

Chapter 3

Problem Solutions

3.1 If a_o were to increase, the bandgap energy would decrease and the material would begin to behave less like a semiconductor and more like a metal. If a_o were to decrease, the bandgap energy would increase and the material would begin to behave more like an insulator.

3.2

Schrodinger's wave equation

$$\frac{-\hbar^2}{2m} \cdot \frac{\partial^2 \Psi(x,t)}{\partial x^2} + V(x) \cdot \Psi(x,t) = j\hbar \frac{\partial \Psi(x,t)}{\partial t}$$

Let the solution be of the form

$$\Psi(x,t) = u(x) \exp \left[j \left(kx - \left(\frac{E}{\hbar} \right) t \right) \right]$$

Region I, $V(x) = 0$, so substituting the proposed solution into the wave equation, we obtain

$$\begin{aligned} \frac{-\hbar^2}{2m} \cdot \frac{\partial}{\partial x} \left\{ jku(x) \exp \left[j \left(kx - \left(\frac{E}{\hbar} \right) t \right) \right] \right. \\ \left. + \frac{\partial u(x)}{\partial x} \exp \left[j \left(kx - \left(\frac{E}{\hbar} \right) t \right) \right] \right\} \\ = j\hbar \left(\frac{-jE}{\hbar} \right) \cdot u(x) \exp \left[j \left(kx - \left(\frac{E}{\hbar} \right) t \right) \right] \end{aligned}$$

which becomes

$$\begin{aligned} \frac{-\hbar^2}{2m} \left\{ (jk)^2 u(x) \exp \left[j \left(kx - \left(\frac{E}{\hbar} \right) t \right) \right] \right. \\ \left. + 2jk \frac{\partial u(x)}{\partial x} \exp \left[j \left(kx - \left(\frac{E}{\hbar} \right) t \right) \right] \right. \\ \left. + \frac{\partial^2 u(x)}{\partial x^2} \exp \left[j \left(kx - \left(\frac{E}{\hbar} \right) t \right) \right] \right\} \\ = +Eu(x) \exp \left[j \left(kx - \left(\frac{E}{\hbar} \right) t \right) \right] \end{aligned}$$

This equation can then be written as

$$-k^2 u(x) + 2jk \frac{\partial u(x)}{\partial x} + \frac{\partial^2 u(x)}{\partial x^2} + \frac{2mE}{\hbar^2} \cdot u(x) = 0$$

Setting $u(x) = u_1(x)$ for region I, this equation becomes

$$\frac{d^2 u_1(x)}{dx^2} + 2jk \frac{du_1(x)}{dx} - (k^2 - \alpha^2) u_1(x) = 0$$

where

$$\alpha^2 = \frac{2mE}{\hbar^2}$$

Q.E.D.

In region II, $V(x) = V_o$. Assume the same form of the solution

$$\Psi(x,t) = u(x) \exp \left[j \left(kx - \left(\frac{E}{\hbar} \right) t \right) \right]$$

Substituting into Schrodinger's wave equation, we obtain

$$\begin{aligned} \frac{-\hbar^2}{2m} \left\{ (jk)^2 u(x) \exp \left[j \left(kx - \left(\frac{E}{\hbar} \right) t \right) \right] \right. \\ \left. + 2jk \frac{\partial u(x)}{\partial x} \exp \left[j \left(kx - \left(\frac{E}{\hbar} \right) t \right) \right] \right. \\ \left. + \frac{\partial^2 u(x)}{\partial x^2} \exp \left[j \left(kx - \left(\frac{E}{\hbar} \right) t \right) \right] \right\} \\ + V_o u(x) \exp \left[j \left(kx - \left(\frac{E}{\hbar} \right) t \right) \right] \\ = Eu(x) \exp \left[j \left(kx - \left(\frac{E}{\hbar} \right) t \right) \right] \end{aligned}$$

This equation can be written as

$$\begin{aligned} -k^2 u(x) + 2jk \frac{\partial u(x)}{\partial x} + \frac{\partial^2 u(x)}{\partial x^2} \\ - \frac{2mV_o}{\hbar^2} u(x) + \frac{2mE}{\hbar^2} u(x) = 0 \end{aligned}$$

Setting $u(x) = u_2(x)$ for region II, this equation becomes

$$\frac{d^2 u_2(x)}{dx^2} + 2jk \frac{du_2(x)}{dx} - \left(k^2 - \alpha^2 + \frac{2mV_o}{\hbar^2} \right) u_2(x) = 0$$

where

$$\alpha^2 = \frac{2mE}{\hbar^2}$$

Q.E.D.

3.3

We have

$$\frac{d^2 u_1(x)}{dx^2} + 2jk \frac{du_1(x)}{dx} - (k^2 - \alpha^2) u_1(x) = 0$$

The proposed solution is

$$u_1(x) = A \exp[j(\alpha - k)x] + B \exp[-j(\alpha + k)x]$$

The first derivative is

$$\frac{du_1(x)}{dx} = j(\alpha - k) A \exp[j(\alpha - k)x] - j(\alpha + k) B \exp[-j(\alpha + k)x]$$

and the second derivative becomes

$$\frac{d^2 u_1(x)}{dx^2} = [j(\alpha - k)]^2 A \exp[j(\alpha - k)x] + [j(\alpha + k)]^2 B \exp[-j(\alpha + k)x]$$

Substituting these equations into the differential equation, we find

$$\begin{aligned} & -(\alpha - k)^2 A \exp[j(\alpha - k)x] \\ & -(\alpha + k)^2 B \exp[-j(\alpha + k)x] \\ & + 2jk \{ j(\alpha - k) A \exp[j(\alpha - k)x] \\ & - j(\alpha + k) B \exp[-j(\alpha + k)x] \} \\ & - (k^2 - \alpha^2) \{ A \exp[j(\alpha - k)x] \\ & + B \exp[-j(\alpha + k)x] \} = 0 \end{aligned}$$

Combining terms, we have

$$\begin{aligned} & \{ -(\alpha^2 - 2\alpha k + k^2) - 2k(\alpha - k) \\ & - (k^2 - \alpha^2) \} A \exp[j(\alpha - k)x] \\ & + \{ -(\alpha^2 + 2\alpha k + k^2) + 2k(\alpha + k) \\ & - (k^2 - \alpha^2) \} B \exp[-j(\alpha + k)x] = 0 \end{aligned}$$

We find that

$$0 = 0 \quad \text{Q.E.D.}$$

For the differential equation in $u_2(x)$ and the proposed solution, the procedure is exactly the same as above.

