

## Chapter 1

1.1. (a) The Lagrangian of the 1D H.O. reads as

$$L = K - V = \frac{1}{2}m\dot{x}^2 - \frac{1}{2}k_x x^2$$

Hence the Lagrange equation of motion,

$$0 = \frac{d}{dt} \left( \frac{\partial L}{\partial \dot{x}} \right) - \frac{\partial L}{\partial x} = \frac{d}{dt} (m\dot{x}) + k_x x = m\ddot{x} + k_x x$$

is in agreement with Newton's or Hamilton's equations of motion, i.e.

$$m\ddot{x} = -k_x x$$

(b) The kinetic and potential energies are given by

$$K = \frac{1}{2}m\dot{x}^2 + \frac{1}{2}m\dot{y}^2 = \frac{p_x^2}{2m} + \frac{p_y^2}{2m}, \quad V = \frac{1}{2}k_x x^2 + \frac{1}{2}k_y y^2$$

and  $H$  and  $L$  read as

$$H = K + V,$$

$$L = K - V.$$

Thus the Hamilton's equations of motion are:

$$\dot{x} = \frac{\partial H}{\partial p_x} = \frac{p_x}{m}$$

$$\dot{p}_x = -\frac{\partial H}{\partial x} = -k_x x$$

so that

$$m\ddot{x} = -k_x x$$

Likewise,

$$\dot{y} = \frac{\partial H}{\partial p_y} = \frac{p_y}{m}$$

$$\dot{p}_y = -\frac{\partial H}{\partial y} = -k_y y$$

and

$$m\ddot{y} = -k_y y$$

One can also write the Lagrange equation of motion as

$$0 = \frac{d}{dt} \left( \frac{\partial L}{\partial \dot{x}} \right) - \frac{\partial L}{\partial x} = m\ddot{x} + k_x x$$

and

$$0 = \frac{d}{dt} \left( \frac{\partial L}{\partial \dot{y}} \right) - \frac{\partial L}{\partial y} = m\ddot{y} + k_y y$$

Thus, Hamilton's and Lagrange's equation of motion lead to results, in complete agreement with each other and also with Newton's equation of motion.

(c) From (b) one can write

$$\ddot{x} + \omega_x^2 x = 0, \quad \omega_x^2 \equiv k_x / m$$

$$\ddot{y} + \omega_y^2 y = 0, \quad \omega_y^2 \equiv k_y / m$$

For the initial condition given, one can obtain the solution as

$$\underline{r}(t) = \hat{x} \cdot x(t) + \hat{y} \cdot y(t)$$

with

$$x(t) = x_0 \cos \omega_x t, \quad y(t) = y_0 \cos \omega_y t$$

It will be interesting to trace and examine  $\underline{r}$  versus  $t$  for various ratios of  $\omega_y / \omega_x$ .

1.2. Consider the x-components of both sides:

$$\begin{aligned} & \nabla \times \nabla \times \underline{A} \Big|_x \\ &= \nabla \times \begin{vmatrix} \hat{x} & \hat{y} & \hat{z} \\ \frac{\partial}{\partial x} & \frac{\partial}{\partial y} & \frac{\partial}{\partial z} \\ A_x & A_y & A_z \end{vmatrix} = \nabla \times \left[ \hat{x} \left( \frac{\partial A_z}{\partial y} - \frac{\partial A_y}{\partial z} \right) + \hat{y} \left( \frac{\partial A_x}{\partial z} - \frac{\partial A_z}{\partial x} \right) + \hat{z} \left( \frac{\partial A_y}{\partial x} - \frac{\partial A_x}{\partial y} \right) \right] \\ &= \begin{vmatrix} \hat{x} & \hat{y} & \hat{z} \\ \frac{\partial}{\partial x} & \frac{\partial}{\partial y} & \frac{\partial}{\partial z} \\ \frac{\partial A_z}{\partial y} - \frac{\partial A_y}{\partial z} & \frac{\partial A_x}{\partial z} - \frac{\partial A_z}{\partial x} & \frac{\partial A_y}{\partial x} - \frac{\partial A_x}{\partial y} \end{vmatrix} = \frac{\partial}{\partial y} \left( \frac{\partial A_y}{\partial x} - \frac{\partial A_x}{\partial y} \right) - \frac{\partial}{\partial z} \left( \frac{\partial A_x}{\partial z} - \frac{\partial A_z}{\partial x} \right) \\ & \quad \left| \frac{\partial A_z}{\partial y} - \frac{\partial A_y}{\partial z} \quad \frac{\partial A_x}{\partial z} - \frac{\partial A_z}{\partial x} \quad \frac{\partial A_y}{\partial x} - \frac{\partial A_x}{\partial y} \right|_x \quad \text{----- (1)} \end{aligned}$$

while

$$\begin{aligned} & \nabla (\nabla \cdot \underline{A}) \Big|_x - \nabla^2 \underline{A} \Big|_x \\ &= \frac{\partial}{\partial x} \left( \frac{\partial A_x}{\partial x} + \frac{\partial A_y}{\partial y} + \frac{\partial A_z}{\partial z} \right) - \left( \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} \right) A_x \quad \text{----- (2)} \\ &= \frac{\partial^2 A_y}{\partial x \partial y} + \frac{\partial^2 A_z}{\partial x \partial z} - \frac{\partial^2 A_x}{\partial y^2} - \frac{\partial^2 A_x}{\partial z^2} \end{aligned}$$

Thus, (1) and (2) are shown identical and one can prove the identities of  $y$  and  $z$  components in the same way.

1.3. (a) The center of mass and relative coordinate systems are defined as

$$(m_1 + m_2) X = m_1 x_1 + m_2 x_2 \quad \text{----- (1)}$$

$$x = x_1 - x_2 \quad \text{----- (2)}$$

(corrections are due for  $X$  definition in the problem)

Expressing  $x_1, x_2$  in terms of  $X, x$  one can write with the operation,  $(1) + m_2 \cdot (2)$  and  $(1) - m_1 \cdot (2)$ ,

$$x_1 = X + \frac{m_2}{m_1 + m_2} x \quad \text{----- (3)}$$

$$x_2 = X - \frac{m_1}{m_1 + m_2} x \quad \text{----- (4)}$$

Thus using (3), (4) H can be expressed as

$$H \equiv \frac{1}{2}m_1\dot{x}_1^2 + \frac{1}{2}m_2\dot{x}_2^2 + \frac{1}{2}k(x_1 - x_2)^2 = \frac{1}{2}M\dot{X}^2 + \frac{1}{2}\mu\dot{x}^2 + \frac{1}{2}kx^2 \quad \text{----- (5)}$$

where

$$M \equiv m_1 + m_2, \quad \mu \equiv \frac{m_1 m_2}{m_1 + m_2}$$

The total kinetic energy consists of those of CM (with total mass  $M$ ) and of relative motion (with reduced mass  $\mu$ ).

One can thus write

$$H = \frac{p^2}{2m} + \frac{p^2}{2\mu} + \frac{1}{2}kx^2,$$

$$P \equiv M\dot{X}, \quad p \equiv \mu\dot{x}$$

(b) The respective Hamilton's equations of motion are:

$$\dot{X} = \frac{\partial H}{\partial P} = \frac{P}{M}$$

$$\dot{P} = -\frac{\partial H}{\partial X} = 0$$

so that

$$M\ddot{X} = 0$$

Also,

$$\dot{x} = \frac{\partial H}{\partial p} = \frac{p}{\mu}$$

$$\dot{p} = -\frac{\partial H}{\partial x} = -kx$$

and

$$\mu\ddot{x} = -kx$$

The CM moves as a free particle while the relative motion executes harmonic oscillation with reduced mass,  $\mu$ .

(c) Note that

$$\omega_c^2 = k/\mu \quad \text{with} \quad \mu \equiv \frac{m_H^2}{m_H + m_H} = \frac{1}{2}m_H$$

Hence,

$$k = (2\pi \cdot 3 \times 10^{13})^2 \frac{1}{2}m_H \cong 29.7 \text{ newton/meter}$$

1.4. The thermal speed is from the equipartition theorem given by

$$\frac{1}{2}m \langle v_T^2 \rangle = \frac{3}{2}k_B T.$$

At room temperature,  $T=300K$ ,

$$k_B T = 1.38 \times 10^{-23} (J/K) \cdot 300K = 4.14 \times 10^{-21} J = 25.86 meV.$$

Thus for electron at 300K

$$v_{Te} = (3k_B T / m)^{1/2} = (3 \cdot 4.14 \times 10^{-21} / 9.109 \times 10^{-31})^{1/2} [m/s] = 1.17 \times 10^5 [m/s]$$

The rest of thermal speeds can be found from  $v_{Te}$  with proper scaling of mass and  $T$ :

$$v_T = v_{Te} \left( \frac{m_e}{m} \cdot \frac{T}{300} \right)^{1/2}$$

1.5. (a) Given

$$\underline{E} = \hat{x} \operatorname{Re} E_0 e^{-i(\omega t - kz)} = \hat{x} E_0 \cos(\omega t - kz)$$

$\underline{H}$  can be found from Maxwell's equation, (1.40):

$$\nabla \times \underline{E} = \begin{vmatrix} \hat{x} & \hat{y} & \hat{z} \\ \frac{\partial}{\partial x} & \frac{\partial}{\partial y} & \frac{\partial}{\partial z} \\ E_0 \cos(\omega t - kz) & 0 & 0 \end{vmatrix} = \hat{y} E_0 k \sin(\omega t - kz) = -\mu \frac{\partial}{\partial t} \underline{H}$$

Integrating both sides w.r.t.  $t$  one finds,

$$\underline{H} = \hat{y} E_0 \left( -\frac{k}{\mu} \right) \left( \frac{-1}{\omega} \right) \cos(\omega t - kz) = \hat{y} \frac{1}{\mu v} E_0 \cos(\omega t - kz) = \hat{y} \frac{1}{\eta} E_0 \cos(\omega t - kz)$$

where

$$\omega = vk, \quad v = 1/\sqrt{\epsilon\mu}, \quad \eta = \sqrt{\mu/\epsilon}$$

Thus the Poynting vector is given by

$$\underline{P} = \underline{E} \times \underline{H} = \hat{z} \left( \frac{E_0^2}{\eta} \right) \cos^2(\omega t - kz)$$

(b) Given  $\lambda = 632.8 \text{ nm}$

$$v = \frac{c}{\lambda} = \frac{3 \times 10^8 \text{ m/s}}{632.8 \times 10^{-9} \text{ m}} \cong 4.75 \times 10^{15} / \text{s}$$

$$\frac{1}{\lambda} = 1.53 \times 10^6 / \text{m} = 1.53 \times 10^{-3} / \text{nm}$$

In an optical medium with the index of refraction  $n$  given by  $n^2 = \epsilon_r$  the frequency remains the same, while

$$\lambda = \frac{\lambda_{vac}}{n} = 316 \text{ nm}$$

## Chapter 2

2.1 (a) Given a photon of wavelength  $\lambda$  the energy and momentum are specified as

$$\varepsilon = h\nu = h \cdot \frac{c}{\lambda}, \quad p = \frac{\varepsilon}{c}$$

$\lambda$	$\varepsilon$ (eV)	$p$ (meVs/m)
10m (radiowave)	$1.24 \times 10^{-7}$	$4.13 \times 10^{-13}$
1m (microwave)	$1.24 \times 10^{-6}$	$4.13 \times 10^{-12}$
$10^4$ nm (infrared)	$1.24 \times 10^{-1}$	$4.13 \times 10^{-7}$
600nm (visible)	$2.07 \times 10^0$	$6.90 \times 10^{-6}$
200nm (UV)	$6.21 \times 10^0$	$2.07 \times 10^{-5}$
50nm (EUV)	$2.48 \times 10$	$8.27 \times 10^{-5}$
1nm (X-ray)	$1.24 \times 10^3$	$4.13 \times 10^{-3}$

2.2 (a) The total power generated is

$$\begin{aligned} & 3.7 \times 10^{26} W [J/s] \\ & = 3.7 \times 10^{26} / (1.602 \times 10^{-19}) [eV/s] \\ & = 2.31 \times 10^{45} [eV/s] \end{aligned}$$

The equivalent number of photons generated per second at 500nm, i.e. at photon energy of  $hc/\lambda = 2.5eV$  is  $9.24 \times 10^{44}/s$ . Thus, at the surface of the sun, for instance, the flux of photons per area and per time is given by

$$\frac{9.24 \times 10^{44}}{4\pi R_s^2}$$

with  $R_s$  denoting the radius of the sun.

(b) The total number of photons reaching the earth per second is approximately given by

$$\frac{9.24 \times 10^{44}}{4\pi d_{SE}^2} \cdot \pi R_E^2$$

where  $d_{SE}$  is the average distance between the sun and earth and  $R_E$  the radius of the earth.

2.3 (a) The thermal speed of the electron at room temperature is given from the equipartition theorem by

$$\frac{1}{2} m_e v_T^2 = \frac{3}{2} k_B T.$$

That is,

$$v_T = \left( \frac{3k_B T}{m_e} \right)^{1/2} \approx 1.17 \times 10^5 m/s$$

at  $T=300K$ . Thus the de Broglie wavelength is found to be

$$\lambda = \frac{h}{m_e \cdot v_T} = 6.22 \times 10^{-9} m = 6.22 nm$$

The de Broglie wavelengths of other particles with mass  $m$  can be found in terms of that of electron:

$$\lambda = \frac{h}{m \cdot \left(\frac{3k_B T}{m}\right)^{1/2}} = \frac{h}{m^{1/2} \cdot (3k_B T)^{1/2}} = \frac{h}{m_e^{1/2} \cdot (3k_B T)^{1/2}} \cdot \left(\frac{m_e}{m}\right)^{1/2}$$

$$= 6.22(m_e/m)^{1/2} \text{ nm}$$

with  $m_e$  denoting the rest mass of electron. Thus for the case of proton, for example,

$$\left(\frac{m_e}{m_p}\right)^{1/2} \approx 2.37 \times 10^{-2}$$

and the corresponding de Broglie wavelength is shorter by the same factor.

(b) Given kinetic energy  $E$  the associated velocity of electron is given in non-relativistic limit by

$$\frac{1}{2}mv^2 = E,$$

so that

$$v = \left(2E/m\right)^{1/2}$$

Thus for  $E=200\text{eV}$

$$v = \left(\frac{2 \times 200 \times 1.6 \times 10^{-19}}{9.1 \times 10^{-31}}\right)^{1/2} \approx 8.3 \times 10^6 \text{ m/s}$$

and de Broglie wavelength is given by

$$\lambda = \frac{h}{mv} \approx 8.8 \times 10^{-11} \text{ m} \approx 0.088 \text{ nm}$$

For K.E. larger than 200eV, the electron velocity could enter into the relativistic regime. In this case K.E. is specified as

$$E = \frac{m_0 c^2}{\sqrt{1-(v/c)^2}} - m_0 c^2 = E_0 \left[ \frac{1}{\sqrt{1-(v/c)^2}} - 1 \right], \quad E_0 = m_0 c^2$$

with  $m_0, E_0$  denoting the rest mass and rest energy of electron, respectively.

Finding  $v$  in terms of  $E$  one can write

$$\frac{v}{c} = \frac{\left(\frac{2E}{E_0}\right)^{1/2} \cdot \left(1 + \frac{E}{2E_0}\right)^{1/2}}{1 + \frac{E}{E_0}}, \quad E_0 = m_0 c^2 \approx 0.5 \text{ MeV}$$

Hence for  $E \ll E_0$ ,  $v \approx (2E/m_0)^{1/2}$  as it should and one can incorporate the relativistic effect by retaining terms proportional to  $E/E_0$ .

Once  $v$  is found, de Broglie wavelength is specified by

$$\lambda = \frac{h}{m_0 v / \sqrt{1-(v/c)^2}}$$

Insert the value of  $v/c$  found without neglecting terms proportional to  $E/E_0$  and find the relativistic corrections in  $\lambda$ .

(c) One can find the de Broglie wavelength of proton by replacing the rest mass and rest energy of electron with those of proton in (b).

(d) Use (2.33), (2.34) in the text, obtaining

$$K.E. \equiv \frac{1}{2}mv^2 = -E_n = \frac{E_0}{n^2}$$

with  $E_0 = 13.6\text{eV}$  denoting the ionization energy of H-atom.

Thus, for  $n = 1$

$$v = \left( \frac{2E_0}{m} \right)^{1/2} = \left( \frac{2 \times 13.6\text{eV} \times 1.6 \times 10^{-19}\text{J/eV}}{9.1 \times 10^{-31}} \right)^{1/2} = 2.2 \times 10^6\text{m/s}$$

Hence,

$$\lambda = \frac{h}{mv} \approx 0.33\text{nm}$$

Here,  $v$  is in mildly relativistic range and one can incorporate its effect in a manner discussed in (b). For  $n = 100$

$$v = \frac{2.2 \times 10^6}{10^4} = 2.2 \times 10^2\text{m/s}$$

and

$$\lambda = 0.33\text{nm} \times 10^4 = 3.3 \times 10^3\text{nm}$$

2.4 The ionization energy of the donor atom can be found from that of H-atom using the scaling relation,

$$E_0 = 13.6\text{eV} \times \left( \frac{\epsilon_0}{\epsilon} \right)^2 \times \frac{m_n}{m_0}$$

Hence,

$$E_0 \approx \begin{cases} 8.7 \times 10^{-2}\text{eV} & m_n/m_0 = 0.9 \\ 9.6 \times 10^{-3}\text{eV} & m_n/m_0 = 0.1 \end{cases}$$

With these values of  $E_0$ , one readily finds de Broglie wavelength in a way discussed in the problem (2.3).

2.5 Given kinetic energy,  $E$  one can find corresponding  $v$  by using the formula derived in problem (2.3).

$$\frac{v}{c} = \frac{\left( \frac{2E}{E_0} \right)^{1/2} \cdot \left( 1 + \frac{E}{2E_0} \right)^{1/2}}{1 + \frac{E}{E_0}}, \quad E_0 = m_0c^2$$

Thus, for 10KeV electron,  $E_0 \approx 0.5\text{MeV}$  and

$$\frac{v}{c} \approx 0.14$$

The relativistic correction as exhibited by

$$\frac{m}{m_0} = \frac{1}{\sqrt{1 - \left( \frac{v}{c} \right)^2}}$$

is then shown to be about 10%.

Likewise for proton,  $E_0 \approx 918\text{MeV}$  and  $v/c \approx 1.5 \times 10^{-2}$ , therefore  $m/m_0 \approx 1.01$ .

For the ground state electron in H-atom, the K.E. is 13.6 eV (see (2.35) in the text) and  $v/c \approx 7 \times 10^{-3}$ ,  $m/m_0 \approx 1.00$

2.6 (a) Given the wavelength,  $\lambda=300\text{nm}$ , the photon energy is

$$E = h\nu = h \frac{c}{\lambda} = 4.14\text{eV}$$

Hence, the photon is capable of inducing photoelectric effect in Li and Be.

The corresponding stopping power is:

$$4.14 - 2.3 = 1.8V \quad \text{for Li}$$

$$4.14 - 3.9 = 0.24V \quad \text{for Be}$$

(b) For a photon with  $\lambda=253.7\text{nm}$ , its energy is

$$E = h \frac{c}{\lambda} = 4.9\text{eV}$$

Thus, the observed stopping power of  $-0.24\text{V}$  in copper indicates that the copper work function;  $q\phi_m$  is

$$4.9 - q\phi_m = 0.24,$$

i.e.

$$q\phi_m = 4.66\text{eV}.$$

Hence, the longest wavelength of the photon capable of producing photoelectric effect is given by

$$\frac{hc}{\lambda} = 4.66\text{eV}.$$

that is,

$$\lambda = 266\text{nm}.$$

(c) There are typographical errors:

Stopping power of  $-2.3\text{V}$  for  $\lambda=194\text{nm}$  (instead of  $200\text{nm}$ ) and of  $-0.9\text{V}$  for  $\lambda=248\text{nm}$  (instead of  $313\text{nm}$ ).

From the conservation of energy one can write

$$h \frac{c}{\lambda_1} = q\phi_m + 2.3, \quad \lambda_1 = 194\text{nm}$$

$$h \frac{c}{\lambda_2} = q\phi_m + 0.9, \quad \lambda_2 = 248\text{nm}$$

Subtracting the second equation from the first one,

$$h \left( \frac{c}{\lambda_1} - \frac{c}{\lambda_2} \right) = 2.3 - 0.9$$

and

$$h = \frac{(2.3 - 0.9)\text{eV}}{\left( \frac{c}{\lambda_1} - \frac{c}{\lambda_2} \right) \text{s}^{-1}} \approx 4.125 \times 10^{-15} \text{eVs}$$

Substituting  $h$  back into any of the two energy conservation equations, the work function is obtained:

$$q\phi_m \approx 4.1\text{eV}$$

2.7 (a) Use (2.31) in the text, i.e.

$$r_n = r_B \cdot n^2$$

with  $r_B$  denoting the Bohr radius of  $0.053\text{nm}$ . Thus, one finds



$$r_n = \begin{cases} 0.053nm & \text{for } n=1 \\ 0.21nm & \text{for } n=2 \end{cases}$$

(b) The angular momentum is quantized as

$$l_n = n\hbar$$

Thus,

$$l_n = \begin{cases} 6.58 \times 10^{-16} \text{ eVs} & \text{for } n=1 \\ 13.2 \times 10^{-16} \text{ eVs} & \text{for } n=2 \end{cases}$$

Since  $\underline{r}_n$  is perpendicular to  $\underline{p}_n$  for circular orbit,

$$p_n = l_n / r_n = \frac{1.055 \times 10^{-34} n \text{ Js}}{0.053 \times 10^{-9} n^2 \text{ m}} \approx 20 \times 10^{-25} \frac{1}{n}$$

Hence,

$$p_n = \begin{cases} 2 \times 10^{-24} \text{ kgm/s for } n=1 \\ 1 \times 10^{-24} \text{ kgm/s for } n=2 \end{cases}$$

(c) The kinetic, potential and total energy associated can be readily found as discussed in the text.

2.8 (a) Use (2.22) in the text:

$$\Delta\lambda = 4\pi\lambda_e \sin^2\left(\frac{\theta}{2}\right)$$

with  $\lambda_e = 4 \times 10^{-13} \text{ m}$ . For  $\theta = \pi/2$

$$\Delta\lambda = 2.5 \times 10^{-12} \text{ m} = 2.5 \times 10^{-3} \text{ nm}$$

(b) The incident X-ray has the wavelength given by

$$h\nu = 2 \times 10^5 \text{ eV} = h \frac{c}{\lambda_i},$$

so that

$$\lambda_i = 6.2 \times 10^{-3} \text{ nm}$$

Hence the wavelength of scattered X-ray is given by

$$\lambda_f = \lambda_i + \Delta\lambda = 8.7 \times 10^{-3} \text{ nm}$$

and

$$E_f = h \frac{c}{\lambda_f} = 1.43 \times 10^4 \text{ eV}$$

Thus the recoil energy of electron is given from the conservation of energy as

$$\Delta E = E_i - E_f = (20 - 1.43) \times 10^4 \text{ eV} = 1.86 \times 10^5 \text{ eV}$$

2.9 With atomic number  $Z=2$ , the energy spectrum of  $\text{He}^+$  is specified from (2.35) by

$$E_n = -E_0 \frac{1}{n^2} = 13.6 \times Z^2 \times \frac{1}{n^2} \text{ eV} = 54.4 \times \frac{1}{n^2} \text{ eV}$$

where

$$E_0 = \frac{Z^2 e_M^2 m}{2\hbar^2} = 13.6 \times Z^2 \text{ eV} = 54.4 \text{ eV}$$

and is shown to be larger than that of H-atom by the factor of 4.

The shortest radius corresponding to the ground state is to be obtained by scaling the Bohr radius:

$$r_1 = \frac{\hbar^2}{m e_M^2 Z} = r_B \cdot \frac{1}{Z} \cong \frac{0.05}{2} nm = 0.025 nm$$

It is clear from (2.36) in the text that the wavelengths corresponding to the Balmer series are shorter than those in H-atom by the factor of  $Z^2$ , i.e. by the factor of 4.

2.10 A charged particle under acceleration, a dissipates power as

$$P = \frac{2}{3} \frac{e_M^2}{c^3} a^2, \quad e_M^2 = \frac{e^2}{4\pi\epsilon_0} \text{----- (1)}$$

An electron in circular orbit around proton in H-atom is under acceleration given (from (2.30) by

$$a = v\omega = \frac{v^2}{r} \text{----- (2)}$$

where  $r$  is the radius of the circular orbit.

Thus, the power dissipated is specified by

$$P = \frac{2}{3} \frac{e_M^2}{c^3} \left( \frac{v^2}{r} \right)^2 \text{----- (3)}$$

Since the energy of electron in circular orbit of radius  $r$  is given from (2.34) by

$$E = -\frac{e_M^2}{2r}, \quad e_M^2 = \frac{e^2}{4\pi\epsilon_0} \text{----- (4)}$$

the rate with which  $r$  decreases in time due to power dissipation is described by

$$\frac{dE}{dt} = \frac{e_M^2}{2r^2} \frac{dr}{dt} = -\frac{2}{3} \frac{e_M^2}{c^3} \left( \frac{v^2}{r} \right)^2 \text{----- (5)}$$

Or

$$\frac{dr}{dt} = -\frac{4}{3} \frac{v^4}{c^3} \text{----- (6)}$$

For given  $r$ , the centrifugal and centripetal Coulomb forces are balanced according to

$$\frac{mv^2}{r} = \frac{e_M^2}{r^2} \text{----- (7)}$$

Inserting (7) into (6) and rearranging one finds

$$\frac{dr}{dt} = -\frac{4}{3c^3} \left( \frac{e_M^2}{mr} \right)^2$$

That is,

$$dr r^2 = -\frac{4e_M^4}{3c^3 m^2} dt$$

Integrating both sides

$$\frac{1}{3} (r_i^3 - r_f^3) = \frac{4e_M^4}{3c^3 m^2} t$$

where  $r_i$ ,  $r_f$  denote respectively the initial and final values of the electron radius. Since  $r_i$  is the Bohr radius,  $r_B$  and  $r_f$  is the radius of the nucleus one can put  $r_f \cong 0$  and write the time in which the electron spirals into the nucleus as

$$t \cong \frac{c^3 m^2}{4e_M^4} r_B^3 \cong 1.32 \times 10^{-11} s$$

where the Coulomb constant

has been used.

$$\frac{1}{4\pi\epsilon_0} = 8.988 \times 10^9 \text{ Nm}^2 / \text{C}^2$$

### Chapter 3

3.1 (a) Given the wavefunction,

$$\psi(\underline{r}, t) = \exp\left[-\frac{i}{\hbar} \int_0^t \hat{H}(t') dt'\right] \psi(\underline{r}, 0)$$

One can write by definition

$$\begin{aligned} & \frac{\partial}{\partial t} \psi(\underline{r}, t) \\ &= \lim_{\Delta t \rightarrow 0} \frac{\psi(\underline{r}, 0)}{\Delta t} \left\{ \exp\left[-\frac{i}{\hbar} \int_0^{t+\Delta t} \hat{H}(t') dt'\right] - \exp\left[-\frac{i}{\hbar} \int_0^t \hat{H}(t') dt'\right] \right\} \\ &= \lim_{\Delta t \rightarrow 0} \frac{\psi(\underline{r}, 0)}{\Delta t} \left\{ \exp\left[-\frac{i}{\hbar} \int_t^{t+\Delta t} \hat{H}(t') dt'\right] - 1 \right\} \exp\left[-\frac{i}{\hbar} \int_0^t \hat{H}(t') dt'\right] \\ &= \lim_{\Delta t \rightarrow 0} \frac{-\frac{i}{\hbar} \hat{H}(t) \Delta t}{\Delta t} \psi(\underline{r}, t) \\ &= -\frac{i}{\hbar} \hat{H}(t) \psi(\underline{r}, t) \end{aligned}$$

Hence

$$i\hbar \frac{\partial \psi(\underline{r}, t)}{\partial t} = \hat{H}(t) \cdot \psi(\underline{r}, t)$$

(b) If  $\hat{H}(t) = \hat{H}_0$ , one can write

$$\psi(\underline{r}, t) = e^{-\frac{i}{\hbar} \hat{H}_0 t} \cdot \psi(\underline{r}, 0) = e^{-i\omega_0 t} \cdot \psi(\underline{r}, 0)$$

where

$$\omega_0 \equiv \hat{H}_0 / \hbar$$

in agreement with the solution entering in the separation of variable technique.

