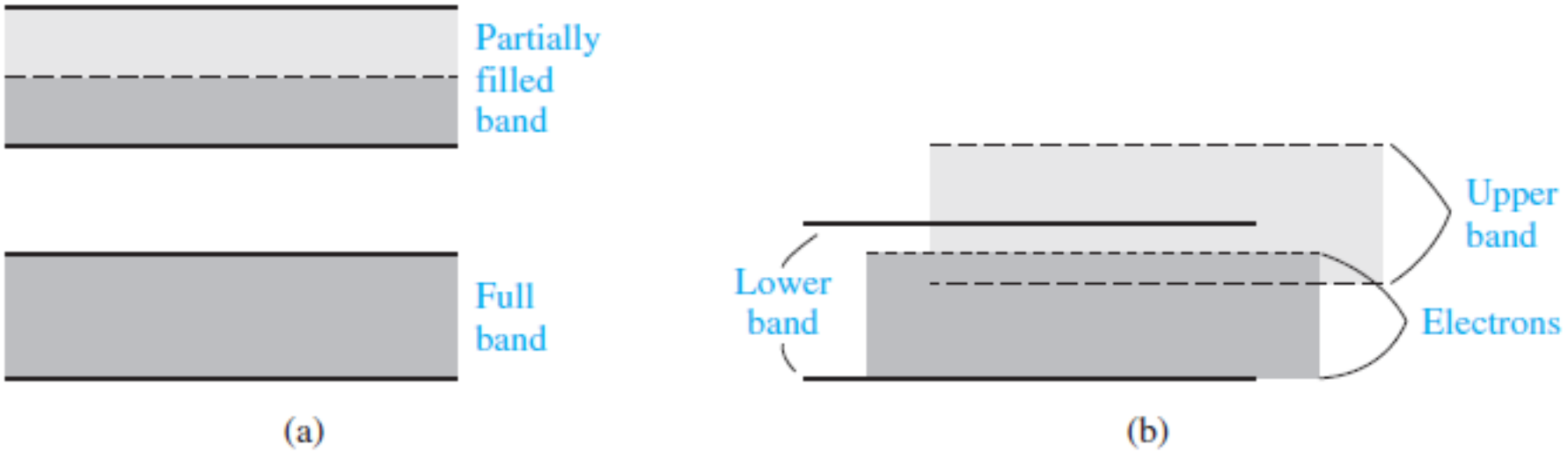


Figure 3.21 | Two possible energy bands of a metal showing (a) a partially filled band and (b) overlapping allowed energy bands.

Density of state (DOS) function

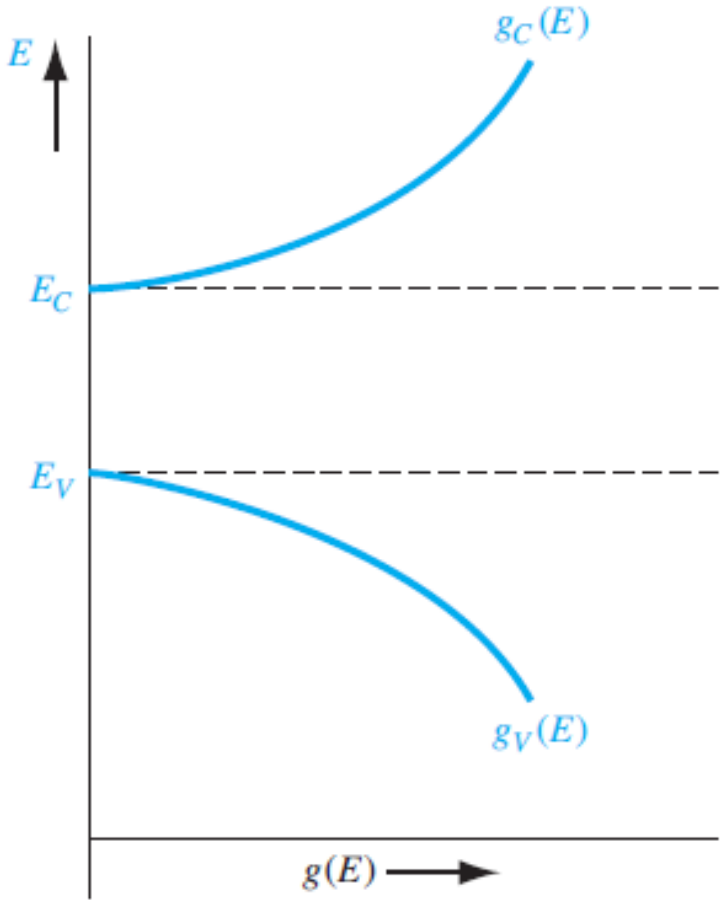
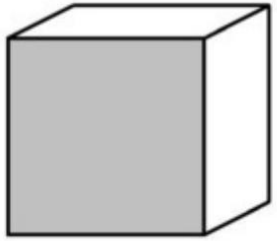