3.4

We have the solutions

$$u_1(x) = A \exp[j(\alpha - k)x] + B \exp[-j(\alpha + k)x] \quad \text{for } 0 < x < a$$

$$u_2(x) = C \exp[j(\beta - k)x] + D \exp[-j(\beta + k)x] \quad \text{for } -b < x < 0$$

The boundary conditions:

$$u_1(0) = u_2(0)$$

which yields

$$A + B - C - D = 0$$

Also

$$\left. \frac{du_1}{dx} \right|_{x=0} = \left. \frac{du_2}{dx} \right|_{x=0}$$

which yields

$$(\alpha - k)A - (\alpha + k)B - (\beta - k)C + (\beta + k)D = 0$$

The third boundary condition is

$$u_1(a) = u_2(-b)$$

which gives

$$\begin{aligned} & A \exp[j(\alpha - k)a] + B \exp[-j(\alpha + k)a] \\ & = C \exp[j(\beta - k)(-b)] + D \exp[-j(\beta + k)(-b)] \end{aligned}$$

This becomes

$$\frac{A \exp[j(\alpha - k)a] + B \exp[-j(\alpha + k)a] - C \exp[-j(\beta - k)b] - D \exp[j(\beta + k)b]}{0} = 0$$

The last boundary condition is

$$\left. \frac{du_1}{dx} \right|_{x=a} = \left. \frac{du_2}{dx} \right|_{x=-b}$$

which gives

$$\begin{aligned} & j(\alpha - k) A \exp[j(\alpha - k)a] \\ & - j(\alpha + k) B \exp[-j(\alpha + k)a] \\ & = j(\beta - k) C \exp[j(\beta - k)(-b)] \\ & - j(\beta + k) D \exp[-j(\beta + k)(-b)] \end{aligned}$$

This becomes

$$\frac{(\alpha - k) A \exp[j(\alpha - k)a] - (\alpha + k) B \exp[-j(\alpha + k)a] - (\beta - k) C \exp[-j(\beta - k)b] + (\beta + k) D \exp[j(\beta + k)b]}{0} = 0$$

3.5 Computer plot

3.6 Computer plot

3.7

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

Let $ka = y$, $\alpha a = x$

Then

$$P' \frac{\sin x}{x} + \cos x = \cos y$$

Consider $\frac{d}{dy}$ of this function

$$\frac{d}{dy} \left\{ \left[P' \cdot (x)^{-1} \cdot \sin x \right] + \cos x \right\} = -\sin y$$

We obtain

$$P' \left\{ (-1)(x)^{-2} \sin x \frac{dx}{dy} + (x)^{-1} \cos x \frac{dx}{dy} \right\} - \sin x \frac{dx}{dy} = -\sin y$$

Then

$$\frac{dx}{dy} \left\{ P' \left[\frac{-1}{x^2} \sin x + \frac{\cos x}{x} \right] - \sin x \right\} = -\sin y$$

For $y = ka = n\pi$, $n = 0, 1, 2, \dots$

$$\Rightarrow \sin y = 0$$

So that, in general, then

$$\frac{dx}{dy} = 0 = \frac{d(\alpha a)}{d(ka)} = \frac{d\alpha}{dk}$$

And

$$\alpha = \sqrt{\frac{2mE}{\hbar^2}} \Rightarrow \frac{d\alpha}{dk} = \frac{1}{2} \left(\frac{2mE}{\hbar^2} \right)^{-1/2} \left(\frac{2m}{\hbar^2} \right) \frac{dE}{dk}$$

This implies that

$$\frac{d\alpha}{dk} = 0 = \frac{dE}{dk} \text{ for } k = \frac{n\pi}{a}$$

3.8

$$f(\alpha a) = 9 \frac{\sin \alpha a}{\alpha a} + \cos \alpha a = \cos ka$$

(a) $ka = \pi \Rightarrow \cos ka = -1$

1st point: $\alpha a = \pi$; 2nd point: $\alpha a = 1.66\pi$
(2nd point by trial and error)

Now

$$\alpha a = a \sqrt{\frac{2mE}{\hbar^2}} \Rightarrow E = \left(\frac{\alpha a}{a} \right)^2 \cdot \frac{\hbar^2}{2m}$$

So

$$E = \frac{(\alpha a)^2}{(5 \times 10^{-10})^2} \cdot \frac{(1.054 \times 10^{-34})^2}{2(9.11 \times 10^{-31})} \Rightarrow$$

$$E = (\alpha a)^2 [2.439 \times 10^{-20}] \text{ (J)}$$

or

$$E = (\alpha a)^2 (0.1524) \text{ (eV)}$$

So

$$\alpha a = \pi \Rightarrow E_1 = 1.504 \text{ eV}$$

$$\alpha a = 1.66\pi \Rightarrow E_2 = 4.145 \text{ eV}$$

Then

$$\Delta E = 2.64 \text{ eV}$$

(b)

$$ka = 2\pi \Rightarrow \cos ka = +1$$

$$1^{\text{st}} \text{ point: } \alpha a = 2\pi$$

$$2^{\text{nd}} \text{ point: } \alpha a = 2.54\pi$$

Then

$$E_3 = 6.0165 \text{ eV}$$

$$E_4 = 9.704 \text{ eV}$$

so

$$\Delta E = 3.69 \text{ eV}$$

(c)