3.2 Given the Hamiltonian,

$$\hat{H} = -\frac{\hbar^2}{2m} \nabla^2 + V(\underline{r})$$

the fact that  $V(\underline{r})$  is real ensures that

$$V(\underline{r}) = V^*(\underline{r})$$

Thus, one can write for arbitrary but well behaving function  $f, g$

$$\int d\underline{r} f^* V g \equiv \int d\underline{r} (V f)^* g$$

indicating that  $V$  is Hermitian.

The x-component of the Laplacian operator, for example, can also be shown to be Hermitian by performing the integration by parts repeated twice in succession:

$$\begin{aligned}
\int dr f^* \frac{\partial^2}{\partial x^2} g &= f^* \frac{\partial}{\partial x} g \Big|_{-\infty}^{\infty} - \int dr \left( \frac{\partial}{\partial x} g \right) \left( \frac{\partial}{\partial x} f^* \right) \\
&= -g \frac{\partial f^*}{\partial x} \Big|_{-\infty}^{\infty} + \int dr g \frac{\partial^2}{\partial x^2} f^* \\
&= \int dr \left( \frac{\partial^2 f^*}{\partial x^2} \right) g
\end{aligned}$$

Here use has been made of  $f(\pm\infty) = g(\pm\infty) = 0$ . Hence  $\hat{H}$  is hermitian.

3.3 (a) If  $\hat{B}$  is Hermitian adjoint of  $\hat{A}$ , i.e.  $\hat{B} = \hat{A}^+$ , it satisfies the relation

$$\int dr f^* \hat{A} g \equiv \int dr (Bf)^* g \text{ ----- (1)}$$

The relation (1) also specifies the Hermitian operator. That is, if  $\hat{A}$  is Hermitian it should satisfy

$$\int dr f^* \hat{A} g \equiv \int dr (Af)^* g \text{ ----- (2)}$$

where  $f, g$  are arbitrary but physically well behaving functions. Hermitian operator is therefore its own Hermitian adjoint:

$$\hat{A} = \hat{A}^+$$

As a corollary take the complex conjugate of (1), obtaining

$$\int dr f (\hat{A} g)^* = \int dr (\hat{B} f)^* g^* \text{ ----- (3)}$$

Or equivalently,

$$\int dr g^* \hat{B} f = \int dr (\hat{A} g)^* f \text{ ----- (4)}$$

Therefore,  $\hat{A}$  is shown the Hermitian adjoint of  $\hat{B}$ , i.e.

$$\hat{A} = \hat{B}^+$$

and one can thus write

$$B = A^+ = (B^+)^+$$

(b) From (a) one can write using the definition of the Hermitian adjoint for any  $\hat{A}^+$

$$\begin{aligned}
i \int dr f^* \hat{A}^+ g &\equiv i \int dr \left[ (\hat{A}^+)^+ f \right]^* g \\
&= i \int dr (\hat{A} f)^* g \text{ ----- (5)} \\
&= \int dr (-i A f)^* g
\end{aligned}$$

while

$$\begin{aligned}
-i \int dr f^* \hat{A} g &\equiv -i \int dr (\hat{A}^+ f)^* g \text{ ----- (6)} \\
&= \int dr (i \hat{A}^+ f)^* g
\end{aligned}$$

Combining (5), (6)

$$\int dr f^* i(\hat{A}^+ - \hat{A})g = \int dr \left[ i(\hat{A}^+ - \hat{A})f \right]^* g$$

q.e.d.

$$(c) i\langle f | \hat{A}^+ g \rangle \equiv i\langle (\hat{A}^+)^+ f | g \rangle = i\langle \hat{A}f | g \rangle = \langle -i\hat{A}f | g \rangle$$

while

$$-i\langle f | \hat{A}g \rangle = -i\langle \hat{A}^+ f | g \rangle = \langle i\hat{A}^+ f | g \rangle$$

Hence,

$$\langle f | i(\hat{A}^+ - \hat{A})g \rangle = \langle i(\hat{A}^+ - \hat{A})f | g \rangle$$

3.4 (a) Consider

$$xp_x^n f - p_x^n xf = (-i\hbar)^n \left[ x \frac{\partial^n}{\partial x^n} f - \frac{\partial^n}{\partial x^n} (xf) \right]$$

Now,

$$\begin{aligned} \frac{\partial^n}{\partial x^n} xf &= x \frac{\partial^n f}{\partial x^n} + {}_n C_1 \frac{\partial^{n-1} f}{\partial x^{n-1}} \frac{\partial}{\partial x} x + {}_n C_2 \frac{\partial^{n-2} f}{\partial x^{n-2}} \frac{\partial^2}{\partial x^2} x + \dots \\ &= x \frac{\partial^n f}{\partial x^n} + n \frac{\partial^{n-1} f}{\partial x^{n-1}} \end{aligned}$$

with  ${}_n C_r$  denoting the combinatorial coefficient,  ${}_n C_r = \binom{n}{r}$

Thus,

$$\begin{aligned} (-i\hbar)^n \cdot \left[ x \frac{\partial^n}{\partial x^n} f - \frac{\partial^n}{\partial x^n} (xf) \right] &= i\hbar n \cdot \left( -i\hbar \frac{\partial}{\partial x} \right)^{n-1} \cdot f \\ &= i\hbar n \cdot p_x^{n-1} \cdot f \end{aligned}$$

That is,

$$[x, p_x^n] = i\hbar n \cdot p_x^{n-1}$$

(b) Consider

$$\begin{aligned} p_x x^n f - x^n p_x f &= -i\hbar \frac{\partial}{\partial x} (x^n f) - x^n \left( -i\hbar \frac{\partial}{\partial x} f \right) \\ &= -i\hbar \left( nx^{n-1} f + x^n \frac{\partial}{\partial x} f \right) - x^n \left( -i\hbar \frac{\partial}{\partial x} f \right) \\ &= -i\hbar nx^{n-1} f \end{aligned}$$

Hence,

$$[p_x, x^n] = -i\hbar n \cdot x^{n-1}$$

3.5 Using the uncertainty relation,

$$\Delta x \Delta p_x \simeq \hbar, \quad \Delta y \Delta p_y \simeq \hbar, \quad \Delta z \Delta p_z \simeq \hbar$$

the minimum K.E. of an electron is to be expressed as

$$\Delta E \approx \frac{1}{2m} (\Delta p_x^2 + \Delta p_y^2 + \Delta p_z^2) = \frac{\hbar^2}{2m} \left( \frac{1}{\Delta x^2} + \frac{1}{\Delta y^2} + \frac{1}{\Delta z^2} \right) = \frac{3\hbar^2}{2m} \frac{1}{L^2}$$

with  $L$  representing the length of the cube.

$$\Delta E = \begin{cases} 9.15 \times 10^{-23} \text{ J} = 5.7 \times 10^{-4} \text{ eV} & \text{for } L = 10 \text{ nm} \\ 9.15 \times 10^{-21} \text{ J} = 5.7 \times 10^{-2} \text{ eV} & \text{for } L = 1 \text{ nm} \\ 3.66 \times 10^{-21} \text{ J} = 2.28 \times 10^{-1} \text{ eV} & \text{for } L = 0.5 \text{ nm} \end{cases}$$

3.6(a) For electron, its K.E. in the nucleus with diameter  $D$  is to be estimated by

$$\Delta E \approx \frac{\hbar^2}{2m} \frac{1}{D^2}, \quad D = 10^{-14} \text{ m}$$

$$\approx 6.1 \times 10^{-11} \text{ J} = 3.8 \times 10^8 \text{ eV}$$

(b) For proton  $\Delta E$  is to be found in terms of that of electron and the ratio of rest masses:

$$\Delta E = 3.8 \times 10^8 \text{ eV} \cdot \frac{m_e}{m_p} = 2.06 \times 10^5 \text{ eV}$$

The proton can thus be contained within the nucleus, while the electron cannot be confined therein.

3.7 The atomic transition frequency from the first excited state to the ground is given by

$$h\nu = E_2 - E_1 = 13.6 \left( 1 - \frac{1}{4} \right) \text{ eV}$$

Hence

$$\nu = \frac{10.2 \text{ eV}}{h} \approx 2.47 \times 10^{15} / \text{s}$$

The spread in  $\nu$  due to the finite lifetime of electron is to be estimated as

$$h\Delta\nu \approx \frac{\hbar}{\tau}$$

That is,

$$\Delta\nu \approx \frac{\hbar}{\tau \cdot h} \approx 1.6 \times 10^7 / \text{s}$$

## Chapter 4

4.1 (a) The electron is free to move along, say  $x$ -direction, while spatially confined in  $y, z$  direction  
Thus, the total energy is given by

$$E_{n_x, n_y} = \frac{\hbar^2 k_x^2}{2m} + E_{n_x} + E_{n_y}$$

where

$$E_{n_x} = \frac{\hbar^2 \pi^2}{2mL^2} n_x^2, \quad n_x = 1, 2, \dots$$

$$E_{n_y} = \frac{\hbar^2 \pi^2}{2mL^2} n_y^2, \quad n_y = 1, 2, \dots$$

Here, the quantum wire has been modeled by infinite square well potentials in  $y, z$  directions.  
For  $L=1\text{nm}$

$$E_0 \equiv \frac{\hbar^2 \pi^2}{2mL^2} \approx 6.03 \times 10^{-20} \text{ J} = 3.77 \times 10^{-1} \text{ eV}.$$

Thus, the lowest 4 quantized levels are:

$$E_{1,1} = E_0(1^2 + 1^2) = 7.54 \times 10^{-1} \text{ eV}$$

$$E_{2,1} = E_{1,2} = E_0(2^2 + 1^2) = 1.89 \text{ eV}$$

$$E_{2,2} = E_0(2^2 + 2^2) = 3.02 \text{ eV}$$

$$E_{3,1} = E_{1,3} = E_0(3^2 + 1^2) = 3.77 \text{ eV}$$

And the frequency of emitted photon,

$$\nu = \Delta E / h$$

when occurring in cascade is given by

$$\nu = \begin{cases} 1.82 \times 10^{14} / \text{s} & \text{for } E_{3,1} \rightarrow E_{2,2} \\ 2.73 \times 10^{14} / \text{s} & \text{for } E_{2,2} \rightarrow E_{2,1} \\ 2.75 \times 10^{14} / \text{s} & \text{for } E_{2,1} \rightarrow E_{1,1} \end{cases}$$

(b) For quantum well one can write

$$E = \frac{\hbar^2 k_x^2}{2m} + \frac{\hbar^2 k_y^2}{2m} + \frac{\hbar^2 \pi^2}{2mL^2} n^2$$

Thus, the lowest 4 quantized energy level is given by

$$E = E_0, 4E_0, 9E_0 \text{ and } 16E_0$$

and the frequency of photons when emitted in cascade is given by

$$\nu = \begin{cases} 6.38 \times 10^{14} / \text{s} & \text{for } E_4 \rightarrow E_3 \\ 4.56 \times 10^{14} / \text{s} & \text{for } E_3 \rightarrow E_2 \\ 2.73 \times 10^{14} / \text{s} & \text{for } E_2 \rightarrow E_1 \end{cases}$$

4.2 The energy eigenfunctions satisfying the stationary boundary condition are given from (4.17) by

$$u = \left(\frac{2}{L}\right)^{\frac{3}{2}} \sin\left(\frac{n_x \pi}{L} x\right) \sin\left(\frac{n_y \pi}{L} y\right) \sin\left(\frac{n_z \pi}{L} z\right)$$

where the quantum numbers satisfy the boundary conditions,



$$k_x L = n_x \pi \quad n_x = 1, 2, \dots$$

$$k_y L = n_y \pi \quad n_y = 1, 2, \dots$$

$$k_z L = n_z \pi \quad n_z = 1, 2, \dots$$

Hence the total number of states between  $k$  and  $k+dk$  is obtained by

$$\frac{(4\pi k^2 dk) / 8}{(\pi / L)^3}$$

Here,  $k_x$ ,  $k_y$ ,  $k_z$  values should be confined to positive values, hence the spherical shell is divided by 8.

The number of states per volume is then specified including the spin by

$$g_{3D}(k)dk \equiv 2 \frac{4\pi k^2 dk}{8(\pi / L)^3} \frac{1}{L^3} = \frac{k^2 dk}{\pi^2}$$

In term of energy,

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

one can therefore write

$$g_{3D}(E)dE = \frac{\sqrt{2}m^{3/2}E^{1/2}dE}{\pi^2 \hbar^3}$$

in complete agreement with the result derived using the periodic boundary condition.

4.3 The Hamiltonian of the particle in 1D box and/or wire is given by

$$\hat{H} = -\frac{\hbar^2}{2m} \nabla^2 + V(x, y, z)$$

where

$$V(x, y, z) = \begin{cases} 0 & \text{for } 0 \leq x \leq L_x \\ & 0 \leq y \leq L_y \\ \infty & \text{otherwise} \end{cases}$$

The energy eigenequation then reads as

$$\left[ -\frac{\hbar^2}{2m} \nabla^2 + V(x, y, z) \right] \varphi(x, y, z) = E\varphi(x, y, z) \quad \text{----- (1)}$$

The eigenfunction can be found, using the usual separation of variable technique, that is, by looking for the solution in the form

$$\varphi = u(x)u(y)u(z) \quad \text{----- (2)}$$

Inserting (2) into (1) and singling out  $x$ ,  $y$ , and  $z$  components in the usual manner there results

$$\begin{aligned} u''(x) + V(x)u(x) &= E_x u(x) \\ u''(y) + V(y)u(y) &= E_y u(y) \quad \text{----- (3)} \end{aligned}$$

$$u''(z) + k^2 u(z) = 0, \quad k^2 \equiv \frac{2mE_z}{\hbar^2}$$

where primes denote the differentiations w.r.t. the variables involved and

$$V(x) = \begin{cases} 0 & 0 \leq x \leq L_x \\ \infty & \text{otherwise} \end{cases} \quad (4a)$$

$$V(y) = \begin{cases} 0 & 0 \leq y \leq L_y \\ \infty & \text{otherwise} \end{cases} \quad (4b)$$

$$E = E_x + E_y + E_z \text{ ----- (5)}$$

One can readily solve (3) using the stationary boundary condition, obtaining

$$\varphi = N \sin\left(\frac{n_x \pi}{L} x\right) \sin\left(\frac{n_y \pi}{L} y\right) e^{ikz}$$

with N representing the normalization constant and

$$E = \frac{\hbar^2 \pi^2}{2m} \left( \frac{n_x^2}{L_x} + \frac{n_y^2}{L_y} \right) + \frac{\hbar^2 k^2}{2m} \text{ ----- (6)}$$

For  $L_x = L_y = L$ ,  $E$  reduces to

$$E_{n_x, n_y} = \frac{\hbar^2 \pi^2}{2mL^2} (n_x^2 + n_y^2) + \frac{\hbar^2 k^2}{2m}$$

The ground state energy thus corresponds to the case, where  $n_x = n_y = 1$ .

The first excited state is doubly degenerate, corresponding to  $n_x = 2, n_y = 1$  &  $n_x = 1, n_y = 2$ .

The second excited state with  $n_x = n_y = 2$  is non-degenerate, while the third excited state is again doubly degenerate with  $n_x = 3, n_y = 1$  &  $n_x = 1, n_y = 3$ .

One can specify the degeneracy of higher lying states in a similar manner.

4.4 (a) The energy eigenequation for this quantum well reads as

$$\left[ -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + V(x) \right] u(x) = Eu(x) \text{ ----- (1)}$$

where for the bound state  $E < 0$  and one may put

$$E = -|E|$$

Also,  $V(x)$  can be put in the form

$$V(x) = \begin{cases} -V & -\frac{1}{2}d \leq x \leq \frac{1}{2}d, \text{ I} \\ 0 & \frac{1}{2}d < x, \text{ II} \end{cases}$$

Thus, (1) can be recast in regions, I, II as

$$\begin{aligned} u''(x) + k^2 u(x) &= 0, & k^2 &= \frac{2m}{\hbar^2} (V - |E|) \\ u''(x) - k^2 u(x) &= 0, & \kappa^2 &= \frac{2m}{\hbar^2} |E| \end{aligned} \text{ ----- (2)}$$

The solutions of (2) is readily obtained as

$$u(x) = \begin{cases} A \sin kx + B \cos kx & , \text{ I} \\ C e^{-\kappa x} & , \text{ II} \end{cases}$$

The boundary conditions for  $u(x)$  to satisfy are:

$$u\left(-\frac{1}{2}d\right) = 0$$

since  $V(-\frac{1}{2}d) = \infty$  and  $u$  and  $u'$  should be continuous at  $x = \frac{1}{2}d$ . Thus,

$$-A \sin\left(\frac{kd}{2}\right) + B \cos\left(\frac{kd}{2}\right) = 0 \quad \dots \quad (3a)$$

$$A \sin\left(\frac{kd}{2}\right) + B \cos\left(\frac{kd}{2}\right) = C e^{-\frac{\kappa d}{2}} \quad \dots \quad (3b)$$

$$k \left[ A \cos\left(\frac{kd}{2}\right) - B \sin\left(\frac{kd}{2}\right) \right] = -\kappa C e^{-\frac{\kappa d}{2}} \quad \dots \quad (3c)$$

From (3a) one finds B in terms of A, i.e.

$$B = A \tan\left(\frac{kd}{2}\right)$$

and insert it into (3b), (3c), obtaining

$$2A \sin\left(\frac{kd}{2}\right) - C e^{-\frac{\kappa d}{2}} = 0 \quad \dots \quad (4a)$$

$$A \left[ \cos\left(\frac{kd}{2}\right) - \frac{\sin^2\left(\frac{kd}{2}\right)}{\cos\left(\frac{kd}{2}\right)} \right] + \frac{\kappa}{k} C e^{-\frac{\kappa d}{2}} = 0 \quad \dots \quad (4b)$$

Note In (4) that the coupled equations for A, C are sourceless, that is, homogeneous and A, C are therefore trivial, i.e.  $A = C = 0$  unless the secular equation holds true:

$$\begin{vmatrix} 2 \sin\left(\frac{kd}{2}\right) & -e^{-\frac{\kappa d}{2}} \\ \cos\left(\frac{kd}{2}\right) - \frac{\sin^2\left(\frac{kd}{2}\right)}{\cos\left(\frac{kd}{2}\right)} & \frac{\kappa}{k} e^{-\frac{\kappa d}{2}} \end{vmatrix} = 0 \quad \dots \quad (5)$$

Since the parameters,  $k$ ,  $\kappa$  are functions of  $|E|$ , the bound state energy eigenvalue is found from this secular equation, (5). Once  $|E|$  is found A, C are in turn to be determined from (4), leading to the explicit solution of the eigenfunction.

(b) For the case of infinite square well potential of width,  $d$  the energy eigenvalues are given from (4.11b) as

$$E_n = \frac{\hbar^2 \pi^2}{2md^2} n^2, \quad n = 1, 2, \dots \quad \dots \quad (6)$$

It will therefore be interesting and instructive to compare a few energy eigenvalues found from the secular equation for given depth  $V$  and width  $d$  with  $E_1$  or  $E_2$  in (6) and examine the reasons for the difference in eigenvalues.

4.5 The method for tackling this problem has been detailed in the text and solving the problem consists of repeating what has been discussed in detail in the text and obtaining concrete values of the quantities for given  $V, W, T$

4.6 (a) Given

$$V(x) = \begin{cases} V & x < -d, & \text{I} \\ V/2 & -d < x < 0, & \text{II} \\ 0 & 0 < x < d, & \text{III} \\ V & d < x, & \text{IV} \end{cases}$$

One can readily set up in the usual manner the energy eigenequation and corresponding eigenfunctions.

(i) for  $E > V$

$$\begin{aligned} u_I &= i_0 e^{ik_1 x} + r e^{-ik_1 x}, & \frac{\hbar^2 k_1^2}{2m} &= E - V \\ u_{II} &= A_2 e^{ik_2 x} + B_2 e^{-ik_2 x}, & \frac{\hbar^2 k_2^2}{2m} &= E - \frac{V}{2} \\ u_{III} &= A_3 e^{ik_3 x} + B_3 e^{-ik_3 x}, & \frac{\hbar^2 k_3^2}{2m} &= E \\ u_{IV} &= t e^{ik_1 x} \end{aligned}$$

(ii) for  $V > E > V/2$

$$\begin{aligned} u_I &= A_1 e^{\kappa x}, & \frac{\hbar^2 \kappa^2}{2m} &= V - E \\ u_{II} &= A_2 e^{ik_2 x} + B_2 e^{-ik_2 x} \\ u_{III} &= A_3 e^{ik_3 x} + B_3 e^{-ik_3 x} \\ u_{IV} &= A_4 e^{-\kappa x} \end{aligned}$$

(iii) for  $E < V/2$

$$\begin{aligned} u_I &= A e^{\kappa x} \\ u_{II} &= A_2 e^{\kappa_2 x} + B_2 e^{-\kappa_2 x}, & \frac{\hbar^2 \kappa_2^2}{2m} &= \frac{1}{2}V - E \\ u_{III} &= A_3 e^{ik_3 x} + B_3 e^{-ik_3 x} \\ u_{IV} &= A_4 e^{-\kappa x} \end{aligned}$$

(b) The boundary conditions at  $x = -d, 0, d$  for the case  $V/2 < E < V$ , for instance, are specified by

$$A_1 e^{-\kappa d} = A_2 e^{-ik_2 d} + B_2 e^{ik_2 d} \quad (1a)$$

$$\kappa A_1 e^{-\kappa d} = ik_2 [A_2 e^{-ik_2 d} - B_2 e^{ik_2 d}] \quad (1b)$$

$$A_2 + B_2 = A_3 + B_3 \quad (1c)$$

$$ik_2 (A_2 - B_2) = ik_3 (A_3 - B_3) \quad (1d)$$

$$A_3 e^{ik_3 d} + B_3 e^{-ik_3 d} = A_4 e^{-\kappa d} \quad (1e)$$

$$ik_3 (A_3 e^{ik_3 d} - B_3 e^{-ik_3 d}) = -\kappa A_4 e^{-\kappa d} \quad (1f)$$

(c) There are 6 conditions to be satisfied as specified in, (1), and there are 7 or 6 constants appearing in eigenfunctions, depending on E considered.

For the case of (i), one can find  $r, A_2, B_2, A_3, B_3, t$  in terms of  $i_0$  and obtain the reflection and

transmission coefficient, in terms of  $r / i_0$  and  $t / i_0$ , as was discussed in the text.

For the case of (ii) or (iii) the six coupled equations are homogeneous and eigenfunctions are therefore trivial unless the secular equation is satisfied.

From the secular equation, the bound state energy eigenvalues are found.

The secular equation for (1) is found as follows.

From (1a), (1b),  $A_2$ ,  $B_2$  are found in terms of  $A_1$  as

$$A_2 = \frac{1}{2} A_1 e^{-\kappa d} \left( 1 + \frac{\kappa}{ik_2} \right) e^{ik_2 d} \text{ ----- (2a)}$$

$$B_2 = \frac{1}{2} A_1 e^{-\kappa d} \left( 1 - \frac{\kappa}{ik_2} \right) e^{-ik_2 d} \text{ ----- (2b)}$$

Likewise from (1e), (1f),

$$A_3 = \frac{1}{2} A_4 e^{-\kappa d} \left( 1 - \frac{\kappa}{ik_3} \right) e^{-ik_3 d} \text{ ----- (3a)}$$

$$B_3 = \frac{1}{2} A_4 e^{-\kappa d} \left( 1 + \frac{\kappa}{ik_3} \right) e^{ik_3 d} \text{ ----- (3b)}$$

Inserting (2), (3) into (1c), (1d),

$$A_1 \left[ \left( 1 + \frac{\kappa}{ik_2} \right) e^{ik_2 d} + \left( 1 - \frac{\kappa}{ik_2} \right) e^{-ik_2 d} \right] - A_4 \left[ \left( 1 - \frac{\kappa}{ik_3} \right) e^{-ik_3 d} + \left( 1 + \frac{\kappa}{ik_2} \right) e^{ik_3 d} \right] = 0 \text{ ----- (4a)}$$

$$A_1 \left[ \left( 1 + \frac{\kappa}{ik_2} \right) e^{ik_2 d} - \left( 1 - \frac{\kappa}{ik_2} \right) e^{-ik_2 d} \right] - A_4 \frac{k_3}{k_2} \left[ \left( 1 - \frac{\kappa}{ik_3} \right) e^{-ik_3 d} - \left( 1 + \frac{\kappa}{ik_3} \right) e^{ik_3 d} \right] = 0 \text{ ----- (4b)}$$

Indeed the coupled equations for  $A_1$ ,  $A_4$  are homogenous and therefore the  $2 \times 2$  determinant involving the coefficients should be zero for the wavefunction not to be trivial and the secular equation reads as,

$$\begin{vmatrix} \left( 1 + \frac{\kappa}{ik_2} \right) e^{ik_2 d} + \left( 1 - \frac{\kappa}{ik_2} \right) e^{-ik_2 d} & - \left( 1 - \frac{\kappa}{ik_3} \right) e^{-ik_3 d} - \left( 1 + \frac{\kappa}{ik_2} \right) e^{ik_3 d} \\ \left( 1 + \frac{\kappa}{ik_2} \right) e^{ik_2 d} - \left( 1 - \frac{\kappa}{ik_2} \right) e^{-ik_2 d} & - \frac{k_3}{k_2} \left[ \left( 1 - \frac{\kappa}{ik_3} \right) e^{-ik_3 d} - \left( 1 + \frac{\kappa}{ik_3} \right) e^{ik_3 d} \right] \end{vmatrix} = 0$$

## Chapter 5

5.1 (a) Let  $\alpha \equiv e^{-ikW/2}$ ,  $\gamma \equiv e^{-ik_0W/2}$ .