Figure 3.27 | The density of energy states in the conduction band and the density of energy states in the valence band as a function of energy.

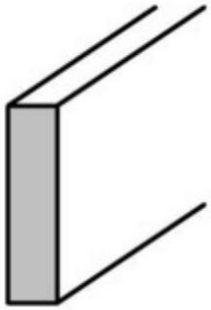
$$g_c(E) = \frac{4\pi(2m_n{}^*)^{3/2}}{h^3}\sqrt{E - E_c} \qquad (3.72)$$

$$g_v(E) = \frac{4\pi(2m_p{}^*)^{3/2}}{h^3}\sqrt{E_v - E} \qquad (3.75)$$

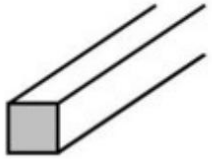
Density of state (DOS) function



Bulk

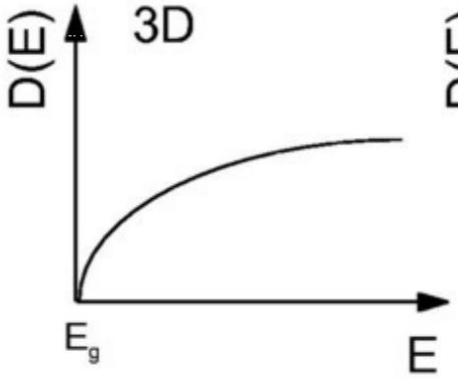


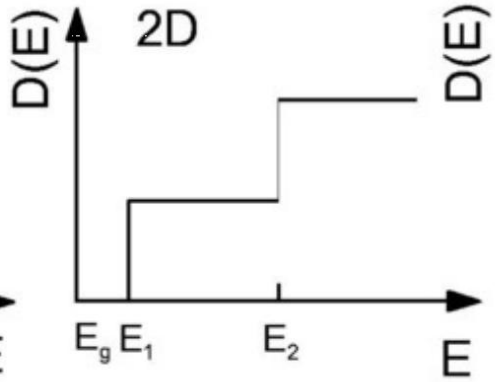
Quantum Well