$$ka = 3\pi \Rightarrow \cos ka = -1$$

$$1^{\text{st}} \text{ point: } \alpha a = 3\pi$$

$$2^{\text{nd}} \text{ point: } \alpha a = 3.44\pi$$

Then

$$E_5 = 13.537 \text{ eV}$$

$$E_6 = 17.799 \text{ eV}$$

so

$$\Delta E = 4.26 \text{ eV}$$

(d)

$$ka = 4\pi \Rightarrow \cos ka = +1$$

$$1^{\text{st}} \text{ point: } \alpha a = 4\pi$$

$$2^{\text{nd}} \text{ point: } \alpha a = 4.37\pi$$

Then

$$E_7 = 24.066 \text{ eV}$$

$$E_8 = 28.724 \text{ eV}$$

so

$$\Delta E = 4.66 \text{ eV}$$

3.9

(a) $0 < ka < \pi$

For $ka = 0 \Rightarrow \cos ka = +1$

By trial and error: 1st point: $\alpha a = 0.822\pi$

2nd point: $\alpha a = \pi$

From Problem 3.8, $E = (\alpha a)^2 (0.1524) \text{ (eV)}$

Then

$$E_1 = 1.0163 \text{ eV}$$

$$E_2 = 1.5041 \text{ eV}$$

so

$$\Delta E = 0.488 \text{ eV}$$

(b)

$\pi < ka < 2\pi$

Using results of Problem 3.8

1st point: $\alpha a = 1.66\pi$

2nd point: $\alpha a = 2\pi$

Then

$$E_3 = 4.145 \text{ eV}$$

$$E_4 = 6.0165 \text{ eV}$$

so

$$\underline{\Delta E = 1.87 \text{ eV}}$$

(c)

$$2\pi < ka < 3\pi$$

$$1^{\text{st}} \text{ point: } \alpha a = 2.54\pi$$

$$2^{\text{nd}} \text{ point: } \alpha a = 3\pi$$

Then

$$E_5 = 9.704 \text{ eV}$$

$$E_6 = 13.537 \text{ eV}$$

so

$$\underline{\Delta E = 3.83 \text{ eV}}$$

(d)

$$3\pi < ka < 4\pi$$

$$1^{\text{st}} \text{ point: } \alpha a = 3.44\pi$$

$$2^{\text{nd}} \text{ point: } \alpha a = 4\pi$$

Then

$$E_7 = 17.799 \text{ eV}$$

$$E_8 = 24.066 \text{ eV}$$

so

$$\underline{\Delta E = 6.27 \text{ eV}}$$

3.10

$$6 \frac{\sin \alpha a}{\alpha a} + \cos \alpha a = \cos ka$$

Forbidden energy bands

(a) $ka = \pi \Rightarrow \cos ka = -1$

$$1^{\text{st}} \text{ point: } \alpha a = \pi$$

$$2^{\text{nd}} \text{ point: } \alpha a = 1.56\pi \text{ (By trial and error)}$$

From Problem 3.8, $E = (\alpha a)^2 (0.1524) \text{ eV}$

Then

$$E_1 = 1.504 \text{ eV}$$

$$E_2 = 3.660 \text{ eV}$$

so

$$\underline{\Delta E = 2.16 \text{ eV}}$$

(b)

$$ka = 2\pi \Rightarrow \cos ka = +1$$

$$1^{\text{st}} \text{ point: } \alpha a = 2\pi$$

$$2^{\text{nd}} \text{ point: } \alpha a = 2.42\pi$$

Then

$$E_3 = 6.0165 \text{ eV}$$

$$E_4 = 8.809 \text{ eV}$$

so

$$\underline{\Delta E = 2.79 \text{ eV}}$$

(c)

$$ka = 3\pi \Rightarrow \cos ka = -1$$

$$1^{\text{st}} \text{ point: } \alpha a = 3\pi$$

$$2^{\text{nd}} \text{ point: } \alpha a = 3.33\pi$$

Then

$$E_5 = 13.537 \text{ eV}$$

$$E_6 = 16.679 \text{ eV}$$

so

$$\underline{\Delta E = 3.14 \text{ eV}}$$

(d)

$$ka = 4\pi \Rightarrow \cos ka = +1$$

$$1^{\text{st}} \text{ point: } \alpha a = 4\pi$$

$$2^{\text{nd}} \text{ point: } \alpha a = 4.26\pi$$

Then

$$E_7 = 24.066 \text{ eV}$$

$$E_8 = 27.296 \text{ eV}$$

so

$$\underline{\Delta E = 3.23 \text{ eV}}$$

3.11

Allowed energy bands

Use results from Problem 3.10.

(a)

$$0 < ka < \pi$$

$$1^{\text{st}} \text{ point: } \alpha a = 0.759\pi \text{ (By trial and error)}$$

$$2^{\text{nd}} \text{ point: } \alpha a = \pi$$

We have

$$E = (\alpha a)^2 (0.1524) \text{ eV}$$

Then

$$E_1 = 0.8665 \text{ eV}$$

$$E_2 = 1.504 \text{ eV}$$

so

$$\underline{\Delta E = 0.638 \text{ eV}}$$

(b)

$$\pi < ka < 2\pi$$

$$1^{\text{st}} \text{ point: } \alpha a = 1.56\pi$$

$$2^{\text{nd}} \text{ point: } \alpha a = 2\pi$$

Then

$$E_3 = 3.660 \text{ eV}$$

$$E_4 = 6.0165 \text{ eV}$$

so

$$\underline{\Delta E = 2.36 \text{ eV}}$$

(c)

$$2\pi < ka < 3\pi$$

$$1^{\text{st}} \text{ point: } \alpha a = 2.42\pi$$

$$2^{\text{nd}} \text{ point: } \alpha a = 3\pi$$

Then

$$E_5 = 8.809 \text{ eV}$$

$$E_6 = 13.537 \text{ eV}$$

so

$$\underline{\Delta E = 4.73 \text{ eV}}$$

(d)