Then (5.25) – (5.28) read as

$$\alpha A + \alpha^* B = \gamma i_0 + \gamma^* r \quad \text{----- (1)}$$

$$\alpha^* A + \alpha B = \gamma^* t \quad \text{----- (2)}$$

$$\alpha A - \alpha^* B = \frac{k_0}{k} \gamma i_0 - \frac{k_0}{k} \gamma^* r \quad \text{----- (3)}$$

$$\alpha^* A - \alpha B = \frac{k_0}{k} \gamma^* t \quad \text{----- (4)}$$

Thus, by performing the operation (1)  $\pm$  (3), (2)  $\pm$  (4), A, B are found in terms of  $i_0$ ,  $r$ :

$$A = \frac{r}{2\alpha} \left(1 + \frac{k_0}{k}\right) i_0 + \frac{\gamma^*}{2\alpha} \left(1 - \frac{k_0}{k}\right) r \quad \text{----- (5)}$$

$$B = \frac{r}{2\alpha^*} \left(1 - \frac{k_0}{k}\right) i_0 + \frac{\gamma^*}{2\alpha^*} \left(1 + \frac{k_0}{k}\right) r \quad \text{----- (6)}$$

and

$$A = \frac{\gamma^*}{2\alpha^*} \left(1 + \frac{k_0}{k}\right) t \quad \text{----- (7)}$$

$$B = \frac{\gamma^*}{2\alpha} \left(1 - \frac{k_0}{k}\right) t \quad \text{----- (8)}$$

Next, equating the right hand sides of (5), (7) and (6), (8), respectively and rearranging the terms one finds

$$\frac{\gamma^*}{\alpha^*} \frac{k + k_0}{2k} t - \frac{\gamma^*}{\alpha} \frac{k - k_0}{2k} r = \frac{\gamma}{\alpha} \frac{k + k_0}{2k} i_0 \quad \text{----- (9)}$$

$$\frac{\gamma^*}{\alpha} \frac{k - k_0}{2k} t - \frac{\gamma^*}{\alpha^*} \frac{k + k_0}{2k} r = \frac{\gamma}{\alpha^*} \frac{k - k_0}{2k} i_0 \quad \text{----- (10)}$$

Thus, one can find  $r$ ,  $t$  in terms of  $i_0$  by solving (9), (10), the results of which are in agreement with (5.29), (5.30).

(b) The transmission coefficient is then specified as

$$\begin{aligned} T &\equiv \frac{\hbar k_0 / m \left| t \right|^2}{\hbar k_0 / m \left| i_0 \right|^2} = \frac{(2k_0 k)^2}{(2k_0 k \cos(kW))^2 + (k_0^2 + k^2)^2 \sin^2 kW} \\ &= \frac{1}{\cos^2 kW + \left( \frac{k_0^2 + k^2}{2k_0 k} \right)^2 \sin^2 kW} = \frac{1}{1 + \left( \frac{k_0 - k}{2k_0 k} \right)^2 \sin^2 kW} \\ &= \frac{1}{1 + \frac{V^2}{4E(E+V)} \sin^2 [W \sqrt{\frac{2m}{\hbar^2}} (E+V)]} \end{aligned}$$

where  $\cos^2 x + \sin^2 x = 1$  has been used and  $k$ ,  $k_0$  have been spelled out in terms of  $E$ ,  $V$ .

One can similarly obtain  $R$  given in (5.34)

5.2 (a) The energy eigenequation of the particle reads as

$$\left[ -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + V(x) \right] u(x) = Eu(x)$$

where

$$V(x) = \begin{cases} 0 & x < 0 \\ V_1 & 0 \leq x \leq d_1 \\ V_2 & d_1 < x \end{cases}$$

Equivalently, the equation is compacted as

$$u'' + \alpha^2 u = 0$$

with

$$\alpha = \begin{cases} k_0, & \hbar^2 k_0^2 / 2m = E \\ k_1, & \hbar^2 k_1^2 / 2m = E - V_1 \\ k_2, & \hbar^2 k_2^2 / 2m = E - V_2 \end{cases}$$

The eigenfunction is readily obtained as

$$u = \begin{cases} i_0 e^{ik_0 x} + r e^{-ik_0 x} \\ A e^{ik_1 x} + B e^{-ik_1 x} \\ t e^{ik_2 x} \end{cases}$$

(b) The constants of integration are determined by the boundary conditions, operative at  $x=0, d_1$ :

$$i_0 + r = A + B \text{ ----- (1a)}$$

$$ik_0(i_0 - r) = ik_1(A - B) \text{ ----- (1b)}$$

$$A e^{ik_1 d_1} + B e^{-ik_1 d_1} = t e^{ik_2 d_1} \text{ ----- (1c)}$$

$$ik_1(A e^{ik_1 d_1} - B e^{-ik_1 d_1}) = ik_2 t e^{ik_2 d_1} \text{ ----- (1d)}$$

Clearly,  $r, t, A, B$  can be specified in terms of  $i_0$ , using (1a) ~ (1d).

Perform the operation, (1a)  $\pm$  (1b) /  $ik_1$ , obtaining

$$A = \frac{1}{2} \left[ i_0 \left( 1 + \frac{k_0}{k_1} \right) + r \left( 1 - \frac{k_0}{k_1} \right) \right] \text{ ----- (2a)}$$

$$B = \frac{1}{2} \left[ i_0 \left( 1 - \frac{k_0}{k_1} \right) + r \left( 1 + \frac{k_0}{k_1} \right) \right] \text{ ----- (2b)}$$

Similarly from (1c), (1d) one finds

$$A = \frac{1}{2} e^{-ik_1 d_1 + ik_2 d_1} \left( 1 + \frac{k_2}{k_1} \right) t \text{ ----- (3a)}$$

$$B = \frac{1}{2} e^{ik_1 d_1 + ik_2 d_1} \left( 1 - \frac{k_2}{k_1} \right) t \text{ ----- (3b)}$$

Thus, by equating the right hand sides of (2a), (3a) and (2b), (3b), there result

$$e^{-ik_1 d_1 + ik_2 d_1} \left( 1 + \frac{k_2}{k_1} \right) t - \left( 1 - \frac{k_0}{k_1} \right) r = \left( 1 + \frac{k_0}{k_1} \right) i_0 \text{ ----- (4a)}$$

$$e^{ik_1 d_1 + ik_2 d_1} \left( 1 - \frac{k_2}{k_1} \right) t - \left( 1 + \frac{k_0}{k_1} \right) r = \left( 1 - \frac{k_0}{k_1} \right) i_0 \text{ ----- (4b)}$$

And  $t, r$  are found in terms of  $i_0$  as

$$\frac{t}{i_0} = e^{-ik_2d_1} \frac{2k_0/k_1}{D} \text{ ----- (5a)}$$

$$\frac{r}{i_0} = \frac{\frac{k_0 - k_2}{k_1} \cos k_1d_1 + i \left(1 - \frac{k_0k_2}{k_1^2}\right) \sin k_1d_1}{D} \text{ ----- (5b)}$$

with

$$D = \frac{k_0 + k_2}{k_1} \cos k_1d_1 - i \left(1 + \frac{k_0k_2}{k_1^2}\right) \sin k_1d_1 \text{ ----- (5c)}$$

Hence the transmission and reflection coefficients are given by

$$T \equiv \frac{\hbar k_2/m}{\hbar k_0/m} \left| \frac{t}{i_0} \right|^2 = \frac{4k_0k_2/k_1^2}{|D|^2} \text{ ----- (6a)}$$

$$R \equiv \frac{\hbar k_0/m}{\hbar k_0/m} \left| \frac{r}{i_0} \right|^2 = \frac{1}{|D|^2} \left[ \left( \frac{k_0 - k_2}{k_1} \right)^2 + \left( 1 - \frac{k_0^2 + k_2^2}{k_1^2} + \frac{k_0^2 k_2^2}{k_1^4} \right) \sin^2(k_1d_1) \right] \text{ -----}$$

(6b)

where

$$|D|^2 = \left( \frac{k_0 + k_2}{k_1} \right)^2 + \left( 1 - \frac{k_0^2 + k_2^2}{k_1^2} + \frac{k_0^2 k_2^2}{k_1^4} \right) \sin^2(k_1d_1)$$

Note from (6a), (6b) that

$$R + T = 1,$$

as it should.

(c) Since  $k_0, k_1, k_2$  are functions of  $E$  with  $V_1, V_2, d_1$  as parameters,  $R$  for instance is shown sensitively dependent on these quantities, in particular  $\sin k_1d_1$ . Evidently it is analogous to antireflection coating.

5.3 (a) Consider the motion of the particle on  $x - z$  plane. The energy eigenequation then reads as

$$\left[ -\frac{\hbar^2}{2m} \left( \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial z^2} \right) + V(z) \right] u(x, z) = Eu(x, z)$$

where

$$V(z) = \begin{cases} V_1 & z \leq 0 \\ V_2 & z > 0 \end{cases}$$

Equivalently one can write

$$u''(x) + k_x^2 u(x) = 0 \text{ ----- (1)}$$

$$u''(z) + k(z)^2 u(z) = 0 \text{ ----- (2)}$$

where primes denote respective differentiations and

$$k_x^2 = \frac{2m}{\hbar^2} E_x \text{ ----- (3a)}$$



$$k_z^2 = \begin{cases} k_{z1}^2, k_{z1}^2 = \frac{2m}{\hbar^2} (E_z - V_1), z \leq 0 \\ k_{z2}^2, k_{z2}^2 = \frac{2m}{\hbar^2} (E_z - V_2), z > 0 \end{cases} \quad \text{----- (3b)}$$

$$E = E_x + E_z \quad \text{----- (3c)}$$

The solutions of (1), (2) can be readily obtained. The particle moves as a free particle along  $x$ -direction, i.e.

$$u(x) \sim e^{ik_x x} \quad \text{----- (4a)}$$

while

$$u(z) = \begin{cases} i_0 e^{ik_{z1} z} + r e^{-ik_{z1} z} \\ t e^{ik_{z2} z} \end{cases} \quad \text{----- (4b)}$$

The boundary conditions for  $u(z)$  to satisfy at  $z=0$  are:

$$\begin{aligned} i_0 + r &= t \\ i_0 - r &= \frac{k_{z2}}{k_{z1}} t \end{aligned}$$

Hence,  $r, t$  can be found in terms of  $i_0$ :

$$r = i_0 \frac{1 - k_{z2}/k_{z1}}{1 + k_{z2}/k_{z1}} \quad \text{----- (5a)}$$

$$t = i_0 \frac{2}{1 + k_{z2}/k_{z1}} \quad \text{----- (5b)}$$

(b) The incident, reflected and transmitted wavefunctions reads then as

$$u_i(x, z) \sim e^{i(k_x x + k_{z1} z)} \quad \text{----- (6a)}$$

$$u_r(x, y) \sim e^{i(k_x x - k_{z1} z)} \quad \text{----- (6b)}$$

$$u_t(x, y) \sim e^{i(k_x x + k_{z2} z)} \quad \text{----- (6c)}$$

Equivalently, one may introduce  $k, \theta_i, \theta_t$  such that

$$k_x = k \cos \theta_i \quad \text{----- (7a)}$$

$$k_{z1} = k \sin \theta_i \quad \text{----- (7b)}$$

$$k_{z2} = k \sin \theta_t \quad \text{----- (7c)}$$

and represent incident wavefunction as

$$u_i(x, z) \sim e^{ik(\cos \theta_i x + \sin \theta_i y)}$$

In which case one can write from (6b)

$$u_r(x, z) \sim e^{ik(\cos \theta_r x - \sin \theta_r y)}$$

so that the incident and reflected angles are shown identical:

$$\theta_i = \theta_r \quad \text{----- (8)}$$

The transmitted wave is likewise to be expressed as

$$u_i(x, z) \sim e^{ik(\cos\theta_i x + \sin\theta_i z)}$$

and one can write

$$\frac{\sin\theta_i}{\sin\theta_t} = \frac{k_{z1}/k}{k_{z2}/k} = \frac{\sqrt{\frac{2m}{\hbar^2}(E_z - V_2)}}{\sqrt{\frac{2m}{\hbar^2}(E_z - V_1)}} = \frac{\sqrt{E_z - V_2}}{\sqrt{E_z - V_1}} \text{----- (9)}$$

(c) The transmission and reflection coefficients are given from (5) by

$$R \equiv \frac{\hbar k_{z1}}{\hbar k_{z1}} \cdot \left| \frac{r}{i_0} \right|^2 = \left[ \frac{1 - k_{z2}/k_{z1}}{1 + k_{z2}/k_{z1}} \right]^2 = \left[ \frac{1 - \sqrt{(E_z - V_2)/(E_z - V_1)}}{1 + \sqrt{(E_z - V_2)/(E_z - V_1)}} \right]^2$$

$$T \equiv \frac{\hbar k_2}{\hbar k_0} \left| \frac{t}{i_0} \right|^2 = \frac{4(k_{z2}/k_{z1})^2}{[1 + (k_{z2}/k_{z1})]^2} = \frac{4\sqrt{(E_z - V_2)/(E_z - V_1)}}{[1 + \sqrt{(E_z - V_2)/(E_z - V_1)}]^2}$$

and

$$R + T = 1$$

as it should.

(d) Evidently (8), (9) are analogous with reflection and refraction of light at a dielectric interface.

5.4 (a) The potential is specified as

$$V(x) = \begin{cases} 0 & x \leq x_i & \text{I} \\ V & x_i < x \leq d + x_i & \text{II} \\ 0 & d + x_i < x \leq d + W + x_i & \text{III} \\ V & d + W + x_i < x \leq 2d + W + x_i & \text{IV} \\ 0 & 2d + W + x_i < x & \text{V} \end{cases}$$

The energy eigenequations are given by

$$u'' + k_i^2 u = 0 \text{----- (1a)}$$

with

$$k_1 = k_3 = k_5 = \sqrt{\frac{2mE}{\hbar^2}} \equiv k_0, \quad \text{I, III, V} \\ k_2 = k_4 = \sqrt{\frac{2m}{\hbar^2}(E - V)} \equiv k, \quad \text{II, IV} \text{----- (1b)}$$

And one can write eigenfunctions as

$$u = \begin{cases} i_0 e^{ik_0 x} + r e^{-ik_0 x}, & \text{I} \\ A e^{ikx} + B e^{-ikx}, & \text{II} \\ C e^{ik_0 x} + D e^{-ik_0 x}, & \text{III} \text{ ----- (2)} \\ F e^{ikx} + G e^{-ikx}, & \text{IV} \\ t e^{ik_0 x} & \text{V} \end{cases}$$

(b) The boundary conditions operative at  $x_i$  between regions I, II are:

$$\begin{aligned} i_0 e^{ik_0 x_i} + r e^{-ik_0 x_i} &= A e^{ikx_i} + B e^{-ikx_i} \\ i_0 e^{ik_0 x_i} - r e^{-ik_0 x_i} &= \frac{k}{k_0} e^{ikx_i} - \frac{k}{k_0} e^{-ikx_i} \end{aligned}$$

One can thus find  $i_0, r$  in terms of  $A, B$ :

$$\begin{aligned} i_0 &= \frac{1}{2} e^{-ik_0 x_i} \left[ A \left( 1 + \frac{k}{k_0} \right) e^{ikx_i} + B \left( 1 - \frac{k}{k_0} \right) e^{-ikx_i} \right] \\ r &= \frac{1}{2} e^{ik_0 x_i} \left[ A \left( 1 - \frac{k}{k_0} \right) e^{ikx_i} + B \left( 1 + \frac{k}{k_0} \right) e^{-ikx_i} \right] \end{aligned}$$

or equivalently

$$\begin{pmatrix} i_0 \\ r \end{pmatrix} = M(k_0, k, x_i) \begin{pmatrix} A \\ B \end{pmatrix} \text{----- (3a)}$$

where the  $2 \times 2$  matrix reads as

$$M(k_0, k, x_i) = \frac{1}{2} \begin{pmatrix} e^{-ik_0 x_i + ikx_i} \left( 1 + \frac{k}{k_0} \right) & e^{-ik_0 x_i - ikx_i} \left( 1 - \frac{k}{k_0} \right) \\ e^{ik_0 x_i + ikx_i} \left( 1 - \frac{k}{k_0} \right) & e^{ik_0 x_i - ikx_i} \left( 1 + \frac{k}{k_0} \right) \end{pmatrix} \text{----- (3b)}$$

One can likewise apply similar boundary conditions at successive interfaces, obtaining

$$\begin{pmatrix} A \\ B \end{pmatrix} = M(k, k_0, x_i + d) \begin{pmatrix} C \\ D \end{pmatrix} \text{----- (3c)}$$

$$\begin{pmatrix} C \\ D \end{pmatrix} = M(k_0, k, x_i + d + W) \begin{pmatrix} F \\ G \end{pmatrix} \text{----- (3d)}$$

$$\begin{pmatrix} F \\ G \end{pmatrix} = M(k, k_0, x_i + 2d + W) \begin{pmatrix} t \\ 0 \end{pmatrix} \text{----- (3e)}$$

Hence one can correlate  $r, t$  with  $i_0$  using (3a) – (3e):

$$\begin{pmatrix} i_0 \\ r \end{pmatrix} = M_T \begin{pmatrix} t \\ 0 \end{pmatrix} \text{----- (4)}$$

where  $M_T$  consists of

$$\begin{aligned} M_T &= M(k_0, k, x_i)M(k, k_0, x_i + d)M(k_0, k, x_i + d + W)M(k, k_0, x_i + 2d + W) \\ &= \begin{pmatrix} m_{11} & m_{12} \\ m_{21} & m_{22} \end{pmatrix} \text{----- (5)} \end{aligned}$$

(c) Now that the matrix elements of  $M_T$  have been specified explicitly,  $R$ ,  $T$  can be found from

$$\begin{pmatrix} i_0 \\ r \end{pmatrix} = \begin{pmatrix} m_{11} & m_{12} \\ m_{21} & m_{22} \end{pmatrix} \begin{pmatrix} t \\ 0 \end{pmatrix}$$

Specifically,

$$\begin{aligned} T &= \frac{\hbar k_0 / m}{\hbar k_0 / m} \left| \frac{t}{i_0} \right|^2 = \left| \frac{1}{m_{11}} \right|^2 \\ R &= \frac{\hbar k_0 / m}{\hbar k_0 / m} \cdot \left| \frac{r}{i_0} \right|^2 = \left| \frac{r/t}{i/t} \right|^2 = \left| \frac{m_{21}}{m_{11}} \right|^2 \end{aligned}$$

(d) The matrix element, say  $m_{11}$ , is a function of energy,  $E$  of incoming particle with  $V$ ,  $d$ ,  $W$  as parameters. Thus finding the condition for 100% transmission amounts to finding  $E$  such that  $|m_{11}|^2 = 1$ .

(e) The analysis can be extended to any number of barriers separated by equal distances by introducing corresponding matrices.

Hint: Try 1 barrier first and add one more barrier and find the pattern emerging.

5.5 This problem can be tackled exactly in the same manner as in (5.4) except that  $M_T$  in (5) therein has to be modified as

$$M_T = M(k_0, k, x_i)M(k, k_0, x_i + d)M(k_0, k', x_i + d + W)M'(k', k_0, x_i + 2d + W)$$

where

$$k' \equiv \sqrt{\frac{2m(E + V)}{\hbar^2}}$$

## Chapter 6

6.1 (a) From (4.11(b)) the quantized energy levels are given by

$$E_n = \frac{\hbar^2 \pi^2}{2mW^2} n^2, \quad n = 1, 2, \dots \text{----- (1)}$$

For electrons with rest mass  $m_0$

$$\begin{aligned} E_1 &= \frac{(1.055 \times 10^{-34})^2 (3.14)^2}{2 \cdot 9.1 \times 10^{-31} \cdot (10^{-9})^2 w^2} n^2 [J] \\ &= (0.603 / w^2) \times 10^{-19} [J] \\ &= (0.603 / w^2) \times 1.6 \times 10^{-19} [eV] \\ &= (0.376 / w^2) [eV] \end{aligned}$$

where the width of the well has been scaled w.r.t nanometer, i.e.

$$W = 10^{-9} \cdot w$$

with  $w$  denoting nm.

For  $m_n = 0.2m_0$ ,

$$E_n = \frac{0.37}{w^2} \cdot \left( \frac{m_0}{m_n} \right) n^2 [eV] = (1.86 / w^2) n^2 [eV] \text{----- (2)}$$

(b) Specify  $V(x)$  as

$$V(x) = \begin{cases} V & x < 0 & \text{I} \\ 0 & 0 \leq x \leq W & \text{II} \\ V & W < x & \text{III} \end{cases}$$

Then the bound state eigenfunctions can be expressed as

$$u(x) = \begin{cases} Ae^{\kappa x} & x < 0 \\ Be^{ikx} + Ce^{-ikx} & 0 \leq x \leq W \\ De^{-\kappa x} & W < x \end{cases}$$

where

$$\begin{aligned} k &= \sqrt{\frac{2m}{\hbar^2} E} \\ \kappa &= \sqrt{\frac{2m}{\hbar^2} (V - E)}, \quad E < V \end{aligned}$$

From the boundary conditions for  $u(x)$  to satisfy at  $x=0, W$ , on finds the non-trivial values of  $A, B, C, D$ , provided the secular equation is satisfied. From the secular equation quantized energy levels for bound states are obtained.

It will be interesting and instructive to perform the graphical analysis and compare the results

with (1). It will also be interesting to compare the resulting ground state energy eigenvalue with that of the infinite square well potential and examine the reasons for the difference, if any (see Fig. 4.7 in the text and seek the reasons for difference).

(c) For  $m = m_0$  for example one can write from (1)

$$\frac{0.376}{w^2} eV = \frac{k_B T}{2} \cong \frac{25}{2} meV$$

Hence

$$w = 376/12.5 \approx 5.5 \text{ and } W = 5.5nm$$

(d) Consider the case where  $W=2nm$ , i.e.  $w=2$ . Then from (a)

$$E_n = \frac{0.37}{4} \cdot n^2 [eV] \approx 0.1n^2 [eV]$$

Thus, energy levels up to  $n = 4$  are given by  $\sim 0.1, 0.4, 0.9, 1.6 eV$ , respectively.

For the other limit of  $W = 200nm$ , the energy levels are reduced by a factor,  $10^{-4}$ .

The density of states is then described by step functions, with each step occurring at every quantized energy level at a height specified from (4.29) by

$$g_{2D} = m / \pi \hbar^2$$

6.2 (a) The tunneling probability through the square barrier potential is given from (6.5), (6.6) by

$$T = \frac{1}{1 + \Lambda}$$

$$\Lambda = \frac{V^2}{4E(V-E)} \sinh^2 d \sqrt{\frac{2m}{\hbar^2} (V-E)}$$

Thus,  $T$  can be found explicitly by inserting the given barrier height  $V$  and thicknesses  $d_L, d_R$  and the energy eigenvalues of the well,  $E$ . It will be interesting to compare the tunneling probability through the two barriers with different thickness.

(b) The lifetime is to be specified first by the condition,

$$TN = 1 \text{ ----- (1)}$$

where  $N$  is the average number the electron encounters the barrier for tunneling through. Once  $N$  is found in terms of the tunneling probability,  $T$  the lifetime is found by multiplying the round trip time with  $N$ :

$$\tau = (2W / v)N \text{ ----- (2)}$$

Here  $2W$  is the round trip distance and  $v$  the velocity of electron given in terms of  $E$  as

$$\frac{1}{2}mv^2 = E$$

Since  $d_R$  (10nm)  $\ll d_L$  (50nm),  $T_R \gg T_L$ , so that the electron lifetime is practically determined by the barrier on the right hand side.

Thus using  $T_R$  found in (a) and the values of  $W$  and energy  $E$  of the subband,  $\tau$  can be calculated using (2).

6.3 (a) As discussed in (6.2) the electron lifetime is determined by the tunneling probability through the potential barrier with thickness,  $d_R$  ( $\ll d_L$ ).

The velocity of electron residing in the ground state energy level of the well is given by

$$\frac{1}{2}mv^2 = E_1 = \frac{\hbar^2 \pi^2}{2mW^2} \text{----- (1)}$$

That is,

$$v = \frac{\hbar \pi}{mW} \text{----- (2)}$$

and depends on the width of the well.

With an external electric field  $|E|$  applied, the potential barrier is transformed into either trapezoidal or triangular shape. The tunneling probability is then given from (6.11), (6.12) by

$$T \approx e^{-f} \text{----- (3a)}$$

where

$$f = \begin{cases} \frac{4\sqrt{2m}}{3q|E|} \left[ (V - E_1)^{\frac{3}{2}} - (V - E_1 - q|E|d_R)^{\frac{3}{2}} \right] & \text{----- 3(a)} \\ \frac{4\sqrt{2m}}{2q|E|\hbar} (V - E_1)^{\frac{3}{2}} & \text{----- 3(b)} \end{cases}$$

Thus one can find  $T$  for given  $|E|$ ,  $W$  and find the lifetime:

$$\tau = \frac{2W}{v} \cdot \frac{1}{T} \text{----- (4)}$$

Note here that the velocity of electron,  $v$  as give by (2) can be used, provided  $v$  is greater than the thermal speed,  $v_T$ . Otherwise,  $v_T$  should be used instead in (4)

(b) The potential barrier

$$V(x) = V - q|E|x, \quad V = 3.1eV$$

becomes a triangular barrier to electrons at the ground state, if

$$V - q|E|d_R \leq E_1 = \frac{\hbar^2 \pi^2}{2mW^2}$$

Thus the required electric field can be estimated by putting  $E_1 \approx 0$ , obtaining

$$|E| \approx \frac{V}{q \cdot d_R} \approx \frac{3.1eV \cdot 1.6 \times 10^{-19} J / eV}{1.6 \times 10^{-19} C \cdot 10 \times 10^{-9} m} = 3.1 \times 10^7 V / m = 31mV / nm$$

Consider the case where  $W = 50nm$ .

The ground state energy given from problem 6.1 by

$$E_1 = \frac{0.376eV}{50^2} \approx 0.15meV$$

is then smaller than the thermal energy at room temperature. Hence for estimating the lifetime the thermal velocity of electron should be used.

Thus, form (3), (4) one can write

$$\tau = \frac{2W}{v_T} \cdot \frac{1}{T} \text{----- (5)}$$

where

$$\frac{1}{2}mv_T^2 = \frac{1}{2}k_B T,$$

and

$$T \cong \exp - \frac{4\sqrt{2m}}{3q|E|\hbar} V^{3/2}, \quad V = 3.1eV$$

At room temperature,  $T=300K$  and  $v_T \approx 6.75 \times 10^4 m/s$ . Hence, the electric field required for  $\tau = 10^{-6} s$  is found from

$$10^{-6} = \frac{2 \cdot 50 \times 10^{-9}}{6.75 \times 10^4} \exp \frac{4\sqrt{2m}}{3q|E|\hbar} V^{3/2}$$

so that

$$|E| \approx 1.36 \times 10^9 V/m = 1.36V/nm$$

6.4 (a) Use the F - N tunneling probability for estimating the electric field and write

$$T \approx \exp - \frac{4\sqrt{2m}}{3q|E|\hbar} V^{3/2} \text{----- (1)}$$

where the work function,  $V = 4.5eV$  is the barrier the electron encounters when incident from the metal to the sample. One finds the required electric field,  $|E|$  by putting  $T = 10^{-4}$  in (1)

$$10^{-4} = \exp - \frac{4\sqrt{2m}}{3q|E|\hbar} V^{3/2}$$

or

$$|E| = \exp \frac{4\sqrt{2m} \cdot V^{3/2}}{3q\hbar \cdot 4(\ln 10)} \approx 7.05 \times 10^9 V/m = 7.05V/nm$$

With this electric field applied the electron indeed encounters the triangular potential barrier while tunneling to the sample 1nm distance away, as was assumed.