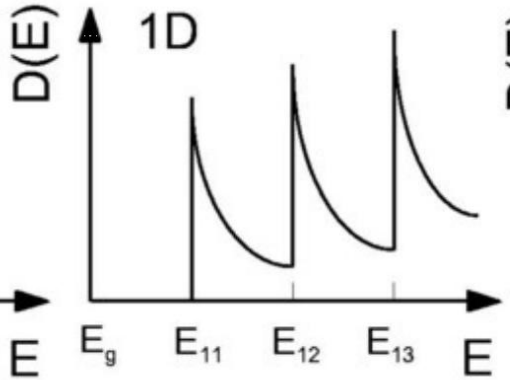


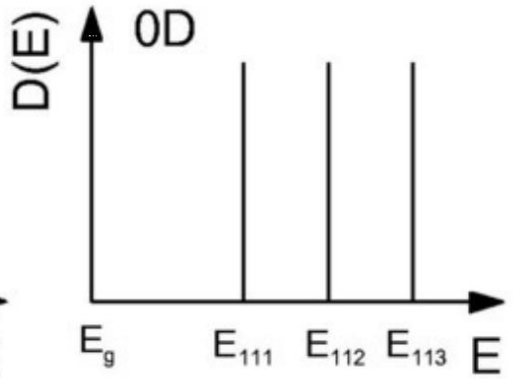
Quantum Wire

Quantum Dot









Si, Ge

Graphene
TMDs

CNT

QLED

Fermi-Dirac distribution function

$$\frac{N(E)}{g(E)} = f_F(E) = \frac{1}{1 + e^{\frac{E - E_F}{kT}}} \tag{3.79}$$

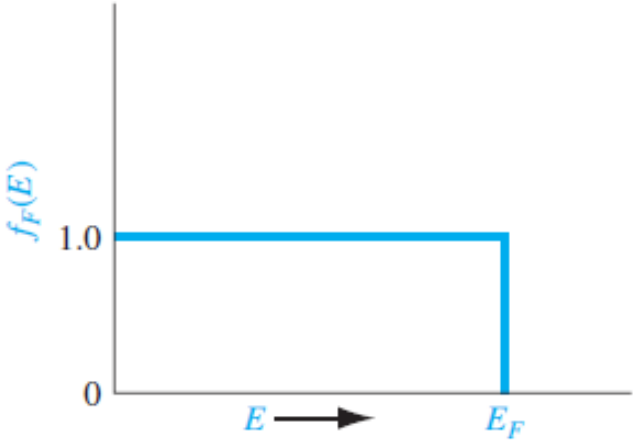


Figure 3.29 | The Fermi probability function versus energy for $T = 0$ K.

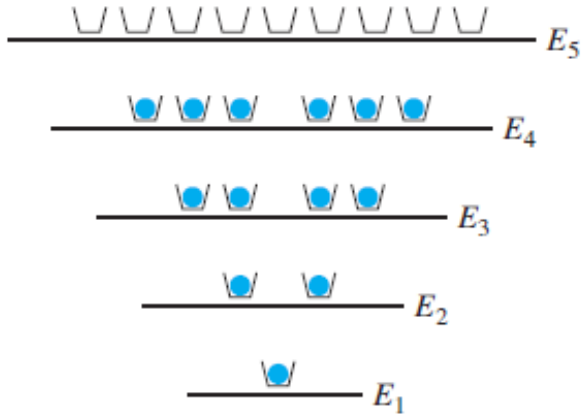


Figure 3.30 | Discrete energy states and quantum states for a particular system at $T = 0$ K.