$$3\pi < ka < 4\pi$$

$$1^{\text{st}} \text{ point: } \alpha a = 3.33\pi$$

$$2^{\text{nd}} \text{ point: } \alpha a = 4\pi$$

Then

$$E_7 = 16.679 \text{ eV}$$

$$E_8 = 24.066 \text{ eV}$$

so

$$\underline{\Delta E = 7.39 \text{ eV}}$$

3.12

$$T = 100\text{K}; E_g = 1.170 - \frac{(4.73 \times 10^{-4})(100)^2}{636 + 100} \Rightarrow$$

$$\underline{E_g = 1.164 \text{ eV}}$$

$$T = 200\text{K} \Rightarrow \underline{E_g = 1.147 \text{ eV}}$$

$$T = 300\text{K} \Rightarrow \underline{E_g = 1.125 \text{ eV}}$$

$$T = 400\text{K} \Rightarrow \underline{E_g = 1.097 \text{ eV}}$$

$$T = 500\text{K} \Rightarrow \underline{E_g = 1.066 \text{ eV}}$$

$$T = 600\text{K} \Rightarrow \underline{E_g = 1.032 \text{ eV}}$$

3.13

The effective mass is given by

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

We have that

$$\frac{d^2 E}{dk^2} (\text{curve A}) > \frac{d^2 E}{dk^2} (\text{curve B})$$

so that

$$\underline{m^* (\text{curve A}) < m^* (\text{curve B})}$$

3.14

The effective mass for a hole is given by

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

We have that

$$\left| \frac{d^2 E}{dk^2} \right| (\text{curve A}) > \left| \frac{d^2 E}{dk^2} \right| (\text{curve B})$$

so that

$$\underline{m_p^* (\text{curve A}) < m_p^* (\text{curve B})}$$

3.15

Points A, B: $\frac{\partial E}{\partial k} < 0 \Rightarrow$ velocity in $-x$ direction;

Points C, D: $\frac{\partial E}{\partial x} > 0 \Rightarrow$ velocity in $+x$ direction;

Points A, D; $\frac{\partial^2 E}{\partial k^2} < 0 \Rightarrow$ negative effective mass;

Points B, C; $\frac{\partial^2 E}{\partial k^2} > 0 \Rightarrow$ positive effective mass;

3.16

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

$$\text{At } k = 0.1 (A^\circ)^{-1} \Rightarrow \frac{1}{k} = 10 A^\circ = 10^{-9} \text{ m}$$

So

$$k = 10^{+9} \text{ m}^{-1}$$

For A:

$$(0.07)(1.6 \times 10^{-19}) = \frac{(10^9)^2 (1.054 \times 10^{-34})^2}{2m}$$

which yields

$$m = 4.96 \times 10^{-31} \text{ kg}$$

so

$$\underline{\text{curve A; } \frac{m}{m_0} = 0.544}$$

For B:

$$(0.7)(1.6 \times 10^{-19}) = \frac{(10^9)(1.054 \times 10^{-34})^2}{2m}$$

which yields

$$m = 4.96 \times 10^{-32} \text{ kg}$$

so

$$\underline{\text{Curve B: } \frac{m}{m_0} = 0.0544}$$

3.17

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

$$k = 0.1 (A^*)^{-1} \Rightarrow 10^9 m^{-1}$$

For Curve A:

$$(0.08)(1.6 \times 10^{-19}) = \frac{(10^9)^2 (1.054 \times 10^{-34})^2}{2m}$$

which yields

$$m = 4.34 \times 10^{-31} \text{ kg} \Rightarrow \frac{m}{m_o} = 0.476$$

For Curve B:

$$(0.4)(1.6 \times 10^{-19}) = \frac{(10^9)^2 (1.054 \times 10^{-34})^2}{2m}$$

which yields

$$m = 8.68 \times 10^{-32} \text{ kg} \Rightarrow \frac{m}{m_o} = 0.0953$$

3.18

(a) $E = h\nu$

Then

$$\nu = \frac{E}{h} = \frac{(1.42)(1.6 \times 10^{-19})}{(6.625 \times 10^{-34})} \Rightarrow$$

$$\nu = 3.43 \times 10^{14} \text{ Hz}$$

(b)

$$\lambda = \frac{c}{\nu} = \frac{3 \times 10^8}{3.43 \times 10^{14}} = 8.75 \times 10^{-7} \text{ m}$$

or

$$\lambda = 0.875 \mu\text{m}$$

3.19

(c) Curve A: Effective mass is a constant
Curve B: Effective mass is positive around

$$k = 0, \text{ and is negative around } k = \pm \frac{\pi}{2}.$$

3.20

$$E = E_o - E_1 \cos[\alpha(k - k_o)]$$

$$\frac{dE}{dk} = (-E_1)(-\alpha) \sin[\alpha(k - k_o)]$$

$$= +E_1 \alpha \sin[\alpha(k - k_o)]$$

So

$$\frac{d^2 E}{dk^2} = E_1 \alpha^2 \cos[\alpha(k - k_o)]$$

Then

$$\left. \frac{d^2 E}{dk^2} \right|_{k=k_o} = E_1 \alpha^2$$

We have

$$\frac{1}{m^*} = \frac{1}{\hbar^2} \cdot \frac{d^2 E}{dk^2} = \frac{E_1 \alpha^2}{\hbar^2}$$

or

$$m^* = \frac{\hbar^2}{E_1 \alpha^2}$$

3.21

For the 3-dimensional infinite potential well, $V(x) = 0$ when $0 < x < a$, $0 < y < a$, and $0 < z < a$. In this region, the wave equation is

$$\frac{\partial^2 \psi(x, y, z)}{\partial x^2} + \frac{\partial^2 \psi(x, y, z)}{\partial y^2} + \frac{\partial^2 \psi(x, y, z)}{\partial z^2} + \frac{2mE}{\hbar^2} \psi(x, y, z) = 0$$