(b) Use the direct tunneling probability, put  $T = 10^{-4}$ , and write

$$10^{-4} \cong \exp - \frac{4\sqrt{2m}}{3q|E|\hbar} \left[ V^{3/2} - (V - q|E|d)^{3/2} \right]$$

Since 0.1 V is applied between the tip and sample, one can put  $|q|E|d = 0.1 eV$  and  $d$  can be found by inserting given parameters in the equation,



$$10^{-4} \cong \exp - \frac{4\sqrt{2m}}{3q\hbar} \frac{d}{0.1} \left[ V^{3/2} - (V - 0.1)^{3/2} \right]$$

6.5 (a) Using (6.13), (6.14) and applying the boundary condition,

$$U_j(z_j) = U_{j+1}(z_j)$$

$$\frac{\partial}{\partial z} U_j(z_j) = \frac{\partial}{\partial z} U_{j+1}(z_j)$$

one can write

$$A_j e^{ikz_j} + B_j e^{-ikz_j} = A_{j+1} e^{-\kappa z_j} + B_{j+1} e^{\kappa z_j} \quad \text{----- (1a)}$$

$$A_j e^{ikz_j} - B_j e^{-ikz_j} = \frac{i\kappa}{k} \left[ A_{j+1} e^{-\kappa z_j} - B_{j+1} e^{\kappa z_j} \right] \quad \text{----- (1b)}$$

Solving for  $A_j, B_j$  in terms of  $A_{j+1}, B_{j+1}$  one obtains

$$A_j = \frac{e^{-ikz_j}}{2} \left[ A_{j+1} e^{-\kappa z_j} \left( 1 + \frac{i\kappa}{k} \right) + B_{j+1} e^{\kappa z_j} \left( 1 - \frac{i\kappa}{k} \right) \right] \quad \text{----- (2a)}$$

$$B_j = \frac{e^{ikz_j}}{2} \left[ A_{j+1} e^{-\kappa z_j} \left( 1 - \frac{i\kappa}{k} \right) + B_{j+1} e^{\kappa z_j} \left( 1 + \frac{i\kappa}{k} \right) \right] \quad \text{----- (2b)}$$

One can thus introduce the transfer matrix connecting  $A_j, B_j$  to  $A_{j+1}, B_{j+1}$  as

$$\begin{pmatrix} A_j \\ B_j \end{pmatrix} = \begin{pmatrix} \alpha & \beta \\ \alpha^* & \beta^* \end{pmatrix} \begin{pmatrix} A_{j+1} \\ B_{j+1} \end{pmatrix} \quad \text{----- (3a)}$$

where

$$\alpha = \frac{1}{2} \left( 1 + \frac{i\kappa}{k} \right) e^{i(i\kappa - k)z_j} \quad \text{----- (3b)}$$

$$\beta = \frac{1}{2} \left( 1 - \frac{i\kappa}{k} \right) e^{i(i\kappa + k)z_j} \quad \text{----- (3c)}$$

(b) One can likewise connect  $A_{j+1}, B_{j+1}$  to  $A_{j+2}, B_{j+2}$ , applying the boundary condition at  $z_j + d$  to the wavefunctions,  $U_{j+1}(z), U_{j+2}(z)$ , obtaining

$$\begin{pmatrix} A_{j+1} \\ B_{j+1} \end{pmatrix} = \begin{pmatrix} \gamma & \gamma^* \\ \delta & \delta^* \end{pmatrix} \begin{pmatrix} A_{j+2} \\ B_{j+2} \end{pmatrix} \quad \text{----- (4a)}$$

where

$$\gamma = \left( 1 + \frac{k}{i\kappa} \right) e^{i(k - i\kappa)(z_j + d)} \quad \text{----- (4b)}$$

$$\delta = \left( 1 + \frac{k}{(-i\kappa)} \right) e^{i(k + i\kappa)(z_j + d)} \quad \text{----- (4c)}$$

Combining (3), (4), one can connect  $A_j, B_j$  to  $A_{j+2}, B_{j+2}$ :

$$\begin{aligned} \begin{pmatrix} A_j \\ B_j \end{pmatrix} &= \begin{pmatrix} \alpha & \beta \\ \alpha^* & \beta^* \end{pmatrix} \begin{pmatrix} \gamma & \gamma^* \\ \delta & \delta^* \end{pmatrix} \begin{pmatrix} A_{j+2} \\ B_{j+2} \end{pmatrix} \\ &= \begin{pmatrix} m_{11}(d) & m_{12}(z_j, d) \\ m_{21}(z_j, d) & m_{22}(d) \end{pmatrix} \begin{pmatrix} A_{j+2} \\ B_{j+2} \end{pmatrix} \end{aligned} \quad \text{----- (5a)}$$

with

$$\begin{aligned} m_{11}(d) &= \alpha\gamma + \beta\delta \\ &= e^{ikd} \left( \cosh \kappa d - i \frac{k^2 - \kappa^2}{2k\kappa} \sinh \kappa d \right) \end{aligned} \quad \text{----- (5b)}$$

$$\begin{aligned} &= m_{22}^* \\ m_{12}(z_j, d) &= \alpha\gamma^* + \beta\delta^* \\ &= ie^{-ik(2z_j+d)} \frac{k^2 + \kappa^2}{2k\kappa} \sinh \kappa d \\ &= m_{21}^* \end{aligned} \quad \text{----- (5c)}$$

(c) In the presence of one barrier potential, one can write

$$\begin{pmatrix} A_j \\ B_j \end{pmatrix} = \begin{pmatrix} m_{11}(d) & m_{12}(z_j, d) \\ m_{21}(z_j, d) & m_{22}(d) \end{pmatrix} \begin{pmatrix} A_{j+2} \\ 0 \end{pmatrix} \quad \text{----- (6)}$$

Here  $B_{j+2} = 0$ , since there is no reflection beyond the single barrier. The transmission coefficient can thus be obtained as

$$T = \left| \frac{A_{j+2}}{A_j} \right|^2 = \frac{1}{|m_{11}(d)|^2} \quad \text{----- (7)}$$

where

$$\begin{aligned} |m_{11}(d)|^2 &= \cosh^2 \kappa d + \left( \frac{k^2 - \kappa^2}{2k\kappa} \right)^2 \sinh^2 \kappa d \\ &= 1 + \sinh^2 \kappa d + \left( \frac{k^2 - \kappa^2}{2k\kappa} \right)^2 \sinh^2 \kappa d \\ &= 1 + \frac{(k^2 + \kappa^2)^2}{4k^2\kappa^2} \sinh^2 \kappa d \\ &= 1 + \frac{V^2}{4(V-E)E} \sinh^2 d \sqrt{\frac{2m}{\hbar^2}(V-E)} \end{aligned}$$

in complete agreement with (6.5) in the text.

(d) It also follows from (6) that

$$\begin{aligned}
R &= \left| \frac{B_j}{A_j} \right|^2 = \left| \frac{m_{12}^*(d)A_{j+2}}{m_{11}(z_j, d)A_{j+2}} \right|^2 \\
&= \left| \frac{-ie^{-ik(2z_j+d)} \frac{k^2 + \kappa^2}{2k\kappa} \sinh \kappa d}{e^{ikd} \left[ \cosh \kappa d - i \left( \frac{k^2 - \kappa^2}{2k\kappa} \right) \sinh \kappa d \right]} \right|^2 \\
&= \frac{\left( \frac{k^2 + \kappa^2}{2k\kappa} \right)^2 \sinh^2 \kappa d}{1 + \left( \frac{k^2 + \kappa^2}{2k\kappa} \right)^2 \sinh^2 \kappa d}
\end{aligned}$$

in agreement with (6.7) in the text.

- 6.6. In the presence of two potential barriers  $W$  distance apart, one can put  $B_{j+4} = 0$  because of no reflection after tunneling through the second barrier and write

$$\begin{pmatrix} A_j \\ B_j \end{pmatrix} = \begin{pmatrix} m_{11}(d) & m_{12}(z_j, d) \\ m_{12}^*(z_j, d) & m_{11}^*(d) \end{pmatrix} \begin{pmatrix} m_{11}(d) & m_{12}(z_{j+2}, d) \\ m_{12}^*(z_{j+2}, d) & m_{11}^*(d) \end{pmatrix} \begin{pmatrix} A_{j+4} \\ 0 \end{pmatrix}$$

where

$$z_{j+2} = z_j + W + d$$

Then, as shown in (6.23), (6.24) in the text one can find

$$\frac{A_{j+4}}{A_j} = \frac{-e^{-2ikd} \cdot 4k^2 \kappa^2}{\left[ D_1 - e^{2ikW} (k^2 + \kappa^2) \sinh \kappa d \right]^2} \text{----- (1a)}$$

where

$$\begin{aligned}
D_1 &= \left[ (k^2 - \kappa^2) \sinh \kappa d + 2ik\kappa \cosh \kappa d \right]^2 \\
&= \left[ (k^2 - \kappa^2)^2 \sinh^2 \kappa d + 4k^2 \kappa^2 \cosh^2 \kappa d \right] e^{2i\theta} \text{----- (1b)} \\
&= \left[ 4k^2 \kappa^2 + (k^2 + \kappa^2)^2 \sinh^2 \kappa d \right] e^{2i\theta}
\end{aligned}$$

with

$$\tan \theta = \frac{2k\kappa \cosh \kappa d}{(k^2 - \kappa^2) \sinh \kappa d} \text{----- (1c)}$$

Here  $D_1$  has been put into a phasor representation and use was made of

$$\cosh^2 x = 1 + \sinh^2 x$$

Since the velocities of incident and transmitted electron are the same, one can express the tunneling probability across two potential barriers as

$$\begin{aligned}
T_{2B} &= \left| \frac{A_{j+4}}{A_j} \right|^2 \\
&= \frac{(4k^2 \kappa^2)^2}{|D_1|^2 \left| 1 - e^{2i(kW-\theta)} \cdot \frac{(k^2 + \kappa^2)^2 \sinh^2 \kappa d}{|D_1|} \right|^2} \text{----- (2)} \\
&= \frac{T_{1B}^2}{\left| 1 - e^{2i(kW-\theta)} \cdot R_{1B} \right|^2}
\end{aligned}$$

Here  $T_{2B}$  has been expressed in terms of the tunneling probability through the single barrier,  $T_{1B}$  and the corresponding reflection coefficient, i.e.

$$\begin{aligned}
T_{1B} &\equiv \frac{4k^2 \kappa^2}{|D_1|} \\
R_{1B} &\equiv \frac{(k^2 + \kappa^2)^2 \sinh^2 \kappa d}{|D_1|}
\end{aligned}$$

(2) can be further compacted into a more transparent form by putting the denominator into a phasor notation:

$$\begin{aligned}
&\left| 1 - e^{i\chi} R_{1B} \right|^2 \\
&= \left[ (1 - \cos \chi R_{1B})^2 + \sin^2 \chi R_{1B}^2 \right] e^{2i\varphi} \\
&= \left[ 1 + R_{1B}^2 - 2 \cos \chi R_{1B} \right] e^{2i\varphi} \text{----- (3)} \\
&= \left[ (1 - R_{1B})^2 + 4R_{1B} \sin^2 \frac{\chi}{2} \right] e^{2i\varphi}
\end{aligned}$$

where

$$\tan \varphi = \frac{\sin \chi R_{1B}}{1 - \cos \chi R_{1B}}, \quad \chi \equiv 2(kW - \theta)$$

and use has been made of

$$\cos \chi = 1 - 2 \sin^2 \frac{\chi}{2}$$

Inserting (3) into (2) and identifying  $T_{1B} = 1 - R_{1B}$  one can write

$$T_{2B} = \frac{1}{1 + 4 \frac{R_{1B}}{T_{1B}^2} \sin^2 (kW - \theta)} \text{----- (4)}$$

One can clearly notice from (4) that the resonant tunneling occurs, i.e.

$T_{2B} = 1$  for

$$kW - \theta = n\pi, \quad n = 1, 2, \dots$$

It will be illuminating to plot  $T_{2B}$  versus incident electron energy for various values of the potential barrier and the quantum well in between the two.

## Chapter 7

7.1 (a) Consider the dispersion relation, (7.22) in the text:

$$\cos k_1 a \cosh \kappa b - \frac{k_1^2 - \kappa^2}{2k_1 \kappa} \sin k_1 a \sinh \kappa b = \cos kd \quad \text{----- (1)}$$

In the limit  $b \rightarrow 0$ ,  $V \rightarrow \infty$ , such that the value  $V \times b$  is finite, then

$$\kappa b = \sqrt{\frac{2m}{\hbar^2}} (V - E)b \rightarrow 0$$

so that

$$\begin{aligned} \cosh \kappa b &\approx 1 \\ \sinh \kappa b &\approx \sqrt{\frac{2m}{\hbar^2}} Vb \\ \frac{k_1^2 - \kappa^2}{2k_1 \kappa} &\approx -\frac{2mV/\hbar^2}{2k_1 \sqrt{2mV/\hbar^2}} = \frac{\sqrt{2mV/\hbar^2}}{2k_1} \quad \text{----- (2)} \\ d &= a + b \approx a \end{aligned}$$

Hence the second term on the left of (1) reads as

$$\frac{\sqrt{2mV/\hbar^2}}{2k_1} \cdot \sqrt{2mV/\hbar^2} \cdot b \sin k_1 a \cdot \frac{a}{a} = P \frac{\sin k_1 a}{k_1 a}, \quad P = \frac{mVba}{\hbar^2} \quad \text{----- (3)}$$

Inserting (3) into (1) one can write with the use of (2)

$$P \frac{\sin k_1 a}{k_1 a} + \cos k_1 a = \cos ka \quad \text{----- (4)}$$

(b) The simplified dispersion relation (4) is a handy equation by which to examine the energy band as a function of parameters involved such as  $Vb$ ,  $a$ , etc.

It will be interesting and instructive to examine the widths of allowed bands and energy gap as a function of these parameters and to interpret the results.

7.2 (a) Given the coupled equation (7.41) for  $x_1, x_2$  one can find  $x_1$  for instance using the Kramer's rule:

$$x_1 = \frac{\begin{vmatrix} 0 & 2 \\ 0 & 1 - \lambda \end{vmatrix}}{\begin{vmatrix} 1 - \lambda & 2 \\ 2 & 1 - \lambda \end{vmatrix}} = 0$$

Hence it is evident that  $x_1 = x_2 = 0$  unless the secular equation holds true, i.e.

$$\begin{vmatrix} 1 - \lambda & 2 \\ 2 & 1 - \lambda \end{vmatrix} = 0 \quad \text{----- (1)}$$

(b) Evaluating the determinant (1) one can write

$$(1 - \lambda)^2 = 4$$

so that

$$\lambda_{\pm} = 3, -1 \quad \text{----- (2)}$$

Inserting these two roots into any one of two coupled equations in (7.41) one finds

$$-2x_1 + 2x_2 = 0 \quad \text{for } \lambda = 3 \text{ ----- (3a)}$$

and

$$2x_1 + 2x_2 = 0 \quad \text{for } \lambda = -1 \text{ ----- (3b)}$$

Hence there exists an infinite number of solutions in the coupled equation, provided  $x_1, x_2$  are constrained by (3).

(c) Insert  $\lambda_+ = 3$  for instance into the two coupled equations in (7.41), obtaining

$$-2x_1 + 2x_2 = 0$$

$$2x_1 - 2x_2 = 0$$

Clearly both equations lead to identical constraints.

(d) The two sets of solutions  $(x_1, x_2)$  corresponding to  $\lambda_+$  and  $\lambda_-$  can be represented by column vectors, i.e.

$$X_1 = x_1 \begin{pmatrix} 1 \\ 1 \end{pmatrix}$$

and

$$X_2 = x_1 \begin{pmatrix} 1 \\ -1 \end{pmatrix}$$

The length of the column vector is defined as

$$\widetilde{X}_1 X_1 = x_1^2 (1 \quad 1) \begin{pmatrix} 1 \\ 1 \end{pmatrix} = 2x_1^2$$

$$\widetilde{X}_2 X_2 = x_1^2 (1 \quad -1) \begin{pmatrix} 1 \\ -1 \end{pmatrix} = 2x_1^2$$

Thus if normalization condition is imposed, that is the unit length condition is imposed,

$$2x_1^2 = 1$$

and

$$x_1 = \frac{1}{\sqrt{2}}$$

7.3 (a) Starting from (7.14) in the text, perform the operation,

$$[(7.14a) \pm (7.14b)] / ik_1$$

obtaining

$$A = \frac{1}{2} e^{-ikd} \left[ e^{-\kappa d} \left( 1 + \frac{i\kappa}{k_1} \right) C + e^{\kappa d} \left( 1 - \frac{i\kappa}{k_1} \right) D \right] \text{----- (1a)}$$

$$B = \frac{1}{2} e^{-ikd} \left[ e^{-\kappa d} \left( 1 - \frac{i\kappa}{k_1} \right) C + e^{\kappa d} \left( 1 + \frac{i\kappa}{k_1} \right) D \right] \text{----- (1b)}$$

Also, perform the operation,

$$[(7.15a) \pm (7.15b)] / ik_1$$

obtaining

$$A = \frac{1}{2} e^{-ik_1 a} \left[ e^{-\kappa a} \left( 1 + \frac{i\kappa}{k_1} \right) C + e^{\kappa a} \left( 1 - \frac{i\kappa}{k_1} \right) D \right] \text{----- (2a)}$$

$$B = \frac{1}{2} e^{-ik_1 a} \left[ e^{-\kappa a} \left( 1 - \frac{i\kappa}{k_1} \right) C + e^{\kappa a} \left( 1 + \frac{i\kappa}{k_1} \right) D \right] \text{----- (2b)}$$

Thus, equating (1a), (2a) and (1b), (2b), respectively and rearranging the terms, one can reproduce (7.19), (7.20) in the text.

(b) Once the matrix elements entering in the  $2 \times 2$  determinant are specified explicitly it is a lengthy but straightforward algebra to obtain the dispersion relation given in (7.22) in the text. Here, recognizing the identity,

$$e^{-2ikd} + 1 = 2e^{-ikd} \cos kd$$

is helpful.

(c) It is extremely desirable to carry out the graphical analysis of the dispersion relation, following the method detailed in the text and using the values of the parameters given in the problem.

The problem provides a simple but practical example, the numerical analysis of which can provide a concrete feeling for the subbands. The energy eigenvalues in quantum well or subbands are used extensively for modeling semiconductor devices.

(d) The physical significance of the dispersion relation (7.22) is to find  $E - k$  pair to render the wavefunction in (7.11) non-trivial. Specifically, given a pair of  $E$  and  $k$ ,  $C$  can be found in terms of  $D$  from (7.19) and  $A, B$  can in turn be found in terms of  $D$  from (7.14) or (7.15).

Constructing a few Bloch wavefunctions in this manner could be rather instructive.

(e) Yes, there is a similarity.

Specifically, finding  $\lambda_+, \lambda_-$  in (7.2) corresponds to finding the dispersion relation between  $E, k$  in (7.22).

Also, finding the relation  $x_2 = \pm x_1$  corresponds to finding non-trivial Bloch wavefunction for given  $E, k$  pair.

7.4 The problem consists of graphically analyzing the dispersion relation (7.22) in the text, using typical barrier height, width and the distance of separation between the barriers, i.e. the width of the quantum well.

The resulting energy band configuration provides the general features of the typical energy eigenvalues or subbands in quantum well.

7.5 This problem is the continuation of (7.4), emphasizing the application aspect of the dispersion relation for designing the energy bands.

## Chapter 8

8.1 (a) Consider the energy eigenequation of the Harmonic oscillator:

$$\left[ -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + \frac{1}{2} kx^2 \right] u(x) = Eu(x) \text{----- (1)}$$

Introduce a variable  $\xi$  as

$$\xi = \alpha x, \quad \alpha \equiv \left( \frac{mk}{\hbar^2} \right)^{1/4} = \left( \frac{m\omega}{\hbar} \right)^{1/2}, \quad k = m\omega^2$$

Then the dimension of the constant,  $\alpha$  can be found in terms of mass  $M$ , length  $L$  and time  $T$ :

$$[\alpha] = \left[ \frac{M \frac{1}{T}}{M \left( \frac{L}{T} \right)^2 T} \right]^{1/2} = \left[ \frac{1}{L^2} \right]^{1/2} = \frac{1}{L}$$

Hence  $\xi$  represents a dimensionless displacement of the oscillator from the equilibrium position. Using the chain rule one can perform the differentiation,

$$\frac{\partial}{\partial x} = \frac{\partial}{\partial \xi} \frac{\partial \xi}{\partial x} = \alpha \frac{\partial}{\partial \xi}$$

$$\frac{\partial^2}{\partial x^2} = \alpha^2 \frac{\partial^2}{\partial \xi^2}$$

so that

$$-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} = -\frac{\hbar^2}{2m} \left( \frac{m\omega}{\hbar} \right) \frac{\partial^2}{\partial \xi^2} = \frac{1}{2} \hbar\omega \frac{\partial^2}{\partial \xi^2} \text{----- (2)}$$

Also,

$$\frac{1}{2} kx^2 = \frac{1}{2} m\omega^2 \frac{\xi^2}{\alpha^2} = \frac{1}{2} m\omega^2 \frac{\hbar}{m\omega} \xi^2 = \frac{1}{2} \hbar\omega \xi^2 \text{----- (3)}$$

Inserting (2), (3) into (1) one can write

$$u'' + (\lambda - \xi^2)u = 0, \quad \lambda \equiv \frac{2E}{\hbar\omega} \text{----- (4)}$$

(b) If the solution of  $u$  is sought in the form

$$u(\xi) = H(\xi) e^{-\frac{1}{2}\xi^2} \text{----- (5)}$$

one can perform the differentiation, using the chain rule,

$$u' = (H' - \xi H) e^{-\frac{1}{2}\xi^2} \text{----- (6a)}$$

$$u'' = [H'' - H - \xi H' - \xi(H' - \xi H)] e^{-\frac{1}{2}\xi^2}$$

$$= [H'' - 2\xi H' + (\xi^2 - 1)H] e^{-\frac{1}{2}\xi^2} \text{----- (6b)}$$

Inserting (6) into (4) there results



$$H'' - 2\xi H' + (\lambda - 1)H = 0$$

8.2 (a) Consider the matrix element,

$$\begin{aligned} & \langle u_n | x^2 | u_n \rangle \\ &= \frac{N_n^2}{\alpha^3} \int_{-\infty}^{\infty} d\xi e^{-\frac{\xi^2}{2}} \cdot H_n \xi^2 H_n e^{-\frac{\xi^2}{2}} \end{aligned} \quad \text{----- (1)}$$

Now, using the recurrence relation, (8.32) in the text

$$\xi H_n = \frac{1}{2} H_{n+1} + n H_{n-1}$$

one can write

$$(\xi H_n)^2 = \frac{1}{4} H_{n+1}^2 + n^2 H_{n-1}^2 + H_{n+1} H_{n-1} \quad \text{----- (2)}$$

Inserting (2) into (1) and performing the  $\xi$ -integration with the use of the orthonormality of eigenfunctions (see (8.38)), there results

$$\begin{aligned} & \langle u_n | x^2 | u_n \rangle \\ &= \frac{1}{\alpha^3} \left( \frac{\alpha}{\sqrt{\pi} 2^n n!} \right) \left[ \frac{\sqrt{\pi} 2^{n+1} (n+1)!}{4} + \sqrt{\pi} 2^{n-1} n^2 \right] \\ &= \frac{1}{\alpha^2} \left( \frac{n+1}{2} + \frac{n}{2} \right), \quad \alpha = \left( \frac{m\omega}{\hbar} \right)^{1/2} \quad \text{----- (3)} \\ &= \frac{\hbar}{m\omega} \left( n + \frac{1}{2} \right) \end{aligned}$$

Next, consider the matrix element,

$$\begin{aligned} & \langle u_n | p_x^2 | u_n \rangle \\ &= N_n^2 (-\hbar^2) \alpha \int_{-\infty}^{\infty} d\xi e^{-\frac{\xi^2}{2}} \cdot H_n \frac{\partial^2}{\partial \xi^2} (H_n e^{-\frac{\xi^2}{2}}) \\ &= N_n^2 (-\hbar^2) \alpha \left\{ e^{-\frac{\xi^2}{2}} H_n \frac{\partial}{\partial \xi} (H_n e^{-\frac{\xi^2}{2}}) \Big|_{-\infty}^{\infty} - \int_{-\infty}^{\infty} d\xi \left[ \frac{\partial}{\partial \xi} (e^{-\frac{\xi^2}{2}} H_n) \right]^2 \right\} \quad \text{----- (4)} \\ &= N_n^2 \hbar^2 \alpha \int_{-\infty}^{\infty} d\xi \left[ \frac{\partial}{\partial \xi} (e^{-\frac{\xi^2}{2}} H_n) \right]^2 \end{aligned}$$

Here the integration by parts has been performed. Next, using the recurrence relation (8.30), (8.32) in the text, one can write

$$\begin{aligned} \frac{\partial}{\partial \xi} (e^{-\frac{\xi^2}{2}} H_n) &= (-\xi H_n + H_n') e^{-\frac{\xi^2}{2}} \\ &= \left( -\frac{1}{2} H_{n+1} - n H_{n-1} + 2n H_{n-1} \right) e^{-\frac{\xi^2}{2}} \quad \text{----- (5)} \\ &= \left( -\frac{1}{2} H_{n+1} + n H_{n-1} \right) e^{-\frac{\xi^2}{2}} \end{aligned}$$

Inserting (5) into (4) and performing the integration with the use of orthonormality of eigenfunctions, there results

$$\begin{aligned}
 & \langle u_n | \hat{p}_x^2 | u_n \rangle \\
 &= N_n^2 \hbar^2 \alpha \int_{-\infty}^{\infty} d\xi e^{-\frac{\xi^2}{2}} \cdot \left( -\frac{1}{2} H_{n+1} + n H_{n-1} \right)^2 \\
 &= \hbar^2 \alpha \left( \frac{\alpha}{\sqrt{\pi} 2^n n!} \right) \left[ \frac{1}{4} \sqrt{\pi} 2^{n+1} (n+1)! + n^2 \sqrt{\pi} 2^{n-1} (n-1)! \right] \text{----- (6)} \\
 &= \hbar^2 \alpha^2 \left( n + \frac{1}{2} \right), \quad \alpha^2 = \frac{m\omega}{\hbar} \\
 &= \hbar \omega m \left( n + \frac{1}{2} \right)
 \end{aligned}$$

(b) Consider the variance in x,  $\Delta x$  :

$$\begin{aligned}
 \Delta x^2 &= \langle u_n | (x - \langle x \rangle)^2 | u_n \rangle \\
 &= \langle u_n | x^2 - 2x \langle x \rangle + \langle x \rangle^2 | u_n \rangle \\
 &= \langle u_n | x^2 | u_n \rangle - 2 \langle x \rangle \langle u_n | x | u_n \rangle + \langle x \rangle^2 \langle u_n | u_n \rangle \\
 &= \langle u_n | x^2 | u_n \rangle - \langle x \rangle^2 \\
 &= \langle u_n | x^2 | u_n \rangle
 \end{aligned}$$

Since  $\langle u_n | x | u_n \rangle = \langle x \rangle = 0$  from parity consideration.