when $T = 0$ K, $E < E_F$

$$f_F(E) = \frac{1}{1} = 1$$

when $T = 0$ K, $E > E_F$

$$f_F(E) = \frac{1}{\infty} = 0$$

Fermi-Dirac distribution function

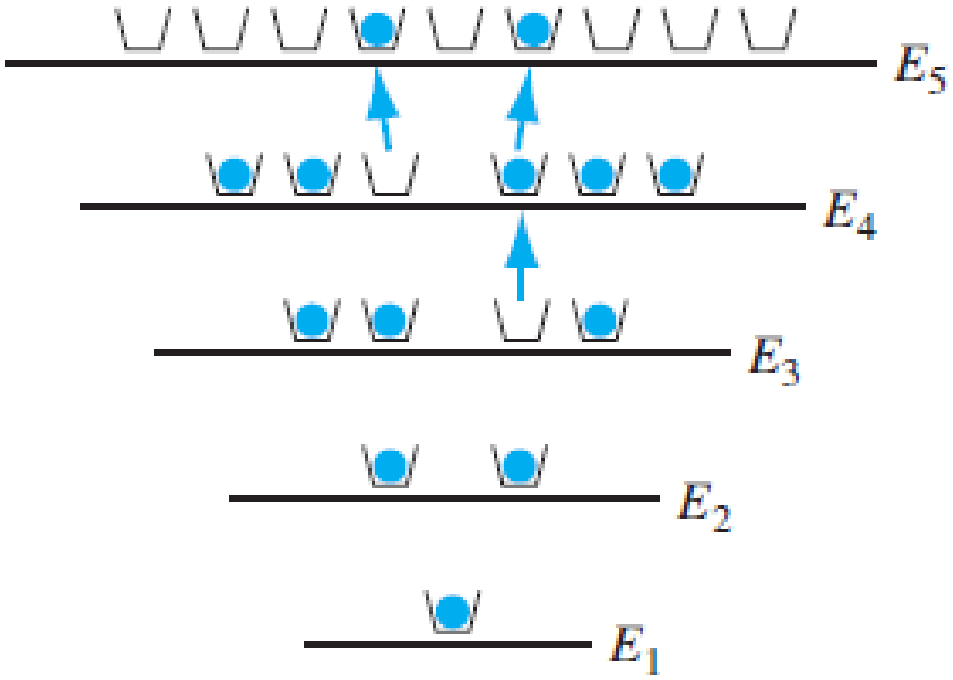


Figure 3.32 | Discrete energy states and quantum states for the same system shown in Figure 3.30 for $T > 0$ K.

Fermi-Dirac distribution function

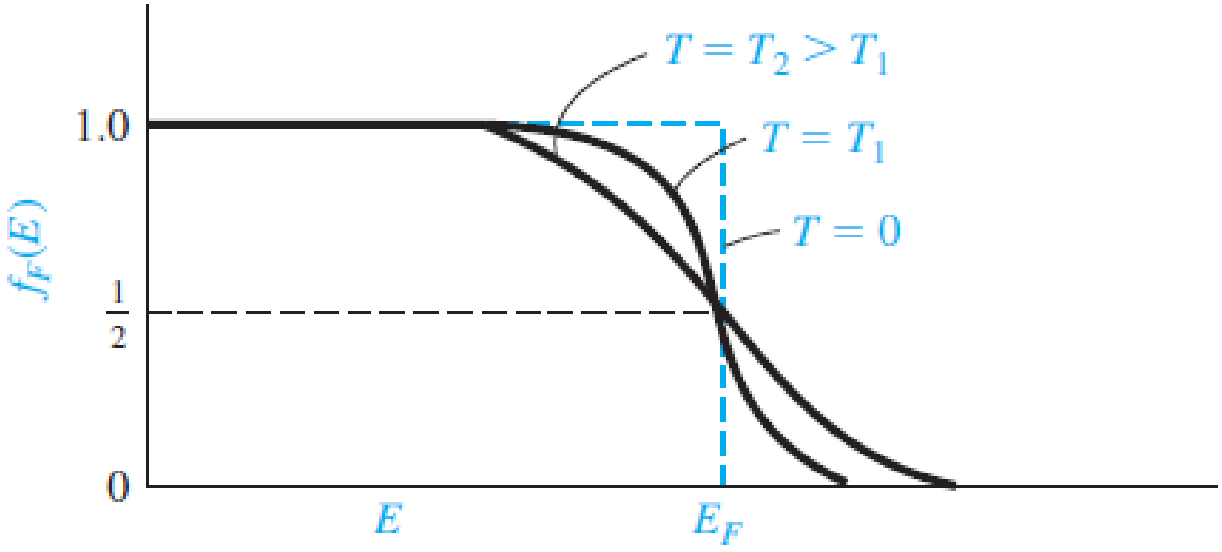


Figure 3.33 | The Fermi probability function versus energy for different temperatures.