Use separation of variables technique, so let

$$\psi(x, y, z) = X(x)Y(y)Z(z)$$

Substituting into the wave equation, we have

$$YZ \frac{\partial^2 X}{\partial x^2} + XZ \frac{\partial^2 Y}{\partial y^2} + XY \frac{\partial^2 Z}{\partial z^2} + \frac{2mE}{\hbar^2} \cdot XYZ = 0$$

Dividing by XYZ , we obtain

$$\frac{1}{X} \cdot \frac{\partial^2 X}{\partial x^2} + \frac{1}{Y} \cdot \frac{\partial^2 Y}{\partial y^2} + \frac{1}{Z} \cdot \frac{\partial^2 Z}{\partial z^2} + \frac{2mE}{\hbar^2} = 0$$

Let

$$\frac{1}{X} \cdot \frac{\partial^2 X}{\partial x^2} = -k_x^2 \Rightarrow \frac{\partial^2 X}{\partial x^2} + k_x^2 X = 0$$

The solution is of the form

$$X(x) = A \sin k_x x + B \cos k_x x$$

Since $\psi(x, y, z) = 0$ at $x = 0$, then $X(0) = 0$ so that $B \equiv 0$.

Also, $\psi(x, y, z) = 0$ at $x = a$, then $X(a) = 0$ so we must have $k_x a = n_x \pi$, where

$$n_x = 1, 2, 3, \dots$$

Similarly, we have

$$\frac{1}{Y} \cdot \frac{\partial^2 Y}{\partial y^2} = -k_y^2 \quad \text{and} \quad \frac{1}{Z} \cdot \frac{\partial^2 Z}{\partial z^2} = -k_z^2$$

From the boundary conditions, we find

$$k_y a = n_y \pi \text{ and } k_z a = n_z \pi$$

where $n_y = 1, 2, 3, \dots$ and $n_z = 1, 2, 3, \dots$

From the wave equation, we have

$$-k_x^2 - k_y^2 - k_z^2 + \frac{2mE}{\hbar^2} = 0$$

The energy can then be written as

$$E = \frac{\hbar^2}{2m} (n_x^2 + n_y^2 + n_z^2) \left(\frac{\pi}{a} \right)^2$$

3.22

The total number of quantum states in the 3-dimensional potential well is given (in k-space) by

$$g_T(k) dk = \frac{\pi k^2 dk}{\pi^3} \cdot a^3$$

where

$$k^2 = \frac{2mE}{\hbar^2}$$

We can then write

$$k = \frac{1}{\hbar} \cdot \sqrt{2mE}$$

Taking the differential, we obtain

$$dk = \frac{1}{\hbar} \cdot \sqrt{2m} \cdot \frac{1}{2} \cdot \frac{1}{\sqrt{E}} \cdot dE = \frac{1}{\hbar} \cdot \sqrt{\frac{m}{2E}} \cdot dE$$

Substituting these expressions into the density of states function, we obtain

$$g_T(E) dE = \frac{\pi a^3}{\pi^3} \left(\frac{2mE}{\hbar^2} \right) \cdot \frac{1}{\hbar} \cdot \sqrt{\frac{m}{2E}} \cdot dE$$

Noting that

$$\hbar = \frac{h}{2\pi}$$

this density of states function can be simplified and written as

$$g_T(E) dE = \frac{4\pi a^3}{h^3} (2m)^{3/2} \cdot \sqrt{E} \cdot dE$$

Dividing by a^3 will yield the density of states, so that

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

3.23

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

Now

$$\begin{aligned} g_T &= \frac{4\pi(2m_n^*)^{3/2}}{h^3} \int_{E_c}^{E_c+kT} \sqrt{E - E_c} \cdot dE \\ &= \frac{4\pi(2m_n^*)^{3/2}}{h^3} \left(\frac{2}{3} \right) (E - E_c)^{3/2} \Big|_{E_c}^{E_c+kT} \\ &= \frac{4\pi(2m_n^*)^{3/2}}{h^3} \left(\frac{2}{3} \right) (kT)^{3/2} \end{aligned}$$

Then

$$\begin{aligned} g_T &= \frac{4\pi [2(0.067)(9.11 \times 10^{-31})]^{3/2}}{(6.625 \times 10^{-34})^3} \left(\frac{2}{3} \right) \\ &\quad \times [(0.0259)(1.6 \times 10^{-19})]^{3/2} \end{aligned}$$

or

$$g_T = 3.28 \times 10^{23} \text{ m}^{-3} = 3.28 \times 10^{17} \text{ cm}^{-3}$$

3.24

$$g_V(E) = \frac{4\pi(2m_p^*)^{3/2}}{h^3} \sqrt{E_V - E}$$

Now

$$\begin{aligned} g_T &= \frac{4\pi(2m_p^*)^{3/2}}{h^3} \int_{E_V-kT}^{E_V} \sqrt{E_V - E} \cdot dE \\ &= \frac{4\pi(2m_p^*)^{3/2}}{h^3} \left(\frac{-2}{3} \right) (E_V - E)^{3/2} \Big|_{E_V-kT}^{E_V} \\ &= \frac{4\pi(2m_p^*)^{3/2}}{h^3} \left(\frac{2}{3} \right) (kT)^{3/2} \end{aligned}$$

$$g_T = \frac{4\pi [2(0.48)(9.11 \times 10^{-31})]^{3/2}}{(6.625 \times 10^{-34})^3} \left(\frac{2}{3} \right)$$

$$\times [(0.0259)(1.6 \times 10^{-19})]^{3/2}$$

or

$$g_T = 6.29 \times 10^{24} \text{ m}^{-3} = 6.29 \times 10^{18} \text{ cm}^{-3}$$