Likewise one can evaluate  $\Delta p_x^2$  as

$$\begin{aligned}
 \Delta p_x^2 &= \langle u_n | (p_x - \langle p_x \rangle)^2 | u_n \rangle \\
 &= \langle u_n | p_x^2 - 2p_x \langle p_x \rangle + \langle p_x \rangle^2 | u_n \rangle \\
 &= \langle u_n | p_x^2 | u_n \rangle
 \end{aligned}$$

Since  $\langle p_x \rangle = 0$ . Hence using (5), (6) one can write

$$\begin{aligned}
 \Delta x \Delta p_x &= \left[ \frac{\hbar}{m\omega} \left( n + \frac{1}{2} \right) \cdot \hbar m\omega \left( n + \frac{1}{2} \right) \right]^{1/2} \\
 &= \hbar \left( n + \frac{1}{2} \right)
 \end{aligned}$$

(c) Consider the x-matrix element:

$$\begin{aligned}
\langle u_l | x | u_{l'} \rangle &= \frac{N_l N_{l'}}{\alpha^2} \int_{-\infty}^{\infty} d\xi e^{-\frac{\xi^2}{2}} \cdot H_l \xi H_{l'} e^{-\frac{\xi^2}{2}}, \quad \xi = \alpha x \\
&= \frac{N_l N_{l'}}{\alpha^2} \int_{-\infty}^{\infty} d\xi e^{-\frac{\xi^2}{2}} \cdot H_l \left( \frac{1}{2} H_{l'+1} + l' H_{l'-1} \right) \\
&= \left( \frac{\alpha}{\sqrt{\pi} 2^l l!} \right)^{1/2} \left( \frac{\alpha}{\sqrt{\pi} 2^{l'} l'!} \right) \frac{1}{\alpha^2} \begin{cases} \frac{1}{2} \sqrt{\pi} 2^{l'} l'! \delta_{l, l'+1} \\ l' \sqrt{\pi} 2^{l'} l'! \delta_{l, l'-1} \\ 0 \quad \text{otherwise} \end{cases}
\end{aligned}$$

which leads to (8.51) in the text. Here the recurrence relation (8.32) has been used.

Consider next the matrix element involving  $p$ :

$$\langle u_l | \frac{\partial}{\partial x} | u_{l'} \rangle = N_l N_{l'} \int_{-\infty}^{\infty} d\xi e^{-\frac{\xi^2}{2}} \cdot H_l \frac{\delta}{\delta \xi} (H_{l'} e^{-\frac{\xi^2}{2}})$$

Using (8.30), (8.32) one can write

$$\begin{aligned}
\frac{\delta}{\delta \xi} (H_{l'} e^{-\frac{\xi^2}{2}}) &= (H_{l'}' - \xi H_{l'}) e^{-\frac{\xi^2}{2}} \\
&= \left( 2l' H_{l'-1} - \frac{1}{2} H_{l'+1} - l' H_{l'-1} \right) e^{-\frac{\xi^2}{2}} \\
&= \left( l' H_{l'-1} - \frac{1}{2} H_{l'+1} \right) e^{-\frac{\xi^2}{2}}
\end{aligned}$$

Hence

$$\begin{aligned}
\langle u_l | x | u_{l'} \rangle &= N_l N_{l'} \int_{-\infty}^{\infty} d\xi e^{-\frac{\xi^2}{2}} \cdot H_l \left( l' H_{l'-1} - \frac{1}{2} H_{l'+1} \right) \\
&= \left( \frac{\alpha}{\sqrt{\pi} 2^l l!} \right)^{1/2} \left( \frac{\alpha}{\sqrt{\pi} 2^{l'} l'!} \right)^{1/2} \begin{cases} l' \sqrt{\pi} 2^{l'} l'! \delta_{l, l'-1} \\ -\left( \frac{1}{2} \right) \cdot \sqrt{\pi} 2^{l'} l'! \delta_{l, l'+1} \\ 0 \quad \text{otherwise} \end{cases}
\end{aligned}$$

which leads to (8.52) in the text.

8.3 (a) The classical oscillator with amplitude  $x_0$  and oscillating in time with  $\omega$  is described by

$$x = x_0 \cos \omega t,$$

in which case one can write

$$v = \dot{x} = -\omega x_0 \sin \omega t.$$

Thus, the kinetic energy averaged over a period of oscillation is given by

$$\langle K \rangle = \frac{1}{2} m \frac{\int_0^{2\pi/\omega} dt v^2(t)}{2\pi/\omega} = \frac{1/2m}{2\pi/\omega} \int_0^{2\pi/\omega} \omega^2 x_0^2 \sin^2 \omega t = \frac{1/2m}{2\pi/\omega} \omega^2 x_0^2 \frac{1}{2} \frac{2\pi}{\omega} = \frac{1}{2} m \frac{x_0^2 \omega^2}{2} \text{-----} \quad (1)$$

Also, the average potential energy is given by

$$\langle V \rangle = \frac{k/2}{2\pi/\omega} \int_0^{2\pi/\omega} x_0^2 \cos^2 \omega t = \frac{1}{2} k \cdot \frac{x_0}{2} = \frac{1}{2} \left( \frac{m\omega^2 x_0^2}{2} \right), \quad k = m\omega^2 \text{-----} \quad (2)$$

Hence it follows from (1), (2) that

$$\langle K \rangle = \langle V \rangle = \frac{1}{2} \langle E \rangle$$

where  $\langle E \rangle$  is the total energy which in this case is time independent. In fact, classically the total energy is independent of time in a conservative system as in harmonic oscillator.

$$\begin{aligned} E &= \frac{1}{2} m v^2 + \frac{1}{2} k x^2 \\ &= \frac{1}{2} m \omega^2 x_0^2 \sin^2 \omega t + \frac{1}{2} k x_0^2 \cos^2 \omega t \\ &= \frac{1}{2} m \omega^2 x_0^2, \quad k = m\omega \end{aligned}$$

Quantum mechanically, the average kinetic energy is given by

$$\langle K \rangle = \frac{1}{2m} \langle u_n | \hat{p}_x^2 | u_n \rangle = \frac{\hbar\omega}{2} \left( n + \frac{1}{2} \right)$$

where the result obtained in (6) in problem (8.2) has been used. Similarly using (3) therein one can write

$$\begin{aligned} \langle V \rangle &= \frac{1}{2} k \langle u_n | x^2 | u_n \rangle = \frac{1}{2} m \omega^2 \frac{\hbar}{m\omega} \left( n + \frac{1}{2} \right), \quad k = m\omega^2 \\ &= \frac{1}{2} \hbar\omega \left( n + \frac{1}{2} \right) \end{aligned}$$

Hence

$$\langle K \rangle = \langle V \rangle = \frac{1}{2} \langle E \rangle$$

(c) Thus, both classical and quantum descriptions are identical in describing the conservative system.

8.4 (a) The energy eigenequation of 3D harmonic oscillator reads as

$$\left[ -\frac{\hbar^2}{2m} \nabla^2 + \frac{1}{2} k_x x^2 + \frac{1}{2} k_y y^2 + \frac{1}{2} k_z z^2 \right] u(x, y, z) = E(x, y, z) \text{-----} \quad (1)$$

and one can look for the solution in the form,

$$u(x, y, z) = u(x)u(y)u(z) \text{-----} \quad (2)$$

Inserting (2) into (1) and dividing both sides by (2) there results

$$\left[ \frac{\left( -\frac{\hbar^2}{2m} \right) \frac{\partial^2 u(x)}{\partial x^2} + \frac{1}{2} kx^2}{u(x)} \right] + \left[ \frac{\left( -\frac{\hbar^2}{2m} \right) \frac{\partial^2 u(y)}{\partial y^2} + \frac{1}{2} ky^2}{u(y)} \right] + \left[ \frac{\left( -\frac{\hbar^2}{2m} \right) \frac{\partial^2 u(z)}{\partial z^2} + \frac{1}{2} kz^2}{u(z)} \right] = E \quad \text{----- (3)}$$

Clearly (3) naturally separates into  $x, y, z$  components as

$$-\frac{\hbar^2}{2m} u''(x) + \frac{1}{2} k_x x^2 u(x) = E_x u(x) \quad \text{----- (4a)}$$

$$-\frac{\hbar^2}{2m} u''(y) + \frac{1}{2} k_y y^2 u(y) = E_y u(y) \quad \text{----- (4b)}$$

$$-\frac{\hbar^2}{2m} u''(z) + \frac{1}{2} k_z z^2 u(z) = E_z u(z) \quad \text{----- (4c)}$$

where primes denote the respective differentiations and

$$E_x + E_y + E_z = E$$

(b) The equation (4a) –(4c) are identical to 1D harmonic oscillator eigenequation and one can therefore write

$$u(x, y, z) = \prod_{j=1} N_j e^{-\frac{\xi_j^2}{2}} H_{n_j}(\xi_j), \quad j = x, y, z \quad \text{----- (5)}$$

with

$$\xi_j = \alpha_j j, \alpha_j = \left( \frac{m k_j}{\hbar^2} \right)^{1/4} = \left( \frac{m \omega_j}{\hbar} \right)^{1/2}$$

$$N_j = \left( \frac{\alpha_j}{\sqrt{\pi} 2^{n_j} n_j!} \right)^{1/2}$$

and the energy eigenvalues are given by

$$E_{n_x, n_y, n_z} = \sum \hbar \omega_j \left( n_j + \frac{1}{2} \right) \quad \text{----- (6)}$$

(c) If  $k_x = k_y = k_z = k$ , then (6) reduces to

$$E_{n_x, n_y, n_z} = \hbar \omega \left( n_x + n_y + n_z + \frac{3}{2} \right), \quad \omega = \sqrt{k/m}$$

The degeneracy of the few excited states is summarized as follows:

$n_x$	$n_y$	$n_z$	$E/\hbar\omega$	degeneracy
0	0	0	3/2	none
1	0	0	5/2	3
0	1	0	5/2	
0	0	1	5/2	
1	1	0	7/2	6

1	0	1	7/2	
0	1	1	7/2	
2	0	0	7/2	
0	2	0	7/2	
0	0	2	7/2	

8.5 The effective spring constant can be specified in terms of hydrogen mass as

$$k = 313.8 = m_H \cdot \omega^2$$

Hence one can write

$$\begin{aligned} \hbar\omega &= \left( \frac{313.8}{m_H} \right)^{1/2} \hbar \\ &= \left( \frac{313.8}{1.673 \times 10^{-27}} \right)^{1/2} 1.055 \times 10^{-34} \text{ J} \\ &= 4.57 \times 10^{-20} \text{ J} \\ &= 4.57 \times 10^{-20} \text{ J} \cdot \frac{1}{1.6 \times 10^{-19}} \frac{\text{eV}}{\text{J}} \\ &= 2.86 \times 10^{-1} \text{ eV} \end{aligned}$$

The frequency of the photon capable of inducing transitions in between vibrational states is therefore given by

$$\nu = \frac{2.86 \times 10^{-1} \text{ eV}}{h} = \frac{2.86 \times 10^{-1} \text{ eV}}{4.136 \times 10^{-15} \text{ eVs}} = 6.9 \times 10^{13} \text{ Hz}$$

8.6 (a) For two atom system coupled via an effective spring constant, the kinetic energy is given by

$$K = \frac{1}{2} m_1 \dot{r}_1^2 + \frac{1}{2} m_2 \dot{r}_2^2 \text{ ----- (1)}$$

Introduce the center of mass and relative coordinates:

$$m_1 \underline{r}_1 + m_2 \underline{r}_2 = M \underline{R}, \quad M = m_1 + m_2$$

$$\underline{r}_1 - \underline{r}_2 = \underline{r}$$

Inverting the relation one can express  $\underline{r}_1, \underline{r}_2$  as

$$\underline{r}_1 = \underline{R} + \frac{m_2}{M} \underline{r} \text{ ----- (2a)}$$

$$\underline{r}_2 = \underline{R} - \frac{m_1}{M} \underline{r} \text{ ----- (2b)}$$

Inserting (2) into (1) one can write

$$\begin{aligned} K &= \frac{1}{2} M \dot{\underline{R}}^2 + \frac{1}{2} \left( \frac{m_1 m_2}{M^2} + \frac{m_2 m_1}{M^2} \right) \dot{\underline{r}}^2 \text{ ----- (3a)} \\ &= \frac{1}{2} M \dot{\underline{R}}^2 + \frac{1}{2} \mu \dot{\underline{r}}^2 \end{aligned}$$

where

$$\mu = \frac{m_1 m_2}{M^2} (m_2 + m_1) = \frac{m_1 m_2}{M} \text{----- (3b)}$$

or

$$\frac{1}{\mu} = \frac{1}{m_1} + \frac{1}{m_2} \text{----- (3c)}$$

Therefore, the Hamiltonian of the system reads as

$$\begin{aligned} H &= K + V \\ &= \frac{1}{2} M \dot{\underline{R}}^2 + \frac{1}{2} \mu \dot{\underline{r}}^2 + \frac{1}{2} k r^2 \\ &= \frac{P^2}{2m} + \frac{p^2}{2\mu} + \frac{1}{2} k r^2 \\ &= -\frac{\hbar^2}{2M} \nabla_R^2 - \frac{\hbar^2}{2\mu} \nabla_r^2 + \frac{1}{2} k r^2 \end{aligned}$$

(b) The energy eigenequation reads then as

$$\left( -\frac{\hbar^2}{2M} \nabla_R^2 - \frac{\hbar^2}{2\mu} \nabla_r^2 + \frac{1}{2} k r^2 \right) \varphi(\underline{R}, \underline{r}) = E \varphi(\underline{R}, \underline{r}) \text{----- (4)}$$

One can thus look for the solution in the form

$$\varphi(\underline{R}, \underline{r}) = u(\underline{R}) u(\underline{r}) \text{----- (5)}$$

and insert (5) into (4) and divide both sides by (5), obtaining

$$\frac{-\frac{\hbar^2}{2M} \nabla_R^2 u(\underline{R})}{u(\underline{R})} + \frac{-\frac{\hbar^2}{2\mu} \nabla_r^2 u(\underline{r})}{u(\underline{r})} + \frac{1}{2} k r^2 = E \text{----- (6)}$$

So that  $u(\underline{R}), u(\underline{r})$  naturally separate as,

$$-\frac{\hbar^2}{2M} \nabla_R^2 u(\underline{R}) = E_{CM} u(\underline{R}) \text{----- (7a)}$$

$$-\frac{\hbar^2}{2\mu} \nabla_r^2 u(\underline{r}) + \frac{1}{2} k r^2 u(\underline{r}) = E_{int} u(\underline{r}) \text{----- (7b)}$$

(7a) is the energy eigenequation for a free particle of mass  $M$ , while (7b) is the standard harmonic oscillator eigenfunction, oscillating with the reduced mass,  $\mu$ .

8.7 (a) The Hamiltonian of the internal motion of the molecule reads as

$$\hat{H} = -\frac{\hbar^2}{2\mu} \nabla^2 + \frac{1}{2} k x^2, \quad \frac{1}{\mu} = \frac{1}{m_C} + \frac{1}{m_O}$$

where  $m_C, m_O$  denote the mass of carbon and oxygen atoms, respectively. The energy spacing between two adjacent vibrational states is given by

$$h\nu = h \frac{c}{\lambda} = hc \cdot \left( \frac{1}{\lambda} \right)$$

Hence,

$$\nu = c \frac{1}{\lambda} = 3 \times 10^8 (m/s) \cdot 2,170/cm = 3 \times 10^8 (m/s) \cdot 217,000/m = 6.51 \times 10^{13} /s$$

And

$$k = \mu\omega^2 = \mu(2\pi\nu)^2$$

Now,

$$\mu = \frac{m_C m_0}{m_C + m_0} = \frac{12 \cdot 16 (1.673 \times 10^{-27})^2}{(12+16)(1.673 \times 10^{-27})} = 1.15 \times 10^{-26} Kg$$

and

$$k = 1.15 \times 10^{-26} (2\pi \cdot 6.51 \times 10^{13})^2 [N/m] = 1.92 \times 10^3 [Newton/m] = 19.2 [Newton/cm]$$

(b) The zero point energy is given by

$$E_0 = \frac{1}{2} h\nu = \frac{1}{2} 4.136 \times 10^{-15} eVs 6.51 \times 10^{13} /s = 1.35 \times 10^{-1} eV$$

8.8

$$\hat{H} = \frac{\hat{p}^2}{2m} + \frac{1}{2} kx^2 \text{ ----- (1a)}$$

Using (8.60), (8.61) in the text, i.e.

$$x = \frac{1}{\sqrt{2}\alpha} (a + a^+), \quad \alpha = \left( \frac{m\omega}{\hbar} \right)^{1/2} \text{ ----- (1b)}$$

$$p = \frac{i\hbar\alpha}{\sqrt{2}} (a^+ - a) \text{ ----- (1c)}$$

one can write

$$\hat{H} = -\frac{\hbar^2\alpha^2}{2} \frac{1}{2m} (a^+ - a)(a^+ - a) + \frac{k}{2} \frac{1}{2\alpha^2} (a^+ + a)(a^+ + a) \text{ ----- (2)}$$

Now,

$$\frac{\hbar^2\alpha^2}{4m} = \frac{\hbar^2 m\omega}{4m\hbar} = \frac{1}{4} \hbar\omega$$

$$\frac{k}{4\alpha^2} = \frac{m\omega^2}{4} \frac{\hbar}{m\omega} = \frac{1}{4} \hbar\omega$$

Hence,  $\hat{H}$  can be expressed in terms of the number operator as



$$\begin{aligned}
\hat{H} &= \frac{\hbar\omega}{4} \left[ -(a^+ - a)(a^+ - a) + (a^+ + a)(a^+ + a) \right] \\
&= \frac{\hbar\omega}{4} \cdot 2(a^+ a + a a^+) \\
&= \frac{\hbar\omega}{2} (a^+ a + 1)
\end{aligned}$$

since  $aa^+ = a^+a + 1$ .

8.9 (a) Given the function,

$$F(x) = e^{xa^+a} a e^{-xa^+a}$$

its derivative reads as

$$\begin{aligned}
\frac{dF(x)}{dx} &= e^{xa^+a} a^+ a a e^{-xa^+a} - e^{xa^+a} a a^+ a e^{-xa^+a} \\
&= e^{xa^+a} (a^+ a - a a^+) a e^{-xa^+a} \quad \text{----- (1)} \\
&= -e^{-xa^+a} a e^{-xa^+a} \\
&= -F(x)
\end{aligned}$$

where use has been made of

$$\begin{aligned}
[a, a^+] &= 1 = a a^+ - a^+ a \\
e^{xa^+a} a^+ a &= a^+ a e^{xa^+a}
\end{aligned}$$

(1) can be recast as

$$\frac{dF(x)}{F(x)} = -dx$$

and upon integrating both sides there results

$$\ln F(x) \Big|_0^x = -x$$

or

$$F(x) = F(0) e^{-x}$$

That is,

$$e^{xa^+a} a e^{-xa^+a} = a e^{-x}$$

(b) Let

$$G(x) = e^{xa^+a} a^+ e^{-xa^+a}$$

Then

$$\begin{aligned}
\frac{dG(x)}{dx} &= e^{xa^+a} (a^+ a a^+ - a^+ a^+ a) e^{-xa^+a} \\
&= e^{xa^+a} a^+ e^{-xa^+a} \\
&= G(x)
\end{aligned}$$

So that one can put

$$\frac{dG(x)}{dx} = dx$$

and upon integrating both sides one can write

$$\ln G(x) \Big|_0^x = x$$

or

$$G(x) = G(0)e^x$$

and

$$e^{xa^+} a^+ e^{-xa^+} = a^+ e^x$$

8.10 (a) Inserting the ground state eigenfunction, (8.72) reads as

$$u_n(x) = \frac{1}{\sqrt{n!}} \left[ \frac{1}{\sqrt{2}} \left( \xi - \frac{\partial}{\partial \xi} \right) \right]^n \left( \frac{\alpha}{\sqrt{\pi}} \right)^{1/2} e^{-\frac{\xi^2}{2}}$$

Hence, for n=1

$$u_1 = \left( \frac{\alpha}{\sqrt{\pi}} \right)^{1/2} \frac{1}{\sqrt{1!}} \frac{1}{\sqrt{2}} \left( \xi - \frac{\partial}{\partial \xi} \right) e^{-\frac{\xi^2}{2}}$$

Now,

$$\left( \xi - \frac{\partial}{\partial \xi} \right) e^{-\frac{\xi^2}{2}} = 2\xi e^{-\frac{\xi^2}{2}} = H_1(\xi) e^{-\frac{\xi^2}{2}}$$

and

$$u_1 = \left( \frac{\alpha}{\sqrt{\pi} \cdot 2 \cdot 1!} \right)^{1/2} H_1 e^{-\frac{\xi^2}{2}} \text{ ----- (1)}$$

Similarly for n=2

$$u_2 = \frac{1}{\sqrt{2!}} \left( \frac{\alpha}{\sqrt{\pi}} \right)^{1/2} \left[ \frac{1}{\sqrt{2}} \left( \xi - \frac{\partial}{\partial \xi} \right) \right]^2 e^{-\frac{\xi^2}{2}} \text{ ----- (2)}$$

Now,

$$\begin{aligned}
& \frac{1}{\sqrt{2}} \left( \xi - \frac{\partial}{\partial \xi} \right) \frac{1}{\sqrt{2}} \left( \xi - \frac{\partial}{\partial \xi} \right) e^{-\frac{\xi^2}{2}} \\
&= \frac{1}{(\sqrt{2})^2} \left( \xi - \frac{\partial}{\partial \xi} \right) H_1 e^{-\frac{\xi^2}{2}} \\
&= \frac{1}{(\sqrt{2})^2} \left[ \xi H_1 - (-\xi H_1 + H_1') \right] e^{-\frac{\xi^2}{2}} \\
&= \frac{1}{(\sqrt{2})^2} (2\xi H_1 - H_1') e^{-\frac{\xi^2}{2}} \\
&= \frac{1}{(\sqrt{2})^2} (H_{1+1} + 2H_{1-1} - 2H_{1-1}) e^{-\frac{\xi^2}{2}} \\
&= \frac{1}{(\sqrt{2})^2} H_2 e^{-\frac{\xi^2}{2}}
\end{aligned}$$

Here the recurrence relation, (8.30), (8.32) have been used. Hence

$$u_2 = \left( \frac{\alpha}{\sqrt{\pi \cdot 2! \cdot 2^2}} \right)^{1/2} H_2 e^{-\frac{\xi^2}{2}}$$

Next,  $u_3$  can likewise be constructed using (1), (2) as

$$\begin{aligned}
u_3 &= \frac{1}{\sqrt{3!}} \left[ \frac{1}{\sqrt{2}} \left( \xi - \frac{\partial}{\partial \xi} \right) \right]^3 \left( \frac{\alpha}{\sqrt{\pi} 1} \right)^{1/2} e^{-\frac{\xi^2}{2}} \\
&= \frac{1}{\sqrt{3}} \frac{1}{\sqrt{2}} \left( \xi - \frac{\partial}{\partial \xi} \right) \cdot \frac{1}{\sqrt{2}} \frac{1}{\sqrt{2}} \left( \xi - \frac{\partial}{\partial \xi} \right) \cdot \frac{1}{\sqrt{1}} \frac{1}{\sqrt{2}} \left( \xi - \frac{\partial}{\partial \xi} \right) \cdot \left( \frac{\alpha}{\sqrt{\pi}} \right)^{1/2} e^{-\frac{\xi^2}{2}} \\
&= \frac{1}{\sqrt{3}} \frac{1}{\sqrt{2}} \left( \xi - \frac{\partial}{\partial \xi} \right) \left( \frac{\alpha}{\sqrt{\pi \cdot 2! \cdot 2^2}} \right)^{1/2} H_2 e^{-\frac{\xi^2}{2}} \\
&= \left( \frac{\alpha}{\sqrt{\pi \cdot 2! \cdot 2^2}} \right)^{1/2} \left( \xi - \frac{\partial}{\partial \xi} \right) H_2 e^{-\frac{\xi^2}{2}}
\end{aligned}$$

Here, 3! has been distributed. Now

$$\begin{aligned}
& \left( \xi - \frac{\partial}{\partial \xi} \right) H_2 e^{-\frac{\xi^2}{2}} \\
&= (2\xi H_2 - H_2') e^{-\frac{\xi^2}{2}} \\
&= (H_3 + 4H_1 - 4H_1) e^{-\frac{\xi^2}{2}} \\
&= H_3 e^{-\frac{\xi^2}{2}}
\end{aligned}$$

Thus,

$$u_3 = \left( \frac{\alpha}{\sqrt{\pi} \cdot 3! \cdot 2^3} \right)^{1/2} H_3 e^{-\frac{\xi^2}{2}} \text{ ----- (3)}$$

in complete agreement with the results obtained by solving the energy eigenequation.

(b) One can show the validity of (8.72) by induction. For this purpose, (8.72) can be decomposed into

$$\begin{aligned} u_n(x) &= \frac{1}{\sqrt{n!}} \left[ \frac{1}{\sqrt{2}} \left( \xi - \frac{\partial}{\partial \xi} \right) \right]^n \left( \frac{\alpha}{\sqrt{\pi}} \right)^{1/2} e^{-\frac{\xi^2}{2}} \\ &= \frac{1}{\sqrt{n}} \left[ \frac{1}{\sqrt{2}} \left( \xi - \frac{\partial}{\partial \xi} \right) \right] \cdot \frac{1}{\sqrt{n-1}} \left[ \frac{1}{\sqrt{2}} \left( \xi - \frac{\partial}{\partial \xi} \right) \right] \cdots \text{ ----- (4)} \\ &\quad \frac{1}{\sqrt{1}} \frac{1}{\sqrt{2}} \left( \xi - \frac{\partial}{\partial \xi} \right) \left( \frac{\alpha}{\sqrt{\pi}} \right)^{1/2} e^{-\frac{\xi^2}{2}} \end{aligned}$$

In view of (1), (2), (3) one can recast (4) as

$$\begin{aligned} u_n(x) &= \frac{1}{\sqrt{n}} \frac{1}{\sqrt{2}} \left( \xi - \frac{\partial}{\partial \xi} \right) \left[ \frac{\alpha}{\sqrt{\pi} 2^{n-1} (n-1)!} \right]^{1/2} H_{n-1} e^{-\frac{\xi^2}{2}} \\ &= \left( \frac{\alpha}{\sqrt{\pi} 2^n n!} \right)^{1/2} (2\xi H_{n-1} - H'_{n-1}) e^{-\frac{\xi^2}{2}} \\ &= \left( \frac{\alpha}{\sqrt{\pi} 2^n n!} \right)^{1/2} [H_{n-1+1} + 2(n-1)H_{n-2} - 2(n-1)H_{n-2}] e^{-\frac{\xi^2}{2}} \\ &= \left( \frac{\alpha}{\sqrt{\pi} 2^n n!} \right)^{1/2} H_n e^{-\frac{\xi^2}{2}} \end{aligned}$$

in exact agreement with (8.40) in the text.