$$f_F(E) = \frac{1}{1 + \exp\left(\frac{E - E_F}{kT}\right)} \qquad (3.79)$$

when $T > 0$ K

$$f_F(E) \neq 1, \quad f_F(E) \neq 0$$

when $E = E_F$

$$f_F(E) = \frac{1}{1 + \exp(0)} = \frac{1}{2}$$

Fermi-Dirac distribution function

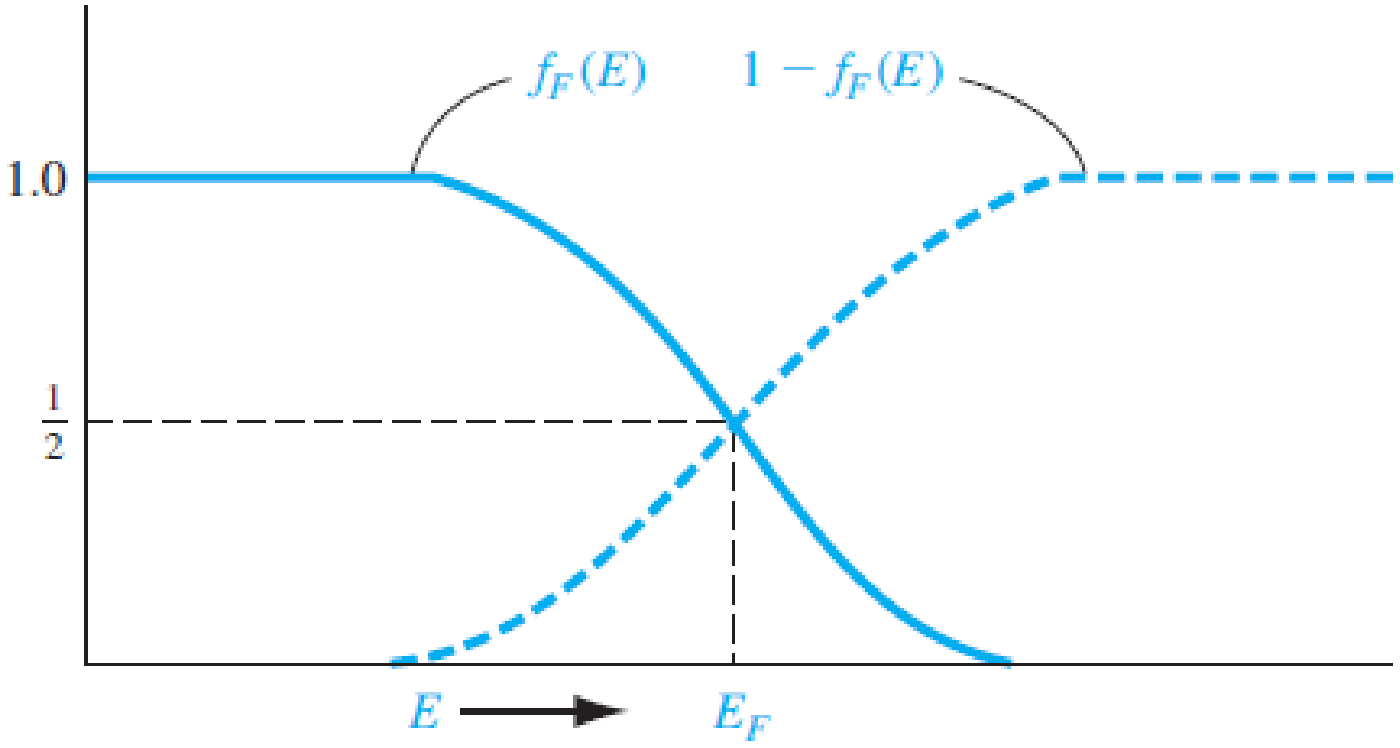


Figure 3.34 | The probability of a state being occupied, $f_F(E)$, and the probability of a state being empty, $1 - f_F(E)$.