3.25

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

$$\begin{aligned} &= \frac{4\pi [2(1.08)(9.11 \times 10^{-31})]^{3/2}}{(6.625 \times 10^{-34})^3} (1.6 \times 10^{-19})^{1/2} \sqrt{E - E_c} \\ &= 4.77 \times 10^{46} \sqrt{E - E_c} \text{ m}^{-3} \text{ J}^{-1} \end{aligned}$$

or

$$g_c(E) = 7.63 \times 10^{21} \sqrt{E - E_c} \text{ cm}^{-3} \text{ eV}^{-1}$$

Then

E	g_c
$E_c + 0.05 \text{ eV}$	$1.71 \times 10^{21} \text{ cm}^{-3} \text{ eV}^{-1}$
$E_c + 0.10 \text{ eV}$	2.41×10^{21}
$E_c + 0.15 \text{ eV}$	2.96×10^{21}
$E_c + 0.20 \text{ eV}$	3.41×10^{21}

$$\begin{aligned} \text{(b)} \quad g_v(E) &= \frac{4\pi(2m_p^*)^{3/2}}{h^3} \sqrt{E_v - E} \\ &= \frac{4\pi[2(0.56)(9.11 \times 10^{-31})]^{3/2}}{(6.625 \times 10^{-34})^3} (1.6 \times 10^{-19})^{1/2} \sqrt{E_v - E} \\ &= 1.78 \times 10^{46} \sqrt{E_v - E} \text{ m}^{-3} \text{ J}^{-1} \\ g_v(E) &= 2.85 \times 10^{21} \sqrt{E_v - E} \text{ cm}^{-3} \text{ eV}^{-1} \end{aligned}$$

E	$g_v(E)$
$E_v - 0.05 \text{ eV}$	$0.637 \times 10^{21} \text{ cm}^{-3} \text{ eV}^{-1}$
$E_v - 0.10 \text{ eV}$	0.901×10^{21}
$E_v - 0.15 \text{ eV}$	1.10×10^{21}
$E_v - 0.20 \text{ eV}$	1.27×10^{21}

3.26

$$\frac{g_c}{g_v} = \frac{(m_n^*)^{3/2}}{(m_p^*)^{3/2}} \Rightarrow \frac{g_c}{g_v} = \left(\frac{m_n^*}{m_p^*} \right)^{3/2}$$

3.27

Computer Plot

3.28

$$\begin{aligned} \frac{g_i!}{N_i!(g_i - N_i)!} &= \frac{10!}{8!(10-8)!} \\ &= \frac{(10)(9)(8!)}{(8!)(2!)} = \frac{(10)(9)}{(2)(1)} \Rightarrow \underline{45} \end{aligned}$$

3.29

$$\text{(a)} \quad f(E) = \frac{1}{1 + \exp\left[\frac{(E_c + kT) - E_c}{kT}\right]}$$

$$= \frac{1}{1 + \exp(1)} \Rightarrow \underline{f(E) = 0.269}$$

(b)

$$\begin{aligned} 1 - f(E) &= 1 - \frac{1}{1 + \exp\left[\frac{(E_v - kT) - E_v}{kT}\right]} \\ &= 1 - \frac{1}{1 + \exp(-1)} \Rightarrow \underline{1 - f(E) = 0.269} \end{aligned}$$

3.30

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

$$\text{(a)} \quad E - E_F = kT, \quad f(E) = \frac{1}{1 + \exp(1)} \Rightarrow$$

$$\underline{f(E) = 0.269}$$

$$\text{(b)} \quad E - E_F = 5kT, \quad f(E) = \frac{1}{1 + \exp(5)} \Rightarrow$$

$$\underline{f(E) = 6.69 \times 10^{-3}}$$

$$\text{(c)} \quad E - E_F = 10kT, \quad f(E) = \frac{1}{1 + \exp(10)} \Rightarrow$$

$$\underline{f(E) = 4.54 \times 10^{-5}}$$

3.31

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

or

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

$$\text{(a)} \quad E_F - E = kT, \quad 1 - f(E) = 0.269$$

$$\text{(b)} \quad E_F - E = 5kT, \quad 1 - f(E) = 6.69 \times 10^{-3}$$

$$\text{(c)} \quad E_F - E = 10kT, \quad 1 - f(E) = 4.54 \times 10^{-5}$$

3.32

$$\text{(a)} \quad T = 300\text{K} \Rightarrow kT = 0.0259 \text{ eV}$$

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

E	$f(E)$
E_c	6.43×10^{-5}
$E_c + (1/2)kT$	3.90×10^{-5}
$E_c + kT$	2.36×10^{-5}
$E_c + (3/2)kT$	1.43×10^{-5}
$E_c + 2kT$	0.87×10^{-5}

(b) $T = 400K \Rightarrow kT = 0.03453$

E	$f(E)$
E_c	7.17×10^{-4}
$E_c + (1/2)kT$	4.35×10^{-4}
$E_c + kT$	2.64×10^{-4}
$E_c + (3/2)kT$	1.60×10^{-4}
$E_c + 2kT$	0.971×10^{-4}

3.33

$$E_n = \frac{\hbar^2 n^2 \pi^2}{2ma^2} = \frac{(1.054 \times 10^{-34})^2 n^2 \pi^2}{2(9.11 \times 10^{-31})(10 \times 10^{-10})^2}$$

or

$$E_n = 6.018 \times 10^{-20} n^2 \text{ J} = 0.376 n^2 \text{ eV}$$

$$\text{For } n = 4 \Rightarrow E_4 = 6.02 \text{ eV},$$

$$\text{For } n = 5 \Rightarrow E_5 = 9.40 \text{ eV}.$$

As a 1st approximation for $T > 0$, assume the probability of $n = 5$ state being occupied is the same as the probability of $n = 4$ state being empty. Then

$$1 - \frac{1}{1 + \exp\left(\frac{E_4 - E_F}{kT}\right)} = \frac{1}{1 + \exp\left(\frac{E_5 - E_F}{kT}\right)}$$

$$\Rightarrow \frac{1}{1 + \exp\left(\frac{E_F - E_4}{kT}\right)} = \frac{1}{1 + \exp\left(\frac{E_5 - E_F}{kT}\right)}$$

or

$$E_F - E_4 = E_5 - E_F \Rightarrow E_F = \frac{E_4 + E_5}{2}$$

Then

$$E_F = \frac{6.02 + 9.40}{2} \Rightarrow E_F = 7.71 \text{ eV}$$

3.34

(a) For 3-Dimensional infinite potential well,

$$\begin{aligned} E &= \frac{\hbar^2 \pi^2}{2ma^2} (n_x^2 + n_y^2 + n_z^2) \\ &= \frac{(1.054 \times 10^{-34})^2 \pi^2}{2(9.11 \times 10^{-31})(10^{-9})^2} (n_x^2 + n_y^2 + n_z^2) \\ &= 0.376 (n_x^2 + n_y^2 + n_z^2) \text{ eV} \end{aligned}$$