## Chapter 9

9.1 (a) Evaluating 9 vector products, e.g.  $\hat{x} \times \hat{x} = \hat{y} \times \hat{y} = \hat{z} \times \hat{z} = 0$ ,  $\hat{x} \times \hat{y} = \hat{z}$ , etc. is tantamount to evaluating the determinant of  $3 \times 3$  matrix, i.e.

$$\begin{aligned} \hat{l} &= \underline{r} \times \underline{p} \\ &= \begin{vmatrix} \hat{x} & \hat{y} & \hat{z} \\ x & y & z \\ p_x & p_y & p_z \end{vmatrix} \\ &= \hat{x}(yp_z - zp_y) + \hat{y}(zp_x - xp_z) + \hat{z}(xp_y - yp_x) \end{aligned}$$

(b) Consider for example the commutation relation between  $\hat{l}_x$ ,  $\hat{l}_y$ :

$$\begin{aligned} [\hat{l}_x, \hat{l}_y] &= [yp_z - zp_y, zp_x - xp_z] \\ &= [yp_z, zp_x] + [zp_y, xp_z] \\ &= yp_x[p_z, z] + p_yx[z, p_z] \\ &= i\hbar(xp_y - yp_x) = \hat{l}_z \end{aligned}$$

where use has been made of

$$[z, p_z] = i\hbar$$

One can likewise prove

$$[\hat{l}_y, \hat{l}_z] = i\hbar\hat{l}_x, \quad [\hat{l}_z, \hat{l}_x] = i\hbar\hat{l}_y$$

9.2. This problem requires a straightforward algebra involving the chain rule for differentiation of elementary trigonometric functions. Performing the analysis and confirming the results is nevertheless important and should be carried out at least once.

9.3 (a) Consider the general case where  $\theta$  is not necessarily confined to  $\pi/4$ .

Since

$$\begin{aligned} \hat{x}' &= \cos \theta \hat{x} + \sin \theta \hat{y} \\ \hat{y}' &= -\sin \theta \hat{x} + \cos \theta \hat{y} \\ \hat{x}' \cdot \hat{x}' &= (\cos \theta \hat{x} + \sin \theta \hat{y}) \cdot (\cos \theta \hat{x} + \sin \theta \hat{y}) \\ &= \cos^2 \theta \hat{x} \cdot \hat{x} + \sin^2 \theta \hat{y} \cdot \hat{y} + 2 \cos \theta \sin \theta \hat{x} \cdot \hat{y} \\ &= \cos^2 \theta + \sin^2 \theta = 1 \end{aligned}$$

One can similarly show that

$$\hat{y}' \cdot \hat{y}' = \sin^2 \theta + \cos^2 \theta = 1$$

and

$$\hat{x}' \cdot \hat{y}' = (\cos \theta \hat{x} + \sin \theta \hat{y}) \cdot (-\sin \theta \hat{x} + \cos \theta \hat{y}) = -\sin \theta \cos \theta + \sin \theta \cos \theta = 0 = \hat{y}' \cdot \hat{x}'$$

Since

$$\hat{x} \cdot \hat{z} = \hat{y} \cdot \hat{z} = 0, \quad \hat{x}' \cdot \hat{z} = \hat{y}' \cdot \hat{z} = 0$$

Hence,  $\hat{x}', \hat{y}', \hat{z}$  constitute an orthonormal unit vector system

(b) From Table 9.1,

$$Y_1^0 = \frac{1}{2} \left( \frac{3}{\pi} \right)^{1/2} \cos \theta$$

$$Y_1^{\pm 1} = \mp \frac{1}{2} \left( \frac{3}{2\pi} \right)^{1/2} \sin \theta e^{\pm i\varphi}$$

Thus, one can write

$$\begin{aligned} \langle Y_1^0 | Y_1^0 \rangle &= \frac{1}{4} \cdot \frac{3}{\pi} \int_0^{2\pi} d\varphi \int_{-1}^1 d\mu \mu^2, \quad \mu \equiv \cos \theta \text{ ----- (1)} \\ &= \frac{1}{4} \cdot \frac{3}{\pi} \cdot 2\pi \cdot \frac{1}{3} \cdot 2 = 1 \end{aligned}$$

Also,

$$\begin{aligned} \langle Y_1^{\pm 1} | Y_1^{\pm 1} \rangle &= \frac{1}{4} \cdot \frac{3}{2\pi} \int_0^{2\pi} d\varphi e^{-i\varphi} e^{+i\varphi} \int_{-1}^1 d\mu (1 - \mu^2), \quad \sin^2 \theta \equiv 1 - \mu^2 \text{ ----- (2)} \\ &= \frac{1}{4} \cdot \frac{3}{2\pi} \cdot 2\pi \cdot \left( 2 - \frac{2}{3} \right) = \frac{1}{4} \cdot \frac{3}{2\pi} \cdot 2\pi \cdot \left( \frac{4}{3} \right) = 1 \end{aligned}$$

(b) Consider for instance

$$\begin{aligned} \langle Y_1^0 | Y_1^1 \rangle &= \frac{-1}{4} \cdot \left( \frac{3}{\pi} \right)^{1/2} \left( \frac{3}{2\pi} \right)^{1/2} \int_0^{2\pi} d\varphi e^{i\varphi} \int_{-1}^1 d\mu \mu \sqrt{1 - \mu^2} = 0 \text{ ----- (3)} \end{aligned}$$

One can likewise show that

$$\langle Y_1^0 | Y_1^{-1} \rangle = \langle Y_1^1 | Y_1^{-1} \rangle = 0 \text{ ----- (4)}$$

(c) It is already shown in (1) that

$$\langle p_z | p_z \rangle = 1$$

It also follows from (2), (3), (4) that

$$\begin{aligned} \langle p_x | p_x \rangle &= \frac{1}{2} \langle Y_1^1 + Y_1^{-1} | Y_1^1 + Y_1^{-1} \rangle \\ &= \frac{1}{2} \left[ \langle Y_1^1 | Y_1^1 \rangle + \langle Y_1^{-1} | Y_1^{-1} \rangle \right] \\ &= 1 \end{aligned}$$

$$\begin{aligned}
& \langle p_y | p_y \rangle \\
&= \frac{1}{2} \langle Y_1^1 - Y_1^{-1} | Y_1^1 - Y_1^{-1} \rangle \\
&= \frac{1}{2} [\langle Y_1^1 | Y_1^1 \rangle + \langle Y_1^{-1} | Y_1^{-1} \rangle] \\
&= 1
\end{aligned}$$

Thus,  $|p_x\rangle$ ,  $|p_y\rangle$  and  $|p_z\rangle$  are normalized.

Also

$$\begin{aligned}
& \langle p_x | p_y \rangle \\
&= \frac{1}{2} \langle Y_1^1 + Y_1^{-1} | Y_1^1 - Y_1^{-1} \rangle \\
&= \frac{1}{2} [\langle Y_1^1 | Y_1^1 \rangle - \langle Y_1^{-1} | Y_1^{-1} \rangle] \\
&= 0
\end{aligned}$$

In view of  $\langle Y_1^0 | Y_1^{\pm 1} \rangle = 0$ ,

$$\langle p_y | p_x \rangle = \langle p_z | p_y \rangle = 0$$

and therefore  $|p_x\rangle$ ,  $|p_y\rangle$  and  $|p_z\rangle$  are orthonormal eigenfunctions.

(d)  $(Y_1^0, Y_1^1, Y_1^{-1})$  and  $(|p_x\rangle, |p_y\rangle, |p_z\rangle)$  are analogous to  $(\hat{x}, \hat{y}, \hat{z})$  and  $(\hat{x}', \hat{y}', \hat{z}')$

(e)

$$\begin{aligned}
& \langle p_z | \hat{l}^2 | p_z \rangle = \langle Y_1^0 | \hat{l}^2 | Y_1^0 \rangle \\
&= \hbar^2 \left( \sqrt{1(1+1)} \right)^2 \langle Y_1^0 | Y_1^0 \rangle \\
&= 2\hbar^2
\end{aligned}$$

$$\langle p_z | \hat{l}_z | p_z \rangle = \hbar 0 \langle p_z | p_z \rangle = 0$$

$$\begin{aligned}
& \langle p_x | \hat{l}^2 | p_x \rangle = \frac{1}{2} \langle Y_1^1 + Y_1^{-1} | \hat{l}^2 | Y_1^1 + Y_1^{-1} \rangle \\
&= \frac{1}{2} \hbar^2 \left( \sqrt{1(1+1)} \right)^2 \langle Y_1^1 + Y_1^{-1} | Y_1^1 + Y_1^{-1} \rangle \\
&= 2\hbar^2
\end{aligned}$$

$$\begin{aligned}
\langle p_x | \hat{l}_z | p_x \rangle &= \frac{1}{2} \langle Y_1^1 + Y_1^{-1} | \hat{l}_z | Y_1^1 + Y_1^{-1} \rangle \\
&= \frac{1}{2} \hbar \langle Y_1^1 + Y_1^{-1} | Y_1^1 - Y_1^{-1} \rangle \\
&= 0
\end{aligned}$$

$$\begin{aligned}
\langle p_y | \hat{l}^2 | p_y \rangle &= \frac{1}{2} \langle Y_1^1 - Y_1^{-1} | \hat{l}^2 | Y_1^1 - Y_1^{-1} \rangle \\
&= \frac{1}{2} \hbar^2 \left( \sqrt{1(1+1)} \right)^2 \langle Y_1^1 - Y_1^{-1} | Y_1^1 - Y_1^{-1} \rangle \\
&= 2\hbar^2
\end{aligned}$$

$$\begin{aligned}
\langle p_y | \hat{l}_z | p_y \rangle &= \frac{1}{2} \langle Y_1^1 - Y_1^{-1} | \hat{l}_z | Y_1^1 - Y_1^{-1} \rangle \\
&= \frac{1}{2} \hbar \langle Y_1^1 - Y_1^{-1} | Y_1^1 + Y_1^{-1} \rangle \\
&= 0
\end{aligned}$$



## Chapter 10

10.1 (a) One can invert the relation,

$$\underline{R} = \frac{1}{M} (m_1 \underline{r}_1 + m_2 \underline{r}_2) \text{----- (1)}$$

$$\underline{r} = \underline{r}_1 - \underline{r}_2 \text{----- (2)}$$

with the operation  $M \times (1) + m_2 \times (2)$ ,  $M \times (1) - m_1 \times (2)$ , obtaining

$$\underline{r}_1 = \underline{R} + \frac{m_2}{M} \underline{r} \text{----- (3)}$$

$$\underline{r}_2 = \underline{R} - \frac{m_1}{M} \underline{r} \text{----- (4)}$$

Thus, one can write

$$\begin{aligned} \dot{\underline{r}}_1^2 &= \left( \dot{\underline{R}} + \frac{m_2}{M} \dot{\underline{r}} \right)^2 \\ &= \dot{\underline{R}}^2 + \left( \frac{m_2}{M} \right)^2 \dot{\underline{r}}^2 + \frac{2m_2}{M} \dot{\underline{R}} \cdot \dot{\underline{r}} \\ \dot{\underline{r}}_2^2 &= \dot{\underline{R}}^2 + \left( \frac{m_1}{M} \right)^2 \dot{\underline{r}}^2 - \frac{2m_1}{M} \dot{\underline{R}} \cdot \dot{\underline{r}} \end{aligned}$$

Hence,

$$\frac{p_1^2}{2m_1} = \frac{1}{2} m_1 \dot{\underline{r}}_1^2 = \frac{1}{2} m_1 \left[ \dot{\underline{R}}^2 + \left( \frac{m_2}{M} \right)^2 \dot{\underline{r}}^2 + \frac{2m_2}{M} \dot{\underline{R}} \cdot \dot{\underline{r}} \right] \text{----- (5)}$$

$$\frac{p_2^2}{2m_2} = \frac{1}{2} m_2 \dot{\underline{r}}_2^2 = \frac{1}{2} m_2 \left[ \dot{\underline{R}}^2 + \left( \frac{m_1}{M} \right)^2 \dot{\underline{r}}^2 - \frac{2m_1}{M} \dot{\underline{R}} \cdot \dot{\underline{r}} \right] \text{----- (6)}$$

and adding (5), (6) there results

$$\begin{aligned} \frac{p_1^2}{2m_1} + \frac{p_2^2}{2m_2} &= \frac{1}{2} M \dot{\underline{R}}^2 + \frac{1}{2M^2} (m_1 m_2^2 + m_1^2 m_2) \dot{\underline{r}}^2 \\ &= \frac{P^2}{2M} + \frac{p^2}{2\mu} \end{aligned} \text{----- (7a)}$$

where

$$\underline{P} \equiv M \underline{R}, \quad M = m_1 + m_2 \text{----- (7b)}$$

$$\underline{p} = \mu \underline{r}, \quad \mu = \frac{m_1 \cdot m_2}{m_1 + m_2} \text{----- (7c)}$$

One can also write

$$\frac{1}{\mu} = \frac{1}{m_1} + \frac{1}{m_2} \text{----- (7d)}$$

(b) From (7c) or (7d)

$$\mu \approx m_1 \quad \text{for } m_2 \gg m_1$$

$$\mu = \frac{1}{2}m \quad \text{for } m_1 = m_2 = m$$

10.2 This problem requires a lengthy but straightforward exercise in differentiation, using the formulas (9.3) – (9.6).

But, it is instructive to carry out the actual derivation in view of its extensive utilizations.

10.3 (a) To find  $a_0$  the only modification required is to replace  $e_M^2 \equiv e^2 / 4\pi\epsilon_0$  by  $Ze_M^2$ , with  $Z$  denoting the atomic number, that is, the number of protons in the nucleus.

Thus, one can write from (10.44)

$$a_0 = \frac{\hbar^2}{\mu Z e_M^2} = \frac{1}{Z} \frac{\hbar^2}{e_M^2} \left( \frac{1}{m_e} + \frac{1}{m_N} \right) = \frac{1}{Z} \frac{\hbar^2}{e_M^2 m_e} \left( 1 + \frac{m_e}{m_N} \right) = \frac{1}{Z} a_B \left( 1 + \frac{m_e}{m_N} \right)$$

Hence for  $Z = 2$   $a_0$  is one half of the Bohr radius,  $a_B$ :

$$a_0 \approx a_B / 2$$

(b) The problem corresponds to the case in which  $Z = 1$ ,  $m_e / m_N = 1$  so that

$$a_0 \approx 2a_B$$

(c) Here the Coulomb potential

$$V = -\frac{e_M^2}{r}$$

is replaced by the gravitational potential

$$V = -\frac{m_n m_n G}{r}$$

with  $m_n$ ,  $G$  denoting the mass of neutron and the gravitational constant, respectively. Thus one can write

$$a_0 = \frac{\hbar^2}{\mu m_n^2 G} = a_B \left( \frac{m_e}{m_N / 2} \right) \left( \frac{e_M^2}{m_n^2 G} \right)$$

It will be an interesting exercise to actually find out the value of  $a_0$  using the gravitational force constant,  $G$ .

10.4 (a) The radius,  $R$  is found from (10.54) as

$$0.9 = \int_0^R dr P(r)$$

$$= N_{nlm}^2 \int_0^{2\pi} d\varphi \int_{-1}^1 d\mu \int_0^R r^2 dr u_{nlm}^2, \quad \mu = \cos \theta$$

Thus, for  $u_{100}$ , for example,

$$\begin{aligned}
0.9 &= \frac{1}{\pi a_0^3} 2\pi \cdot 2 \cdot \int_0^R r^2 e^{-\frac{2r}{a_0}} dr \\
&= \frac{1}{\pi a_0^3} 4\pi \left(\frac{a_0}{2}\right)^3 \left[ 2 - (\rho_0^2 + 2\rho_0 + 2)e^{-\rho_0} \right] \\
&= 1 - \frac{1}{2}(\rho_0^2 + 2\rho_0 + 2)e^{-\rho_0}, \quad \rho_0 \equiv \frac{2R}{a_0}
\end{aligned}$$

From this result one can numerically find  $R$ . Following the same procedure one can likewise find the effective radius for  $u_{200}$ ,  $u_{300}$ .

(b) For the ground state,  $u_{100}$ ,

$$\begin{aligned}
\langle r \rangle &= \int_0^{2\pi} d\varphi \int_{-1}^1 d\mu \int_0^\infty r^2 dr r u_{100}^2 \\
&= \left(\frac{1}{a_0^3 \pi}\right) 4\pi \int_0^\infty dr r^3 e^{-\frac{2r}{a_0}} \\
&= \frac{4\pi}{a_0^3 \pi} \left\{ -\frac{e^{-\frac{2r}{a_0}}}{\left(\frac{a_0}{2}\right)^4} \left[ \left(\frac{2r}{a_0}\right)^3 + 3 \cdot \left(\frac{2r}{a_0}\right)^2 + 6 \left(\frac{2r}{a_0}\right) + 6 \right] \right\}_0^\infty \\
&= \frac{3}{2} a_0
\end{aligned}$$

Likewise,

$$\begin{aligned}
\langle r^2 \rangle &= \int_0^{2\pi} d\varphi \int_{-1}^1 d\mu \int_0^\infty r^2 dr r^2 u_{100}^2 \\
&= \frac{4\pi}{a_0^3 \pi} \int_0^\infty dr r^4 e^{-\frac{2r}{a_0}} \\
&= 3a_0^2
\end{aligned}$$

Hence

$$\begin{aligned}
\langle (r - \langle r \rangle)^2 \rangle &= \langle r^2 \rangle - \langle r \rangle^2 \\
&= a_0^2 (3 - 2.25) \\
&= 0.75 a_0^2
\end{aligned}$$

so that

$$\Delta r / \langle r \rangle \approx 0.6$$

and the variance *w.r.t.*  $\langle r \rangle$  is appreciable. The variances,  $\Delta r$  for other states e.g.  $2s$ ,  $3s$  can be evaluated in a similar way.

10.5 (a)

$$\begin{aligned} 1 &= \langle x | x \rangle \\ &= N^2 \langle (u_{211} + u_{21-1}) | (u_{211} + u_{21-1}) \rangle \\ &= N^2 (1+1) \end{aligned}$$

Hence

$$N = 1/\sqrt{2}$$

Similarly

$$1 = \langle y | y \rangle = N^2 \cdot 2$$

and

$$N = 1/\sqrt{2}$$

(b) Since

$$\langle u_{210} | u_{21\pm 1} \rangle = 0$$

it clearly follows from the definitions of these x-, y-, z-functions that

$$\langle z | x \rangle = \langle z | y \rangle = 0$$

and

$$\langle x | y \rangle \propto \langle (u_{211} + u_{21-1}) | (u_{211} - u_{21-1}) \rangle = 1 - 1 = 0$$

10.6 (a) For the ground state,  $u_{100}$  the average kinetic energy is given by

$$\langle K \rangle = \left\langle u_{100} \left| \frac{-\hbar^2}{2\mu} \nabla^2 \right| u_{100} \right\rangle$$

Now,

$$\begin{aligned} \nabla^2 u_{100} &= \left( \frac{1}{r^2} \frac{\partial}{\partial r} r^2 \frac{\partial}{\partial r} - \frac{1}{r^2} \frac{1}{\hbar^2} \hat{l}^2 \right) u_{100} \\ &= N_{100} \cdot \left( \frac{1}{r^2} \frac{\partial}{\partial r} r^2 \frac{\partial}{\partial r} e^{-\frac{r}{a_0}} \right) \\ &= N_{100} \cdot \left( \frac{1}{a_0^2} e^{-\frac{r}{a_0}} - \frac{2}{a_0 r} e^{-\frac{r}{a_0}} \right) \end{aligned}$$

Hence,

$$\begin{aligned}
\langle K \rangle &= \frac{1}{a_0^3 \pi} \left( \frac{-\hbar^2}{2\mu} \right) \int_0^{2\pi} d\varphi \int_{-1}^1 d\mu \int_0^\infty r^2 dr \left( \frac{1}{a_0^2} - \frac{r}{a_0} \right) e^{-\frac{2r}{a_0}} \\
&= \frac{\hbar^2}{2\mu a_0^2} \\
&= \frac{\hbar^2}{\mu e_M^2} \frac{e_M^2}{2a_0^2}, & e_M^2 &\equiv e^2 / 4\pi\epsilon_0 \\
&= \frac{e_M^2}{2a_0}, & \frac{\hbar^2}{\mu e_M^2} &= a_0
\end{aligned}$$

Also,

$$\begin{aligned}
\langle V \rangle_{100} &= \frac{1}{a_0^3 \pi} \int_0^{2\pi} d\varphi \int_{-1}^1 d\mu \int_0^\infty r^2 dr \left( -\frac{e_M^2}{r} \right) e^{-\frac{2r}{a_0}} \\
&= -\frac{4\pi}{a_0^3 \pi} \cdot e_M^2 \int_0^\infty dr r e^{-\frac{2r}{a_0}} \\
&= -\frac{e_M^2}{a_0}
\end{aligned}$$

Therefore,

$$\langle K \rangle_{100} = -\frac{1}{2} \langle V \rangle_{100}$$

(b) It will be an instructive exercise to carry out similar calculations for  $\langle K \rangle$ ,  $\langle V \rangle$  for the states  $u_{200}$ ,  $u_{210}$ . One can generally show that

$$\langle K \rangle_{nlm} = -\frac{1}{2} \langle V \rangle_{nlm}$$

10.7 (a) Let us first consider the fraction of electron charge cloud contained within the Bohr radius,  $a_0$ :

$$\begin{aligned}
P &\equiv \int_0^{2\pi} d\varphi \int_0^1 d\mu \int_0^{a_0} r^2 dr \cdot u_{100}^2, \quad \mu = \cos \theta \\
&= \frac{1}{\pi a_0^3} \cdot 4\pi \int_0^{a_0} r^2 dr \cdot e^{-Zr/a_0} \\
&= \frac{4}{a_0^3} \left\{ -\frac{e^{-Zr/a_0}}{(2/a_0)^3} \left[ \left( \frac{2r}{a_0} \right)^3 + 3 \left( \frac{2r}{a_0} \right)^2 + 6 \left( \frac{2r}{a_0} \right) + 6 \right] \right\}_0^{a_0} \\
&= 0.85 \\
r &= \underline{r_1} - \underline{r_2} \text{ ----- (2)}
\end{aligned}$$

Hence the fraction of electron cloud lying outside the Bohr radius  $a_B = a_0$  is 15%.

(b) For  $u_{200}$  and  $u_{210}$ , one can similarly calculate  $P$  within  $2a_0$  and find the fraction lying outside  $2a_0$ . It will be interesting to see whether the fraction increases or decreases as the principle

quantum number  $n$  increases.

10.8 (a) For H-atom in which  $Z=1$ , the transition energy involved is given by

$$\Delta E_{n_i, n_f} = -\frac{e_M^2}{2a_0} \left( \frac{1}{n_i^2} - \frac{1}{n_f^2} \right),$$

where  $n_i, n_f$  denote the initial and final state quantum numbers and

$$\frac{e_M^2}{2a_0} = 13.6eV$$

For Lyman series in which  $n_f=1$ , the shortest and longest wavelengths are therefore given by

$$\nu_s = \frac{c}{\lambda_s} = -\frac{e_M^2}{2a_0} \left( \frac{1}{\infty^2} - \frac{1}{1^2} \right)$$

and

$$\nu_l = \frac{c}{\lambda_l} = -\frac{e_M^2}{2a_0} \left( \frac{1}{2^2} - \frac{1}{1^2} \right).$$

That is,

$$\lambda_s \approx 90nm \ \& \ \frac{1}{\lambda_s} \approx 1.1 \times 10^7 / m$$

$$\lambda_l \approx 122nm \ \& \ \frac{1}{\lambda_l} \approx 0.82 \times 10^7 / m$$

For Balmer series, in which  $n_f=2$ , one can likewise obtain

$$\lambda_s \approx 365nm \ \& \ \frac{1}{\lambda_s} \approx 0.27 \times 10^7 / m$$

$$\lambda_l \approx 652nm \ \& \ \frac{1}{\lambda_l} \approx 0.15 \times 10^7 / m$$

One can similarly find  $\lambda_s, \lambda_l$  for other series.

(b) For positronium, the reduced mass is given by

$$\frac{1}{\mu} = \frac{1}{m_0} + \frac{1}{m_0}$$

where  $m_0$  is the electron rest mass, so that  $\mu = m_0/2$ . Hence  $a_0 \propto 1/\mu$  increases by a factor of 2 and the ground state binding energy,  $\propto e_M^2/2a_0$  decreases by the same factor of 2. Thus,  $\lambda_s$  and  $\lambda_l$  found for the case of H-atom have to be increased by 2.

For ionized helium atom,  $Z=2$  and  $\mu$  is essentially same as in H-atom case. Hence the ground state binding energy  $\propto Z^2 e_M^2 / 2a_0$  increases by  $2^2$ , leading to shortening of  $\lambda_s, \lambda_l$  found for H-atom by the factor of 4.

10.9 (a) The ground state binding energy can be analyzed simply using the binding energy of the H-atom as the reference (see (10.43), (10.44) in the text):

$$\begin{aligned}\frac{Z^2 e_M^2}{2a_0} &= \frac{e_M^2}{2a_B} \cdot \frac{Z^2}{1 + \frac{m_e}{m_N}} \\ &= 13.6 \frac{Z^2}{1 + m_e/m_N} eV\end{aligned}$$

where  $m_e$ ,  $m_N$  are the mass of electron and nucleus, respectively.

The transition from  $u_{2lm}$  to  $u_{100}$  corresponds to the longest wavelength in Lyman series or the smallest frequency, *i.e.*  $\lambda = 122 \text{ nm}$  and  $\nu = 2.46 \times 10^{15} / s$  in H-atom.

For deuterium,  $Z=1$  and  $m_D \approx 2m_H$ . Hence, its ground state binding energy is given in terms of that of H-atom as

$$13.6eV \cdot \frac{1 + m_e/m_H}{1 + m_e/m_D} \approx 13.6eV \cdot (1.0003)$$

This indicates that the upward shift of frequency is about 0.03% from the case of H-atom.

(b) The emitted radiation of frequency,  $\nu$  and/or energy  $h\nu$  has the momentum given by

$$p = \hbar k = \hbar \frac{2\pi}{\lambda} = \hbar \frac{2\pi\nu}{c} = \frac{h\nu}{c}$$

If the atom emits a photon of momentum  $p$ , it recoils back to preserve momentum, so that

$$|p| = |P| = M|V|$$

with  $P$  denoting the momentum of the atom. Hence with

$$\begin{aligned}|p| &= \frac{h\nu}{c} = \frac{13.6eV(1 - \frac{1}{4}) \times 1.6 \times 10^{-19} J/eV}{3 \times 10^8 m/s} \\ &\approx 5.44 \times 10^{-27} \text{ kg } m/s\end{aligned}$$

Thus the recoil velocity of H-atom is given by

$$\begin{aligned}|V| &= \frac{5.44 \times 10^{-27} \text{ kg} \cdot m/s}{1.673 \times 10^{-27} \text{ kg}} \\ &\approx 3.25 \text{ m/s}\end{aligned}$$

For deuterium with mass  $2 \times m_H$   $|V| \approx 1.63 \text{ m/s}$ .

(c) For the H-atom, the transition frequency from  $u_{3lm}$  to  $u_{100}$  is given by

$$h\nu_{31} = 13.6eV \left(1 - \frac{1}{3^2}\right),$$

that is

$$\nu_{31} = 2.93 \times 10^{15} / s.$$

For deuterium the frequency is practically same within the error of 0.03%.