Boltzmann approximation

$$f_F(E) = \frac{1}{1 + \exp\left(\frac{E - E_F}{kT}\right)} \tag{3.79}$$

when $E - E_F >> kT$ $\exp((E - E_F)/kT) >> 1$

$$f_F(E) \approx \frac{1}{\exp\left(\frac{E - E_F}{kT}\right)} \approx \exp\left[\frac{-(E - E_F)}{kT}\right] \tag{3.80}$$

Boltzmann approximation

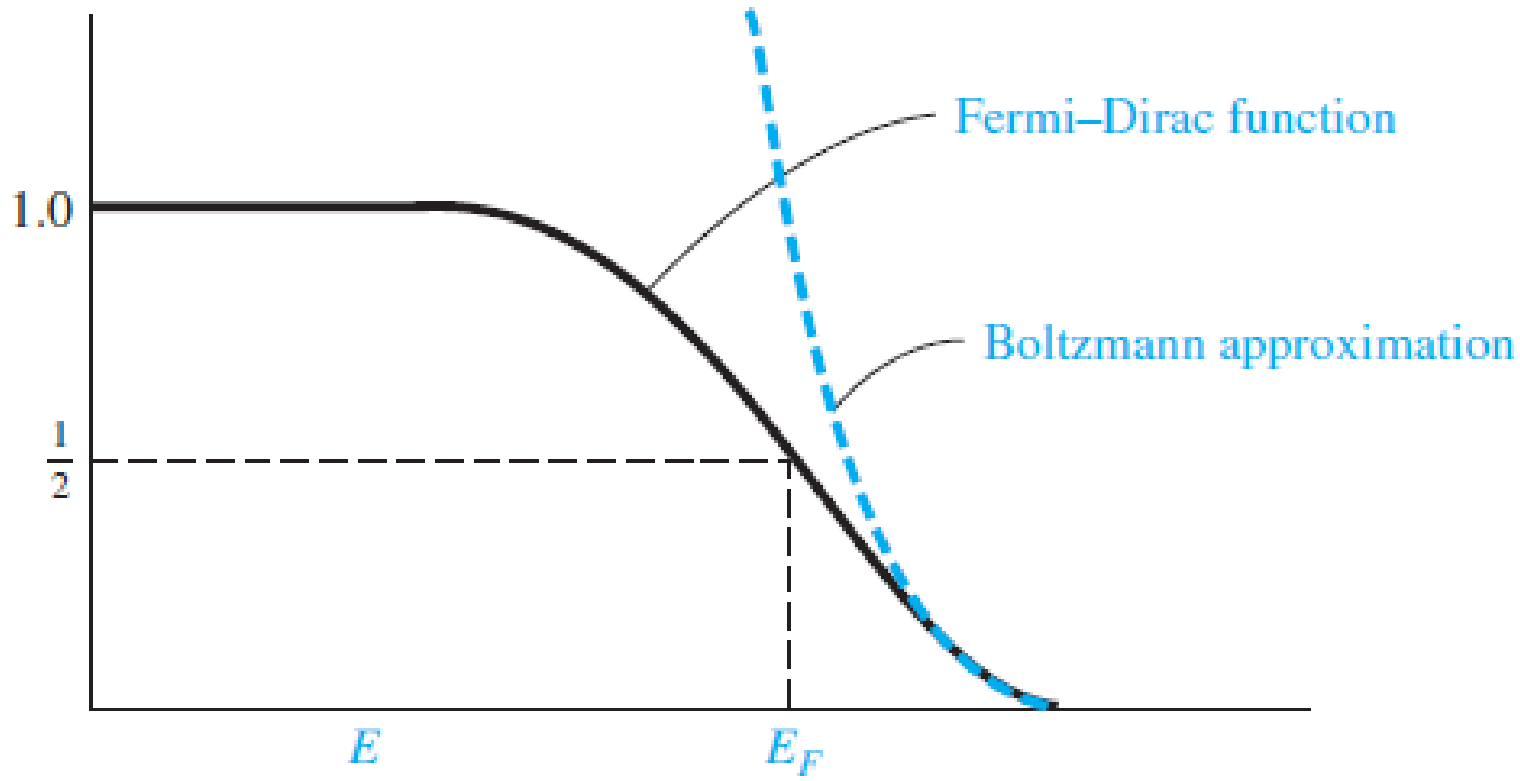


Figure 3.35 | The Fermi–Dirac probability function and the Maxwell–Boltzmann approximation.