For 5 electrons, energy state corresponding to $n_x n_y n_z = 221 = 122$ contains both an electron and an empty state, so

$$E_F = (0.376)(2^2 + 2^2 + 1^2) \Rightarrow$$

$$E_F = 3.384 \text{ eV}$$

(b) For 13 electrons, energy state corresponding to $n_x n_y n_z = 323 = 233$ contains both an electron and an empty state, so

$$E_F = (0.376)(2^2 + 3^2 + 3^2) \Rightarrow$$

$$E_F = 8.272 \text{ eV}$$

3.35

The probability of a state at $E_1 = E_F + \Delta E$ being occupied is

$$f_1(E_1) = \frac{1}{1 + \exp\left(\frac{E_1 - E_F}{kT}\right)} = \frac{1}{1 + \exp\left(\frac{\Delta E}{kT}\right)}$$

The probability of a state at $E_2 = E_F - \Delta E$ being empty is

$$\begin{aligned} 1 - f_2(E_2) &= 1 - \frac{1}{1 + \exp\left(\frac{E_2 - E_F}{kT}\right)} \\ &= 1 - \frac{1}{1 + \exp\left(\frac{-\Delta E}{kT}\right)} = \frac{\exp\left(\frac{-\Delta E}{kT}\right)}{1 + \exp\left(\frac{-\Delta E}{kT}\right)} \end{aligned}$$

or

$$1 - f_2(E_2) = \frac{1}{1 + \exp\left(\frac{+\Delta E}{kT}\right)}$$

Hence, we have that

$$f_1(E_1) = 1 - f_2(E_2) \quad \text{Q.E.D.}$$

3.36

(a) At energy E_1 , we want

$$\frac{\frac{1}{\exp\left(\frac{E_1 - E_F}{kT}\right)} - \frac{1}{1 + \exp\left(\frac{E_1 - E_F}{kT}\right)}}{1 + \exp\left(\frac{E_1 - E_F}{kT}\right)} = 0.01$$

This expression can be written as

$$\frac{1 + \exp\left(\frac{E_1 - E_F}{kT}\right)}{\exp\left(\frac{E_1 - E_F}{kT}\right)} - 1 = 0.01$$

$$\Rightarrow 1 = (0.01) \exp\left(\frac{E_1 - E_F}{kT}\right)$$

or

$$E_1 = E_F + kT \ln(100)$$

Then

$$E_1 = E_F + 4.6kT$$

(b)

$$\text{At } E_1 = E_F + 4.6kT,$$

$$f(E_1) = \frac{1}{1 + \exp\left(\frac{E_1 - E_F}{kT}\right)} = \frac{1}{1 + \exp\left(\frac{4.6kT}{kT}\right)}$$

which yields

$$f(E_1) = 0.00990 \approx 0.01$$

3.37

(a) $E_F = 6.25 \text{ eV}$, $T = 300 \text{ K}$, At $E = 6.50 \text{ eV}$

$$f(E) = \frac{1}{1 + \exp\left(\frac{6.50 - 6.25}{0.0259}\right)} = 6.43 \times 10^{-5}$$

or

$$\underline{6.43 \times 10^{-3} \%}$$

(b)

$$T = 950 \text{ K} \Rightarrow kT = (0.0259) \left(\frac{950}{300}\right)$$

or

$$kT = 0.0820 \text{ eV}$$

Then

$$f(E) = \frac{1}{1 + \exp\left(\frac{6.50 - 6.25}{0.0820}\right)} = 0.0453$$

or

$$\underline{4.53 \%}$$

$$(c) 1 - 0.01 = \frac{1}{1 + \exp\left(\frac{-0.30}{kT}\right)} = 0.99$$

Then

$$1 + \exp\left(\frac{-0.30}{kT}\right) = \frac{1}{0.99} = 1.0101$$

which can be written as

$$\exp\left(\frac{+0.30}{kT}\right) = \frac{1}{0.0101} = 99$$

Then

$$\frac{0.30}{kT} = \ln(99) \Rightarrow kT = \frac{0.30}{\ln(99)} = 0.06529$$

So

$$\underline{T = 756 \text{ K}}$$

3.38

(a)

$$f(E) = \frac{1}{1 + \exp\left(\frac{7.15 - 7.0}{0.0259}\right)} = 0.00304$$

or

$$\underline{0.304 \%}$$

(b)

$$\text{At } T = 1000 \text{ K} \Rightarrow kT = 0.08633 \text{ eV}$$

Then

$$f(E) = \frac{1}{1 + \exp\left(\frac{7.15 - 7.0}{0.08633}\right)} = 0.1496$$

$$\text{or } \underline{14.96 \%}$$

(c)

$$f(E) = \frac{1}{1 + \exp\left(\frac{6.85 - 7.0}{0.0259}\right)} = 0.997$$

or

$$\underline{99.7 \%}$$

(d)

$$\text{At } E = E_F, f(E) = \frac{1}{2} \text{ for all temperatures.}$$

3.39

For $E = E_1$,

$$f(E) = \frac{1}{1 + \exp\left(\frac{E_1 - E_F}{kT}\right)} \approx \exp\left[\frac{-(E_1 - E_F)}{kT}\right]$$