10.10 (a) With  $Z=1$ , the ionization energy is given from (10.43) by

$$E_I = \frac{\mu e_M^4}{2\hbar^2}, \quad e_M^2 = \frac{e^2}{4\pi\epsilon_0}$$

Thus,  $E_I$  can be simply analyzed based on the ionization energy of H-atom:

$$\begin{aligned}
E_I &= 13.6eV \left( \frac{\epsilon_0}{\epsilon_0 \epsilon_r} \right)^2 \left( \frac{m_0}{m_n} \right) \\
&= 13.6 \left( \frac{1}{11.9} \right)^2 (1.1)eV \\
&\approx 0.1eV
\end{aligned}$$

(b) The atomic radius is also conveniently analyzed using radius of the H-atom:

$$\begin{aligned}
a_0 &= \frac{\hbar^2}{\mu e_M^2} = \frac{\hbar^2 4\pi\epsilon_0\epsilon_r}{\mu e^2} \\
&\approx 0.05\epsilon_r \text{ nm} \\
&\approx 0.6 \text{ nm}
\end{aligned}$$

(c) Using the de Broglie relation,

$$\lambda = \frac{h}{p}$$

where the momentum is found from

$$\left\langle \frac{p^2}{2m_n} \right\rangle = -\frac{1}{2} E_I = \frac{0.1}{2} eV$$

one can write

$$\begin{aligned}
p &= (2m_n 0.05eV)^{1/2} \\
&= (2 \cdot 9.1 \times 10^{-31} \cdot 1.1 \cdot 0.05eV \cdot 1.6 \times 10^{-19} J/eV)^{1/2} \\
&= 1.27 \times 10^{-25} \text{ kg} \cdot \text{m} / \text{s}
\end{aligned}$$

and

$$\begin{aligned}
\lambda &= \frac{h}{p} \\
&= \frac{6.626 \times 10^{-34} J \cdot s}{1.27 \times 10^{-25} \text{ kg} \cdot \text{m} / \text{s}} \\
&= 5.22 \times 10^{-9} \text{ m} \\
&= 5.22 \text{ nm}
\end{aligned}$$



## Chapter 11

11.1 (a) The normalization condition of this composite wavefunction has been built in separately:

$$\begin{aligned}
 & \langle \varphi_0(1,2) | \varphi_0(1,2) \rangle \\
 &= \langle u_{100}(1)u_{100}(2)\chi_a | u_{100}(1)u_{100}(2)\chi_a \rangle \\
 &= \langle u_{100}(1) | u_{100}(1) \rangle \langle u_{100}(2) | u_{100}(2) \rangle \langle \chi_a | \chi_a \rangle \\
 &= 1
 \end{aligned}$$

(b) Since  $\hat{S} = \hat{s}_1 + \hat{s}_2$ , one can write using (11.20) – (11.23)

$$\begin{aligned}
 \hat{S}_z &= \hat{s}_{1z} + \hat{s}_{2z} \\
 &= \frac{\hbar}{2} \left[ \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}_1 + \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}_2 \right]
 \end{aligned}$$

$$\begin{aligned}
 \hat{S}^2 &= (\hat{s}_1 + \hat{s}_2) \cdot (\hat{s}_1 + \hat{s}_2) \\
 &= \frac{\hbar^2}{4} (\underline{\sigma}_1 + \underline{\sigma}_2) \cdot (\underline{\sigma}_1 + \underline{\sigma}_2) \\
 &= \frac{\hbar^2}{4} (\sigma_1^2 + \sigma_2^2 + 2 \sigma_1 \cdot \sigma_2) \\
 &= \frac{\hbar^2}{4} \left\{ \begin{pmatrix} 3 & 0 \\ 0 & 3 \end{pmatrix}_1 + \begin{pmatrix} 3 & 0 \\ 0 & 3 \end{pmatrix}_2 + 2 \left[ \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}_1 \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}_2 + \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}_1 \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}_2 + \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}_1 \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}_2 \right] \right\} \\
 & \text{----- (1)}
 \end{aligned}$$

Now

$$\begin{aligned}
 \hat{S}_z | \chi_a \rangle &= (\hat{s}_{1z} + \hat{s}_{2z}) | \chi_a \rangle \\
 &= \frac{1}{2} \hbar \left[ \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}_1 + \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}_2 \right] \frac{1}{\sqrt{2}} \left[ \begin{pmatrix} 1 \\ 0 \end{pmatrix}_1 \begin{pmatrix} 0 \\ 1 \end{pmatrix}_2 - \begin{pmatrix} 1 \\ 0 \end{pmatrix}_2 \begin{pmatrix} 0 \\ 1 \end{pmatrix}_1 \right] \\
 &= \frac{1}{2} \hbar \cdot 0 \frac{1}{\sqrt{2}} \left[ \begin{pmatrix} 1 \\ 0 \end{pmatrix}_1 \begin{pmatrix} 0 \\ 1 \end{pmatrix}_2 - \begin{pmatrix} 1 \\ 0 \end{pmatrix}_2 \begin{pmatrix} 0 \\ 1 \end{pmatrix}_1 \right]
 \end{aligned}$$

Hence

$$\langle \chi_a | \hat{S}_z | \chi_a \rangle = 0$$

Also, using (1) one obtains

$$\begin{aligned}
 \hat{S}^2 | \chi_a \rangle &= \frac{\hbar^2}{4} \cdot (2 \cdot 3 - 2 \cdot 3) | \chi_a \rangle \\
 &= \frac{\hbar^2}{4} \cdot 0 | \chi_a \rangle
 \end{aligned}$$

Therefore,

$$\langle \chi_a | \hat{S}^2 | \chi_a \rangle = 0$$

11.2 (a) Because of the orthonormality of  $u_{nlm}(j)$  the symmetrized and antisymmetrized wave functions are also orthonormal:

$$\frac{1}{2} \langle u_{100}(1)u_{200}(2) \pm u_{100}(2)u_{200}(1) | u_{100}(1)u_{200}(2) \pm u_{100}(2)u_{200}(1) \rangle = 1$$

and

$$\frac{1}{2} \langle u_{100}(1)u_{200}(2) + u_{100}(2)u_{200}(1) | u_{100}(1)u_{200}(2) - u_{100}(2)u_{200}(1) \rangle = 0$$

Also the singlet and triplet states defined in (11.33),(11.34) are orthonormal :

$$\langle \chi_s | \chi_s \rangle = \langle \chi_a | \chi_a \rangle = 1$$

$$\langle \chi_s | \chi_a \rangle = 0$$

(b) In evaluating  $\langle \hat{S}^2 \rangle$ ,  $\langle \hat{S}_z \rangle$ , the spatial integration involving the symmetrized and antisymmetrized wave functions automatically yields unity, and one needs to consider the spin operators acting on the triplet and singlet spin functions.

$$\begin{aligned} & \langle \varphi_s | \hat{S}_z | \varphi_s \rangle \\ &= \langle \chi_a | \hat{s}_{1z} + \hat{s}_{2z} | \chi_a \rangle \\ &= 0 \\ & \langle \varphi_s | \hat{S}^2 | \varphi_s \rangle \\ &= \langle \chi_a | (\hat{s}_1 + \hat{s}_2) \cdot (\hat{s}_1 + \hat{s}_2) | \chi_a \rangle \\ &= 2 \cdot \frac{3\hbar^2}{4} \end{aligned}$$

where use has been made of the results of the previous problems.

Similarly one can write

$$\begin{aligned} & \langle \varphi_a | \hat{S}_z | \varphi_a \rangle \\ &= \langle \chi_s | \hat{s}_{1z} + \hat{s}_{2z} | \chi_s \rangle \\ &= \hbar \cdot m, \quad m = 1, 0, -1 \\ & \langle \varphi_a | \hat{S}^2 | \varphi_a \rangle \\ &= \langle \chi_s | (\hat{s}_1 + \hat{s}_2) \cdot (\hat{s}_1 + \hat{s}_2) | \chi_s \rangle \\ &= \frac{\hbar^2}{4} \cdot (2 \cdot 3 + 2) \\ &= 2\hbar^2 \end{aligned}$$

corresponding to  $\ell(\ell+1)\hbar^2$ ,  $\ell = 1$ .

11.3 Let

$$n_1 = 100 \ 1/2, \quad n_2 = 200 \ 1/2, \quad n_3 = 200 \ -1/2$$

denote the set of quantum numbers including the spin. Then the 3-electron wave function is

represented by the Slater determinant as

$$\begin{aligned}\varphi(1,2,3) &= \frac{1}{\sqrt{3!}} \begin{vmatrix} u_{n_1}(1) & u_{n_1}(2) & u_{n_1}(3) \\ u_{n_2}(1) & u_{n_2}(2) & u_{n_2}(3) \\ u_{n_3}(1) & u_{n_3}(2) & u_{n_3}(3) \end{vmatrix} \\ &= \frac{1}{\sqrt{3!}} \begin{vmatrix} u_{100}(1)\alpha(1) & u_{100}(2)\alpha(2) & u_{100}(3)\alpha(3) \\ u_{200}(1)\alpha(1) & u_{200}(2)\alpha(2) & u_{200}(3)\alpha(3) \\ u_{200}(1)\beta(1) & u_{200}(2)\beta(2) & u_{200}(3)\beta(3) \end{vmatrix}\end{aligned}$$

The wavefunction  $\varphi(1,2,3)$  consists of a linear superposition of 3 quantum states, for instance,  $u_{100}(1)u_{200}(2)u_{200}(3)$ .

Thus,

$$\begin{aligned}\hat{H} u_{100}(1) u_{200}(2) u_{200}(3) \\ = (E_1 + 2E_2) u_{100}(1) u_{200}(2) u_{200}(3)\end{aligned}$$

and all other terms in  $\varphi(1,2,3)$  yield the same energy eigenvalue.

Therefore

$$\langle \varphi(1,2,3) | \hat{H} | \varphi(1,2,3) \rangle = E_1 + 2E_2$$

11.4 (a) The Hamiltonian reads as

$$\hat{H} = \sum_{j=1}^3 \hat{H}_{0j} + \hat{H}'$$

where  $\hat{H}_0$  represents the Hamiltonian of a hydrogenic atom, i.e.

$$\hat{H}_{0j} = -\frac{\hbar^2}{2m} \nabla_j^2 + \frac{e_M^2}{r_j}, \quad e_M^2 = \frac{e^2}{4\pi\epsilon_0}$$

and  $\hat{H}'$  accounts for the Coulomb interactions among 3 electrons :

$$\hat{H}' = e_M^2 \left( \frac{1}{r_{12}} + \frac{1}{r_{13}} + \frac{1}{r_{23}} \right)$$

Thus, if  $\hat{H}'$  is neglected, one can write

$$\begin{aligned}\hat{H} u_{n_1}(1)u_{n_2}(2)u_{n_3}(3) &= \sum_{j=1}^3 \hat{H}_{0j} u_{n_1}(1)u_{n_2}(2)u_{n_3}(3) \\ &= (E_{n_1} + E_{n_2} + E_{n_3}) u_{n_1}(1)u_{n_2}(2)u_{n_3}(3)\end{aligned}$$

(b) Let

$$\begin{aligned}a_1 &= 100\alpha \\ a_2 &= 100\beta \\ a_3 &= 200\alpha \text{ or } 200\beta\end{aligned}$$

denote the set of quantum number,  $n_l m_s$ . Then, the 3-electron wave function in lithium atom is given by

$$\begin{aligned}\varphi(1,2,3) &= \frac{1}{\sqrt{3!}} \begin{vmatrix} u_{a1}(1) & u_{a1}(2) & u_{a1}(3) \\ u_{a2}(1) & u_{a2}(2) & u_{a2}(3) \\ u_{a3}(1) & u_{a3}(2) & u_{a3}(3) \end{vmatrix} \\ &= \frac{1}{\sqrt{3!}} \begin{vmatrix} u_{100}(1)\alpha(1) & u_{100}(2)\alpha(2) & u_{100}(3)\alpha(3) \\ u_{100}(1)\beta(1) & u_{100}(2)\beta(2) & u_{100}(3)\beta(3) \\ u_{200}(1)\alpha(1) & u_{200}(2)\alpha(2) & u_{200}(3)\alpha(3) \end{vmatrix}\end{aligned}$$

(c) Each term appearing in the wavefunction,  $\varphi(1,2,3)$  yields the same energy eigenvalue when acted upon by  $\hat{H}_{01} + \hat{H}_{02} + \hat{H}_{03}$ .

For instance

$$\begin{aligned}\sum_{j=1}^3 \hat{H}_{0j} u_{100}(1) u_{100}(2) u_{200}(3) \\ = (2E_1 + E_2) u_{100}(1) u_{100}(2) u_{200}(3)\end{aligned}$$

so that

$$\begin{aligned}\langle \varphi(1,2,3) | \sum_{j=0}^3 \hat{H}_{0j} | \varphi(1,2,3) \rangle \\ = 2E_1 + E_2\end{aligned}$$

Similarly, each term yields the same spin eigen value. For example

$$\begin{aligned}(\hat{s}_{1z} + \hat{s}_{2z} + \hat{s}_{3z}) \alpha(1)\beta(2)\alpha(3) \\ = \frac{1}{2} \hbar (1 - 1 + 1) \alpha(1)\beta(2)\alpha(3) \\ = \frac{1}{2} \hbar \alpha(1)\beta(2)\alpha(3)\end{aligned}$$

Hence

$$\langle \varphi(1,2,3) | \hat{S}_z | \varphi(1,2,3) \rangle = \frac{1}{2} \hbar$$

11.5 (a) The 11 electrons in Na atom are assigned the following set of quantum numbers:

$$\begin{aligned}100\alpha, 100\beta, 200\alpha, 200\beta \\ 211\alpha, 211\beta, 210\alpha, 210\beta \\ 21-1\alpha, 21-1\beta, 300\alpha \text{ or } \beta\end{aligned}$$

(b) Let  $Z_{\text{eff}}$  represent the effective nuclear charge as acting on the valence electron in  $u_{300}$  state. Then its radial component is sealed approximately

$$\exp\left(-\frac{Z_{\text{eff}} r}{a_0 n}\right), \quad n = 3.$$

The ionization potential of the valence electron is then given from (10.43) by

$$IP_1 = \frac{\mu Z_{eff}^2 e_M^4}{2\hbar^2} \frac{1}{3^2} = 13.6eV \cdot \frac{Z_{eff}^2}{9} = 5.14eV$$

from which one finds  $Z_{eff} \approx 1.84$

Given  $Z_{eff}$ , the atomic size is to be roughly estimated

$$2\langle r \rangle \sim 2 \cdot \frac{a_0 n}{Z_{eff}} \sim \frac{2.3}{1.84} \times 0.05nm \approx 0.16nm$$

which is in reasonable agreement with measured data of 0.17nm

- 11.6 (a) Electrons in solids, in particular in metal are generally modeled as free particles with the quasi-continuous energy spectrum. Thus, the highest energy level  $E_F$  is specified by

$$N = \int_0^{E_F} dE \cdot g_{3D}(E)V$$

where  $N$  is the number of electrons in volume  $V$  and

$$g_{3D}(E) = \frac{\sqrt{2}m^{3/2}}{\pi^2\hbar^3} E^{1/2}$$

is the 3D density of states derived in chapter 4. Performing the integration one finds

$$\frac{N}{V} = \frac{\sqrt{2}m^{3/2}}{\pi^2\hbar^3} \frac{2}{3} E_F^{3/2}$$

or

$$E_F = \frac{\hbar^2}{8m} \left( \frac{3N}{\pi V} \right)^{2/3}$$

For the electron wavefunction one can use the wavefunction of a free particle confined in 3-D box, considered in chapter 4.

- (b) The total energy per volume is then given by

$$\begin{aligned} E_T &= \int_0^{E_F} dE \cdot g(E)E \\ &= \frac{\sqrt{2}m^{3/2}}{\pi^2\hbar^3} \int_0^{E_F} E^{3/2} dE \\ &= \frac{\sqrt{2}m^{3/2}}{\pi^2\hbar^3} \cdot \frac{2}{5} E_F^{5/2} \end{aligned}$$

- (c) To proceed further,  $E_F$  has to be found from (a), using the given values of  $N/V$ , i.e.

$$\begin{aligned} E_F &= \frac{(6.626 \times 10^{-34} Js)^2}{8 \times 9.1 \times 10^{-31} Kg} \cdot \left( \frac{3}{\pi} \cdot 10^{22+6} \right)^{2/3}, \quad \frac{N}{V} = 10^{28}/m^3 \\ &= 2.716 \times 10^{-19} J \\ &\approx 1.7eV \end{aligned}$$

With  $E_F$  thus found the total energy is to be evaluated to be

$$E_T = \frac{\sqrt{2} \cdot (9.1 \times 10^{-31})^{3/2}}{\pi^2 \cdot (1.055 \times 10^{-34})^3} \cdot \frac{2}{5} (2.716 \times 10^{-19})^{5/2} \approx 1.61 \times 10^9 J$$

$E_T$  in turn can be expressed in terms of the average electron energy  $\langle E \rangle$  times  $N/V = 10^{28} / \text{meter}^3$ , i.e.

$$E_T = \left( \frac{N}{V} \right) \cdot \langle E \rangle$$

so that

$$\langle E \rangle \approx \frac{1.61 \times 10^9 \text{ J}}{1.602 \times 10^{-19} \text{ J} \cdot 1 \text{ eV}} \cdot \frac{1}{(N/V)} \approx 1 \text{ eV}$$

(d) The Fermi energy  $E_F$  for 2D electron system is specified by

$$N/V_{2D} = \sum_n \int_{E_n}^{E_F} dE \cdot g_{2D}(E_n), \quad V_{2D} = 1/L^2 \text{ ----- (1)}$$

where the 2D density of states are given from (4.30) as

$$g_{2D}(E) = \frac{m}{\pi \hbar^2}$$

with  $E_n$  denoting the energy eigenvalues in the quantum well.

For simplicity, assume quasi-continuous energy spectrum. Then one can recast (1) as

$$N/V_{2D} = \sum_{E_n=0}^{E_F} \frac{m}{\pi \hbar^2} (E_F - E_n) = \frac{m}{\pi \hbar^2} \cdot \frac{1}{2} E_F$$

Hence

$$\begin{aligned} E_F &= \frac{N}{V_{2D}} \cdot \frac{2\pi \hbar^2}{m} \\ &= \left[ \frac{4.6 \times 10^{18}}{(\text{meter})^2} \right] \cdot \frac{2\pi (1.055 \times 10^{-34})^2}{9.1 \times 10^{-31}} \\ &= 3.53 \times 10^{-19} \text{ J} \\ &= \frac{3.53 \times 10^{-19} \text{ J}}{1.6 \times 10^{-19} \text{ V} / \text{eV}} \\ &= 2.21 \text{ eV} \end{aligned}$$

The total energy is then given by

$$\begin{aligned} E_T &= \sum_{E_n=0}^{E_F} \int_0^{E_F} dE \cdot g_{2D}(E - E_n) \\ &= \sum_{E_n=0}^{E_F} \frac{m}{\pi \hbar^2} \cdot \int_{E_n}^{E_F} dE (E - E_n) \\ &\approx \frac{m E_F^2}{2\pi \hbar^2} \int_0^1 (1 - \xi)^2, \quad \xi = \frac{E_n}{E_F} \\ &= \frac{m E_F^2}{6\pi \hbar^2} \\ &\approx 0.54 \text{ J} \approx 0.34 \times 10^{19} \text{ eV} \end{aligned}$$

Hence the average electron energy is given by

$$0.34 \cdot 10^{19} eV = \frac{N}{V_{2D}} \cdot \langle E \rangle_{2D} = 4.6 \times 10^{18} \cdot \langle E \rangle$$

so that

$$\langle E \rangle_{2D} \cong 0.74 eV$$

For 1D electron system  $E_F$  is found by

$$\frac{N}{V_{1D}} = \sum_{E_n=0}^{E_F} \int_{E_n}^{E_F} dE \cdot g_{1D}(E, E_n), \quad 1/V_{1D} = 1/L \text{ ----- (2)}$$

where the 1D density of states is given from (4.31) in the text by

$$g_{1D}(E, E_n) = \frac{\sqrt{2m}^{1/2}}{\pi\hbar} \cdot \frac{1}{(E - E_n)^{1/2}}$$

Hence, using  $g_{1D}$  in the integral one finds

$$\int_{E_n}^{E_F} dE \cdot g_{1D} = \frac{\sqrt{2m}^{1/2}}{\pi\hbar} \cdot 2(E - E_n)^{1/2} \Big|_{E_n}^{E_F} = \frac{2\sqrt{2m}^{1/2}}{\pi\hbar} (E_F - E_n)^{1/2}$$

Again assuming quasi-continuous energy eigenvalues for this 1D electron system (2) can be recast into

$$\begin{aligned} \frac{N}{V_{1D}} &= \frac{2\sqrt{2m}^{1/2}}{\pi\hbar} \sum_{E_n=0}^{E_F} (E_F - E_n)^{1/2} \\ &= \frac{2\sqrt{2m}^{1/2} E_F^{1/2}}{\pi\hbar} \int_0^1 (1 - \xi)^{1/2} d\xi, \quad \xi = \frac{E_n}{E_F} \\ &= \frac{4\sqrt{2m}^{1/2} E_F^{1/2}}{3\pi\hbar} \end{aligned}$$

Hence

$$\begin{aligned} E_F &= \left( \frac{N}{V_{1D}} \cdot \frac{3\pi\hbar}{4\sqrt{2m}^{1/2} E_F^{1/2}} \right)^2, \quad \frac{N}{V_{1D}} = 2.15 \times 10^9 \\ &\cong 1.57 \times 10^{-19} J \\ &= \frac{1.57 \times 10^{-19} J}{1.6 \times 10^{-19} J/eV} \\ &= 0.98 eV \end{aligned}$$

The total energy is then, given by

$$\begin{aligned}
E_T &= \int_0^{E_F} dE \cdot g_{1D}(E - E_n) \\
&= \sum_{E_n=0}^{E_F} \int_{E_n}^{E_F} dE \cdot \frac{\sqrt{2m}^{1/2}}{\pi\hbar} (E - E_n)^{1/2} \\
&= \sum_{E_n=0}^{E_F} \frac{\sqrt{2m}^{1/2}}{\pi\hbar} \frac{2}{3} (E_F - E_n)^{3/2} \\
&\approx \frac{2\sqrt{2m}^{1/2} E_F^{3/2}}{3\pi\hbar} \int_0^1 (1 - \xi)^{3/2} d\xi, \quad \xi = \frac{E_n}{E_F} \\
&= \frac{4\sqrt{2m}^{1/2} E_F^{3/2}}{15\pi\hbar} \\
&\approx 7 \times 10^{-11} J \\
&\approx 4.38 \times 10^8 eV
\end{aligned}$$

Thus the average electron energy is given by

$$4.38 \times 10^8 = \left( \frac{N}{V_{1D}} \right) \langle E \rangle_{1D}$$

or

$$\langle E \rangle_{1D} \approx 2.03 \times 10^{-1} eV$$



## Chapter 12

12.1 Given the wavefunction,

$$|\varphi_{\pm}\rangle \equiv |u_a(r_1)u_b(r_2) \pm u_b(r_1)u_a(r_2)\rangle$$

one has to evaluate

$$\langle \varphi_{\pm} | \hat{H} | \varphi_{\pm} \rangle$$

where  $\hat{H}$  consists of 2 hydrogenic Hamiltonians plus additional Coulomb interactions:

$$\hat{H} = \hat{H}_1 + \hat{H}_2 + \frac{e_M^2}{R_{ab}} + \frac{(-e_M^2)}{r_{b1}} + \frac{(-e_M^2)}{r_{a2}} + \frac{e_M^2}{r_{12}}$$

(see (12.26) in the text).

It is important to first notice that  $\hat{H}$  is invariant under  $r_1 \leftrightarrow r_2$ .

Also, there are 4 possible combinations of wavefunctions  $u_a, u_b$ :

- I.  $u_a(r_1)u_b(r_2)u_a(r_1)u_b(r_2)$
- II.  $\pm u_a(r_1)u_b(r_2)u_b(r_1)u_a(r_2)$
- III.  $\pm u_b(r_1)u_a(r_2)u_a(r_1)u_b(r_2)$
- IV.  $u_b(r_1)u_a(r_2)u_b(r_1)u_a(r_2)$

Under interchange of the variables of integrations,  $r_1$  and  $r_2$ , one can note I  $\equiv$  IV, II  $\equiv$  III.

Hence the evaluation of  $\langle \hat{H} \rangle$  needs to be done with the use of only I, II and multiply the sum of these two results by 2:

$$\begin{aligned} & \langle u_a(r_1)u_b(r_2) | \hat{H} | u_a(r_1)u_b(r_2) \rangle \\ &= 2E_0 + \frac{e_M^2}{R_{ab}} + 2C + E_{RI} \text{-----} (1) \end{aligned}$$

where

$$\begin{aligned} C &\equiv \langle u_a(r_1) | \frac{-e_M^2}{r_{b1}} | u_a(r_1) \rangle \\ &= \langle u_b(r_2) | \frac{-e_M^2}{r_{a2}} | u_b(r_2) \rangle \\ E_{RI} &\equiv \langle u_a(r_1)u_b(r_2) | \frac{e_M^2}{r_{12}} | u_a(r_1)u_b(r_2) \rangle \end{aligned}$$

Also,

$$\pm \langle u_a(r_1)u_b(r_2) | \hat{H} | u_b(r_1)u_a(r_2) \rangle$$

$$= \pm \left[ 2E_0 S^2 + \frac{e_M^2}{R_{ab}} S^2 + 2DS + E_{CE} \right] \text{----- (2)}$$

where

$$S \equiv \langle u_a(\underline{r}_1) | u_b(\underline{r}_1) \rangle$$

$$= \langle u_a(\underline{r}_2) | u_b(\underline{r}_2) \rangle$$

$$D \equiv \langle u_b(\underline{r}_1) | \frac{-e_M^2}{r_{b1}} | u_a(\underline{r}_1) \rangle$$

$$= \langle u_a(\underline{r}_2) | \frac{-e_M^2}{r_{a2}} | u_b(\underline{r}_2) \rangle$$

$$E_{CE} = \langle u_b(\underline{r}_1) u_a(\underline{r}_2) | \frac{e_M^2}{r_{12}} | u_a(\underline{r}_1) u_b(\underline{r}_2) \rangle$$

Hence, by adding (1), (2) and multiplying the results by 2 one obtains

$$E_{\pm} = \frac{\langle \varphi_{\pm} | \hat{H} | \varphi_{\pm} \rangle}{\langle \varphi_{\pm} | \varphi_{\pm} \rangle}$$

$$= \frac{2 \left[ 2E_0(1 \pm S^2) + \frac{e_M^2}{R_{ab}}(1 \pm S^2) + 2C + E_{RI} \pm 2DS \pm E_{CE} \right]}{2(1 \pm S^2)}$$

$$= 2E_0 + \frac{e_M^2}{R_{ab}} + \frac{2C + E_{RI}}{1 \pm S^2} \pm \frac{2DS + E_{CE}}{1 \pm S^2}$$

12.2(a) Given the wavefunction,

$$\varphi(\underline{r}_a, \underline{r}_b) = N(|u_a\rangle + u_b)$$

the normalization constant is determined by

$$1 = \int d\underline{r} \cdot \varphi^*(\underline{r}_a, \underline{r}_b) \cdot \varphi(\underline{r}_a, \underline{r}_b)$$

$$= N^2 \int d\underline{r} (u_a^* + u_b^*)(u_a + u_b)$$

$$= N^2(1 + 1 + 2S)$$

where the overlap integral is given by

$$S = \langle u_a | u_b \rangle = \langle u_b | u_a \rangle$$

(see (12.8)). Hence

$$N = \frac{1}{[2(1 + S)]^{1/2}}$$

(b) Next consider  $\hat{H}$  acting on  $\varphi(\underline{r}_a, \underline{r}_b)$ ,

$$\hat{H} \cdot \varphi(\underline{r}_a, \underline{r}_b)$$

$$\begin{aligned}
&= \left[ -\frac{\hbar^2}{2m} \nabla^2 - e_M^2 \left( \frac{1}{r_a} + \frac{1}{r_b} \right) \right] N(|u_a\rangle + |u_b\rangle) \\
&= N \left[ E_0 |u_a\rangle - \frac{e_M^2}{r_b} |u_a\rangle + E_0 |u_b\rangle - \frac{e_M^2}{r_a} |u_b\rangle \right] \\
&= E_0 \varphi(\underline{r}_a, \underline{r}_b) - N \left( \frac{e_M^2}{r_b} |u_a\rangle + \frac{e_M^2}{r_a} |u_b\rangle \right)
\end{aligned}$$

Thus,

$$\begin{aligned}
&\langle \varphi(\underline{r}_a, \underline{r}_b) | \widehat{H} | \varphi(\underline{r}_a, \underline{r}_b) \rangle \\
&= E_0 - N^2 e_M^2 \left[ \langle u_a | \frac{1}{r_b} | u_a \rangle + \langle u_a | \frac{1}{r_a} | u_b \rangle + \langle u_b | \frac{1}{r_b} | u_a \rangle + \langle u_b | \frac{1}{r_a} | u_b \rangle \right] \\
&= E_0 + \frac{1}{1+S} (C+D) \text{----- (1)}
\end{aligned}$$

where

$$\begin{aligned}
C &\equiv -e_M^2 \langle u_a | \frac{1}{r_b} | u_a \rangle \\
&= -e_M^2 \langle u_b | \frac{1}{r_a} | u_b \rangle \\
D &\equiv -e_M^2 \langle u_a | \frac{1}{r_a} | u_b \rangle \\
&= -e_M^2 \langle u_b | \frac{1}{r_b} | u_a \rangle
\end{aligned}$$

(see (12.28b),(11.29b)). Clearly (1) is agreement with (12.13) corresponding to the symmetric combination of  $u_a$  and  $u_b$ .