Then

$$f(E_1) = \exp\left(\frac{-0.30}{0.0259}\right) \Rightarrow f(E_1) = 9.3 \times 10^{-6}$$

For $E = E_2$, $E_F - E_2 = 1.12 - 0.3 = 0.82 \text{ eV}$

$$1 - f(E) = 1 - \frac{1}{1 + \exp\left(\frac{-0.82}{0.0259}\right)}$$

or

$$1 - f(E) \approx 1 - \left[1 - \exp\left(\frac{-0.82}{0.0259}\right)\right]$$

$$= \exp\left(\frac{-0.82}{0.0259}\right) \Rightarrow 1 - f(E) = 1.78 \times 10^{-14}$$

(b)

For $E_F - E_2 = 0.4 \Rightarrow E_1 - E_F = 0.72 \text{ eV}$

At $E = E_1$,

$$f(E) = \exp\left[\frac{-(E_1 - E_F)}{kT}\right] = \exp\left(\frac{-0.72}{0.0259}\right)$$

so

$$f(E) = 8.45 \times 10^{-13}$$

At $E = E_2$,

$$1 - f(E) = \exp\left[\frac{-(E_F - E_2)}{kT}\right] = \exp\left(\frac{-0.4}{0.0259}\right)$$

so

$$1 - f(E) = 1.96 \times 10^{-7}$$

3.40

(a) At $E = E_1$,

$$f(E) = \exp\left[\frac{-(E - E_F)}{kT}\right] = \exp\left(\frac{-0.30}{0.0259}\right)$$

or

$$f(E) = 9.3 \times 10^{-6}$$

At $E = E_2$, then

$$E_F - E_2 = 1.42 - 0.3 = 1.12 \text{ eV},$$

So

$$1 - f(E) = \exp\left[\frac{-(E_F - E_2)}{kT}\right] = \exp\left(\frac{-1.12}{0.0259}\right)$$

or

$$1 - f(E) = 1.66 \times 10^{-19}$$

(b)

For $E_F - E_2 = 0.4 \Rightarrow E_1 - E_F = 1.02 \text{ eV}$,

At $E = E_1$,

$$f(E) = \exp\left[\frac{-(E_1 - E_F)}{kT}\right] = \exp\left(\frac{-1.02}{0.0259}\right)$$

or

$$f(E) = 7.88 \times 10^{-18}$$

At $E = E_2$,

$$1 - f(E) = \exp\left[\frac{-(E_F - E_2)}{kT}\right] = \exp\left(\frac{-0.4}{0.0259}\right)$$

or

$$1 - f(E) = 1.96 \times 10^{-7}$$

3.41

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

so

$$\frac{df(E)}{dE} = (-1) \left[1 + \exp\left(\frac{E - E_F}{kT}\right)\right]^{-2}$$

$$\times \left(\frac{1}{kT}\right) \exp\left(\frac{E - E_F}{kT}\right)$$

or

$$\frac{df(E)}{dE} = \frac{-\frac{1}{kT} \exp\left(\frac{E - E_F}{kT}\right)}{\left[1 + \exp\left(\frac{E - E_F}{kT}\right)\right]^2}$$

(a) $T = 0$, For

$$E < E_F \Rightarrow \exp(-\infty) = 0 \Rightarrow \frac{df}{dE} = 0$$

$$E > E_F \Rightarrow \exp(+\infty) = +\infty \Rightarrow \frac{df}{dE} = 0$$

$$\text{At } E = E_F \Rightarrow \frac{df}{dE} \rightarrow -\infty$$

3.42

(a) At $E = E_{midgap}$,

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

Si: $E_g = 1.12 \text{ eV}$,

$$f(E) = \frac{1}{1 + \exp\left[\frac{1.12}{2(0.0259)}\right]}$$

or

$$f(E) = 4.07 \times 10^{-10}$$

Ge: $E_g = 0.66 \text{ eV}$,

$$f(E) = \frac{1}{1 + \exp\left[\frac{0.66}{2(0.0259)}\right]}$$

or

$$f(E) = 2.93 \times 10^{-6}$$

GaAs: $E_g = 1.42 \text{ eV}$,

$$f(E) = \frac{1}{1 + \exp\left[\frac{1.42}{2(0.0259)}\right]}$$

or

$$f(E) = 1.24 \times 10^{-12}$$

(b)

Using results of Problem 3.35, the answers to part (b) are exactly the same as those given in part (a).

3.43

$$f(E) = 10^{-6} = \frac{1}{1 + \exp\left(\frac{0.55}{kT}\right)}$$

Then

$$1 + \exp\left(\frac{0.55}{kT}\right) = \frac{1}{10^{-6}} = 10^{+6} \Rightarrow$$

$$\exp\left(\frac{0.55}{kT}\right) \approx 10^{+6} \Rightarrow \left(\frac{0.55}{kT}\right) = \ln(10^6)$$

or

$$kT = \frac{0.55}{\ln(10^6)} \Rightarrow T = 461K$$

3.44

At $E = E_2$, $f(E_2) = 0.05$

So

$$0.05 = \frac{1}{1 + \exp\left(\frac{E_2 - E_F}{kT}\right)}$$

Then

$$\frac{E_2 - E_F}{kT} = \ln(19)$$

By symmetry, at $E = E_1$, $1 - f(E_1) = 0.05$,

So

$$\frac{E_F - E_1}{kT} = \ln(19)$$

Then

$$\frac{E_2 - E_1}{kT} = 2 \ln(19)$$

(a)

At $T = 300K$, $kT = 0.0259 \text{ eV}$

$$E_2 - E_1 = \Delta E = (0.0259)(2) \ln(19) \Rightarrow$$

$$\Delta E = 0.1525 \text{ eV}$$

(b)

At $T = 500K$, $kT = 0.04317 \text{ eV}$

$$E_2 - E_1 = \Delta E = (0.04317)(2) \ln(19) \Rightarrow$$

$$\Delta E = 0.254 \text{ eV}$$