12.3 Given  $R_e = 0.24nm$ ,  $\nu_e = 1.1 \times 10^{13}/s$  and

$$\frac{1}{\mu} = \frac{1}{m_{Na}} + \frac{1}{m_{Cl}}$$

i.e.  $\mu = 23.3 \times 10^{-27} Kg$  one can determine A,  $\alpha$  and the bonding energy as follows. First, start with (2.32) in the text,

$$\Delta E(R) = A e^{-\alpha R} - \frac{e_M^2}{R} + K,$$

with  $K = 1.49 eV$ ,  $e_M^2 = e^2 / 4\pi\epsilon_0$ .

$R_e$  is determined at the minimum value of  $\Delta E(R)$ , i.e.

$$\left. \frac{\partial \Delta E(R)}{\partial R} \right|_{R_e} = 0 = -A\alpha e^{-\alpha R_e} + \frac{e_M^2}{R_e^2}$$

or

$$A\alpha = \frac{e_M^2}{R_e^2} e^{\alpha R_e} \text{ ----- (1)}$$

Also, the effective spring constant, k is specified as

$$\begin{aligned} k &\equiv \mu\omega_e^2 = \mu(2\pi\nu_e)^2 \\ &= \left. \frac{\partial^2 \Delta E(R)}{\partial R^2} \right|_{R_e} \\ &= A\alpha^2 e^{-\alpha R_e} - 2 \frac{e_M^2}{R_e^3} \text{ ----- (2)} \end{aligned}$$

Combining (1), (2) one can write

$$\alpha \frac{e_M^2}{R_e^2} - 2 \frac{e_M^2}{R_e^3} = \mu\omega_e^2 \text{ ----- (3)}$$

$\alpha$  is thus found from (3) using the known values of  $R_e$ ,  $\omega_e^2$ :

$$\begin{aligned} \alpha &= \frac{2}{R_e} + \frac{\mu\omega_e^2 R_e^2}{e_M^2} \\ &\approx 3.6 \times 10^{10} \text{ meter}^{-1} \end{aligned}$$

With  $\alpha$  thus found A can be determined from (1):

$$\begin{aligned} A &= \frac{1}{\alpha} \frac{e_M^2}{R_e^2} e^{\alpha R_e} \\ &\approx 6.28 \times 10^{-16} \text{ J} \\ &= 3.92 \times 10^3 \text{ eV} \end{aligned}$$

Finally, with A,  $\alpha$  thus determined the bonding energy can be found by evaluating  $\Delta E$  at  $R=R_e$ :

$$\begin{aligned} \Delta E(R_e) &= A e^{-\alpha R_e} - \frac{e_M^2}{R_e} + 1.49 \text{ eV} \\ &\approx -3.82 \text{ eV} \end{aligned}$$

12.4 To recast the coupled Hamiltonian of (12.41),

$$\hat{H} = -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x_1^2} + \frac{1}{2} k x_1^2 - \frac{\hbar^2}{2m} \frac{\partial^2}{\partial x_2^2} + \frac{1}{2} k x_2^2 - \frac{2e_M^2 x_1 x_2}{R^3}$$

introduce new variables

$$\begin{aligned} \xi &= x_1 + x_2 \\ \eta &= x_2 - x_1 \end{aligned}$$

or by inverting

$$\begin{aligned} x_1 &= \frac{1}{2}(\xi - \eta) \\ x_2 &= \frac{1}{2}(\xi + \eta) \end{aligned}$$

Thus one can write

$$\begin{aligned}\frac{\partial}{\partial x_1} &= \frac{\partial}{\partial \xi} \frac{\partial \xi}{\partial x_1} + \frac{\partial}{\partial \eta} \frac{\partial \eta}{\partial x_1} \\ &= \frac{\partial}{\partial \xi} - \frac{\partial}{\partial \eta} \\ \frac{\partial^2}{\partial x_1^2} &= \frac{\partial}{\partial \xi} \left( \frac{\partial}{\partial \xi} - \frac{\partial}{\partial \eta} \right) \frac{\partial x_1}{\partial \xi} + \frac{\partial}{\partial \eta} \left( \frac{\partial}{\partial \xi} - \frac{\partial}{\partial \eta} \right) \frac{\partial \eta}{\partial x_1} \\ &= \frac{\partial^2}{\partial \xi^2} - 2 \frac{\partial^2}{\partial \xi \partial \eta} + \frac{\partial^2}{\partial \eta^2}\end{aligned}$$

Similarly

$$\frac{\partial^2}{\partial x_2^2} = \frac{\partial^2}{\partial \xi^2} + 2 \frac{\partial^2}{\partial \xi \partial \eta} + \frac{\partial^2}{\partial \eta^2}$$

Hence

$$\begin{aligned}& -\frac{\hbar^2}{2m} \left( \frac{\partial^2}{\partial x_1^2} + \frac{\partial^2}{\partial x_2^2} \right) \\ &= -\frac{\hbar^2}{2m} \cdot 2 \left( \frac{\partial^2}{\partial \xi^2} + \frac{\partial^2}{\partial \eta^2} \right)\end{aligned}$$

Also,

$$\begin{aligned}& \frac{1}{2} k (x_1^2 + x_2^2) \\ &= \frac{1}{2} k \left[ \frac{1}{4} (\xi - \eta)^2 + \frac{1}{4} (\xi + \eta)^2 \right] \\ &= \frac{1}{4} k (\xi^2 + \eta^2),\end{aligned}$$

and

$$\begin{aligned}& -\frac{2e_M^2}{R^3} x_1 x_2 \\ &= -\frac{2e_M^2}{R^3} \frac{1}{4} (\xi - \eta)(\xi + \eta) \\ &= -\frac{e_M^2}{2R^3} (\xi^2 - \eta^2)\end{aligned}$$

Therefore,

$$\hat{H} = -\frac{\hbar^2}{2\mu} \frac{\partial^2}{\partial \xi^2} - \frac{\hbar^2}{2\mu} \frac{\partial^2}{\partial \eta^2} + \frac{1}{2} k_- \xi^2 + \frac{1}{2} k_+ \eta^2$$

where

$$\begin{aligned}\frac{1}{\mu} &= \frac{1}{m} + \frac{1}{m}, \quad \mu = m/2 \\ k_{\mp} &= \frac{1}{2} k \mp \frac{e_M^2}{R^3}\end{aligned}$$

12.5 (a) The Hamiltonian consists of two hydrogenic Hamiltonians plus Coulomb interactions between two electrons and two protons (see Fig. 12.7) :

$$\hat{H} = \hat{H}_a + \hat{H}_b + \hat{V}$$

where

$$\hat{H}_a = -\frac{\hbar^2}{2m} \nabla_1^2 - \frac{e_M^2}{r_1}$$

$$\hat{H}_b = -\frac{\hbar^2}{2m} \nabla_2^2 - \frac{e_M^2}{r_2}$$

$$\hat{V} = e_M^2 \left( \frac{1}{r_{12}} + \frac{1}{R} - \frac{1}{|\underline{R} + \underline{r}_2|} - \frac{1}{|\underline{r}_1 - \underline{R}|} \right)$$

Here  $\underline{r}_1, \underline{r}_2$  are the displacements of electrons 1 and 2 from proton a, b respectively and

$$\underline{R} = \underline{R}_b - \underline{R}_a, \quad \underline{r}_{12} = \underline{r}_2 - \underline{r}_1$$

with  $\underline{R}_a, \underline{R}_b$  denoting the positions of protons a and b. Thus,  $|\underline{R} + \underline{r}_2|$  represents the relative distance of electron 2 with respect to proton a and  $|\underline{r}_1 - \underline{R}|$  is the relative distance of electron 1 with respect to proton B.

(b) Since  $r_1, r_2 \ll R$  one can write

$$\begin{aligned} |\underline{R} + \underline{r}_2|^{-1} &= [(\underline{R} + \underline{r}_2) \cdot (\underline{R} + \underline{r}_2)]^{-1/2} \\ &= [R^2 + 2\underline{r}_2 \cdot \underline{R} + r_2^2]^{-1/2} \\ &= R^{-1} \left( 1 + \frac{2\underline{r}_2 \cdot \underline{R}}{R^2} + \frac{r_2^2}{R^2} \right)^{-1/2} \\ &= R^{-1} \left( 1 - \frac{\underline{r}_2 \cdot \underline{R}}{R^2} - \frac{1}{2} \frac{r_2^2}{R^2} + \dots \right) \\ |\underline{r}_1 - \underline{R}|^{-1} &= [(\underline{r}_1 - \underline{R}) \cdot (\underline{r}_1 - \underline{R})]^{-1/2} \\ &= R^{-1} \left( 1 + \frac{\underline{r}_1 \cdot \underline{R}}{R^2} + \frac{1}{2} \frac{r_1^2}{R^2} + \dots \right) \end{aligned}$$

where use has been made of

$$(1 + \epsilon)^n = 1 + n\epsilon + \dots, \quad \epsilon \ll 1$$

Also

$$\begin{aligned} r_{12}^{-1} &\equiv \frac{1}{|\underline{r}_2 + \underline{R}_b - (\underline{r}_1 + \underline{R}_a)|} \\ &= \frac{1}{|\underline{r}_2 - \underline{r}_1 + \underline{R}|} \end{aligned}$$

$$\begin{aligned}
&= \left[ (R + r_2 - r_1) \cdot (R + r_2 - r_1) \right]^{-1/2} \\
&= R^{-1} \left( 1 - \frac{(r_2 - r_1) \cdot R}{R^2} + \frac{(r_2 - r_1)^2}{R^2} + \dots \right)
\end{aligned}$$

Hence, inserting these expansions into  $\hat{V}$  expression there results

$$\begin{aligned}
\hat{V} &= e_M^2 \frac{1}{2R^3} \left[ (r_2 - r_1) \cdot (r_2 - r_1) - (r_1^2 + r_2^2) \right] \\
&= -\frac{e_M^2}{R^3} r_1 \cdot r_2 \\
&= -\frac{e_M^2}{R^3} (x_1 x_2 + y_1 y_2 + z_1 z_2)
\end{aligned}$$

(c) If  $\hat{H}_a$ ,  $\hat{H}_b$  are replaced by 3D harmonic oscillators, the Hamiltonian reads as

$$\begin{aligned}
\hat{H} &= \hat{H}_1 + \hat{H}_2 + \hat{V} \\
\hat{H}_i &= -\frac{\hbar^2}{2m} \nabla_i^2 - \frac{1}{2} k r_i^2, \quad i=1,2
\end{aligned}$$

Here the perturbing Hamiltonian couples the coordinates of these 3D oscillators:

$$\begin{aligned}
\hat{V} &= -\frac{e_M^2}{R^3} (x_1 x_2 + y_1 y_2 + z_1 z_2) \\
&= -\frac{e_M^2}{R^3} r_1 \cdot r_2
\end{aligned}$$

Next, introduce new variables,

$$\begin{aligned}
\underline{\xi} &= \underline{r}_1 + \underline{r}_2 \\
\underline{\eta} &= -\underline{r}_1 + \underline{r}_2
\end{aligned}$$

or inverting the relation one can write

$$\begin{aligned}
\underline{r}_1 &= \frac{1}{2} (\underline{\xi} - \underline{\eta}) \\
\underline{r}_2 &= \frac{1}{2} (\underline{\xi} + \underline{\eta})
\end{aligned}$$

Then the Laplacian operators transform as

$$\begin{aligned}
&-\frac{\hbar^2}{2m} (\nabla_1^2 + \nabla_2^2) \\
&= -\frac{\hbar^2}{2m} \left[ \left( \frac{\partial^2}{\partial x_1^2} + \frac{\partial^2}{\partial y_1^2} + \frac{\partial^2}{\partial z_1^2} \right) + \left( \frac{\partial^2}{\partial x_2^2} + \frac{\partial^2}{\partial y_2^2} + \frac{\partial^2}{\partial z_2^2} \right) \right] \\
&= -\frac{\hbar^2}{2\mu} \left[ \left( \frac{\partial^2}{\partial \xi_x^2} + \frac{\partial^2}{\partial \xi_y^2} + \frac{\partial^2}{\partial \xi_z^2} \right) + \left( \frac{\partial^2}{\partial \eta_x^2} + \frac{\partial^2}{\partial \eta_y^2} + \frac{\partial^2}{\partial \eta_z^2} \right) \right]
\end{aligned}$$

$$= -\frac{\hbar^2}{2\mu}(\nabla_{\xi}^2 + \nabla_{\eta}^2)$$

where

$$\frac{1}{\mu} = \frac{1}{m} + \frac{1}{m}$$

i.e.

$$\mu = \frac{2}{m}$$

Also the potential energy is recast into

$$\begin{aligned} & \frac{1}{2}k(r_1^2 + r_2^2) \\ &= \frac{1}{2}k \left[ \frac{1}{4}(\underline{\xi} - \underline{\eta}) \cdot (\underline{\xi} - \underline{\eta}) + \frac{1}{4}(\underline{\xi} + \underline{\eta}) \cdot (\underline{\xi} + \underline{\eta}) \right] \\ &= \frac{1}{4}k(\xi^2 + \eta^2), \\ \hat{V} &= -\frac{e_M^2}{R^3}(\underline{r}_1 \cdot \underline{r}_2) \\ &= -\frac{e_M^2}{R^3} \frac{1}{4}(\underline{\xi} - \underline{\eta}) \cdot (\underline{\xi} + \underline{\eta}) \\ &= -\frac{e_M^2}{4R^3}(\xi^2 + \eta^2) \end{aligned}$$

Hence the Hamiltonian reads in terms of  $\xi, \eta$  as

$$\begin{aligned} \hat{H} &= -\frac{\hbar^2}{2\mu} \nabla_{\xi}^2 - \frac{\hbar^2}{2\mu} \nabla_{\eta}^2 + \frac{1}{2}k(\xi^2 + \eta^2) - \frac{e_M^2}{4R^3}(\xi^2 + \eta^2) \\ &= -\frac{\hbar^2}{2\mu} \nabla_{\xi}^2 + \frac{1}{2}k_{-}\xi^2 - \frac{\hbar^2}{2\mu} \nabla_{\eta}^2 + \frac{1}{2}k_{+}\eta^2 \end{aligned}$$

where

$$k_{\mp} = \frac{1}{2}k \left( 1 \mp \frac{e_M^2}{2kR^3} \right)$$

Clearly,  $\hat{H}$  now consists of two 3D harmonic oscillators, which are uncoupled and oscillating at two different frequencies. The energy eigenvalues are therefore given by

$$\begin{aligned} E_{n_1, n_2} &= \hbar\omega_{-} \left( n_{1x} + n_{1y} + n_{1z} + \frac{3}{2} \right) + \hbar\omega_{+} \left( n_{2x} + n_{2y} + n_{2z} + \frac{3}{2} \right) \\ n_{1x}, \dots, n_{2z} &= 1, 2, \dots \end{aligned}$$

The characteristic frequencies are given by

$$\omega_{\mp}^2 = \frac{k_{\mp}}{\mu}$$

Thus, the ground state energy reads as



$$E_{oo} = \frac{3}{2}(\hbar\omega_- + \hbar\omega_+)$$

Now,

$$\begin{aligned} \omega_{\mp} &= \left[ \frac{k/2}{m/2} \left( 1 \mp \frac{e_M^2}{2kR^3} \right) \right]^{1/2} \\ &= \omega_c \left[ 1 \mp \frac{1}{2} \frac{e_M^2}{2kR^3} + \frac{(1/2)(-1/2)}{2} \left( \frac{e_M^2}{2kR^3} \right)^2 + \dots \right] \end{aligned}$$

where

$$\omega_c \equiv (k/m)^{1/2}$$

Hence

$$E_{oo} = 3\hbar\omega_c - K \frac{1}{R^6} \text{----- (1)}$$

with

$$\begin{aligned} K &= \frac{3}{2} \hbar\omega_c \cdot \frac{1}{4} \cdot \left( \frac{e_M^2}{2k} \right)^2 \\ &= \frac{3\hbar\omega_c e_M^4}{32 k^2} \end{aligned}$$

The first term in (1) represents the ground state energy of two uncoupled 3D harmonic oscillators, while the second term represents Van der Waals attraction proportional to  $1/R^6$ .

12.6 (a) Given the Hamiltonian,

$$\begin{aligned} H &= H_0 + Eer \cos \theta \\ H_0 &= -\frac{\hbar^2}{2m} \nabla^2 - \frac{e_M^2}{r}, \quad e_M^2 = \frac{e^2}{4\pi\epsilon_0} \end{aligned}$$

and a trial wavefunction,

$$\varphi = c_1 |u_{100}\rangle + c_2 |u_{210}\rangle$$

with  $|u_{100}\rangle$ ,  $|u_{210}\rangle$  denoting the eigenfunctions of hydrogenic Hamiltonian,  $H_0$ , one can write the energy eigenequation as

$$\begin{aligned} H\varphi &= E_1 c_1 |u_{100}\rangle + Eer \cos \theta c_1 |u_{100}\rangle \\ &\quad + E_2 c_2 |u_{210}\rangle + Eer \cos \theta c_2 |u_{210}\rangle \\ &= E (c_1 |u_{100}\rangle + c_2 |u_{210}\rangle) \end{aligned}$$

Here use has been made of

$$H_0 |u_{100}\rangle = E_1 |u_{100}\rangle, \quad H_0 |u_{210}\rangle = E_2 |u_{210}\rangle$$

Rearranging, one can write

$$(E_1 - E + Eer \cos \theta) c_1 |u_{100}\rangle + (E_2 - E + Eer \cos \theta) c_2 |u_{210}\rangle = 0 \text{----- (1)}$$

Taking the inner product of (1) w.r.t.  $\langle u_{100} |$ ,  $\langle u_{210} |$ , there result

$$(E_1 - E)c_1 + m_{12}c_2 = 0 \text{ ----- (2a)}$$

$$m_{12}^* c_1 + (E_2 - E)c_2 = 0 \text{ ----- (2b)}$$

where

$$m_{12} = \langle u_{100} | Eer \cos \theta | u_{210} \rangle$$

$$m_{12}^* = \langle u_{210} | Eer \cos \theta | u_{100} \rangle$$

In deriving (2a) (2b) the orthonormality of  $|u_{100}\rangle$  and  $|u_{210}\rangle$  was used, i.e.  $\langle u_{100} | u_{100} \rangle = \langle u_{210} | u_{210} \rangle = 1$  and  $\langle u_{100} | u_{210} \rangle = 0$

(b) The coupled equations (2a),(2c) would yield trivial solutions, i.e.  $c_1 = c_2 = 0$ , hence trivial wavefunctions  $\varphi$ , unless the secular equation holds true:

$$\begin{vmatrix} E_1 - E & m_{12} \\ m_{12}^* & E_2 - E \end{vmatrix} = 0$$

Or expanding the determinant,

$$E^2 - (E_1 + E_2)E + E_1E_2 - |m_{12}|^2 = 0$$

The solution of this quadratic equation for  $E$  yields

$$\begin{aligned} E_{\pm} &= \frac{1}{2} \left\{ (E_1 + E_2) \pm \left[ (E_1 + E_2)^2 - 4(E_1E_2 - |m_{12}|^2) \right]^{\frac{1}{2}} \right\} \\ &= \frac{1}{2} \left\{ (E_1 + E_2) \pm \left[ (E_2 - E_1)^2 + 4|m_{12}|^2 \right]^{\frac{1}{2}} \right\} \\ &= \frac{1}{2} \left\{ (E_1 + E_2) \pm \left[ \Delta E^2 + 4|m_{12}|^2 \right]^{\frac{1}{2}} \right\} \text{ ----- (3)} \end{aligned}$$

with

$$\Delta E = E_2 - E_1$$

Inserting (3) into either (2a) or (2b) one finds  $c_1, c_2$ . For example, insert  $E_+$  into (2a), obtaining

$$\alpha_+ \equiv \frac{c_2}{c_1} \Big|_+ = -\frac{E_1 - E_+}{m_{12}} = \frac{\left[ \Delta E + \left( \Delta E^2 + 4|m_{12}|^2 \right)^{1/2} \right]}{2m_{12}} \text{ ----- (4a)}$$

Likewise, insert  $E_+$  into (2b) and obtain

$$\begin{aligned} \alpha_+ &\equiv \frac{c_2}{c_1} \Big|_+ = -\frac{m_{12}^*}{E_2 - E_+} \\ &= -\frac{2m_{12}^*}{\left[ \Delta E - \left( \Delta E^2 + 4|m_{12}|^2 \right)^{1/2} \right]} \text{ ----- (4b)} \end{aligned}$$

Indeed the right hand sides of (4a), (4b) are seen identical, as they should.

One can also find  $c_2$  in terms of  $c_1$  by inserting  $E_-$  in (3) into, say (2b) :

$$\alpha_- \equiv \frac{c_2}{c_1} \Big|_- = - \frac{2m_{12}^*}{\left[ \Delta E + \left( \Delta E^2 + 4|m_{12}|^2 \right)^{1/2} \right]}$$

Using (4), (5) one can write

$$\varphi_{\pm} = c_1 \left( |u_{100}\rangle + \alpha_{\pm} |u_{210}\rangle \right)$$

where  $c_1$  can be used for normalizing the wavefunction, if necessary.

(c) Consider first

$$\begin{aligned} \langle \varphi_{\pm} | \varphi_{\pm} \rangle &= |c_1|^2 \langle u_{100} + \alpha_{\pm} u_{210} | u_{100} + \alpha_{\pm} u_{210} \rangle \\ &= |c_1|^2 \left( 1 + |\alpha_{\pm}|^2 \right) \end{aligned}$$

Next, consider

$$\begin{aligned} \langle \underline{r}_{\pm} \rangle &= \langle \varphi_{\pm} | \underline{r} | \varphi_{\pm} \rangle \\ &= |c_1|^2 \langle u_{100} + \alpha_{\pm} u_{210} | \underline{r} | u_{100} + \alpha_{\pm} u_{210} \rangle \\ &= |c_1|^2 \left[ \alpha_{\pm} \langle u_{100} | \underline{r} | u_{210} \rangle + c.c. \right] \end{aligned}$$

Hence

$$\langle \underline{r}_{\pm} \rangle = \frac{\alpha_{\pm} \langle u_{100} | \underline{r} | u_{210} \rangle + c.c.}{1 + |\alpha_{\pm}|^2}$$

The atom – dipole is thus specified as

$$\mu_{ind} = -e \langle \underline{r}_{\pm} \rangle$$

and inasmuch as  $\alpha_{\pm} \propto E$ ,  $\mu_{ind} \propto E$  as expected.

## Chapter 13

13.1 The first order level shift and modification in the wave function are given from (13.18),(13.19) as

$$W_1 = \langle u_m | \hat{H}' | u_m \rangle \text{----- (1a)}$$

$$\varphi^{(1)} = |u_m\rangle + \sum_{k \neq m} \frac{\langle u_k | \hat{H}' | u_m \rangle}{E_m - E_k} \text{----- (1b)}$$

Given  $\hat{H}' = k_2 x^3 + k_3 x^4$ , the matrix elements  $\propto \langle u_k | x^3 | u_m \rangle, \langle u_k | x^4 | u_m \rangle$  have to be evaluated. In so doing the orthonormality of  $\{u_m\}$  and the recurrence relation, (8.32) can be usefully employed.

Repeating the relation (8.32) repeatedly, one can write

$$\begin{aligned} \xi H_m &= \frac{1}{2} H_{m+1} + m H_{m-1} \\ \xi^2 H_m &= \frac{1}{2} \left[ \frac{1}{2} H_{m+2} + (m+1) H_m \right] + m \left[ \frac{1}{2} H_m + (m-1) H_{m-2} \right] \\ &= \frac{1}{4} H_{m+2} + (m + \frac{1}{2}) H_m + m(m-1) H_{m-2} \\ \xi^3 H_m &= \frac{1}{4} \left[ \frac{1}{2} H_{m+3} + (m+2) H_{m+1} \right] + (m + \frac{1}{2}) \left[ \frac{1}{2} H_{m+1} + m H_{m-1} \right] \\ &\quad + m(m-1) \left[ \frac{1}{2} H_{m-1} + (m-2) H_{m-3} \right] \\ &= \frac{1}{8} H_{m+3} + \frac{3m+3}{4} H_{m+1} + \frac{3m^2}{2} H_{m-1} + m(m-1)(m-2) H_{m-3} \text{----- (2a)} \end{aligned}$$

$$\begin{aligned} \xi^4 H_m &= \frac{1}{16} H_{m+4} + \frac{1}{4} (2m+3) H_{m+2} + \frac{1}{4} (6m^2 + 6m + 3) H_m \\ &\quad + \frac{1}{2} (4m^3 - 6m^2 + 2m) H_{m-2} + m(m-1)(m-2)(m-3) H_{m-4} \text{----- (2b)} \end{aligned}$$

Hence (1a) can be evaluated by using (2a),(2b) and the orthonormality of  $\{u_m\}$  (see (8.38), (8.40)):

$$\begin{aligned} W_1 &= \int_{-\infty}^{\infty} dx u_m^* (k_2 x^3 + k_3 x^4) u_m \\ &= \frac{N_m^2 k_2}{\alpha^4} \int_{-\infty}^{\infty} d\xi e^{-\xi^2} H_m \xi^3 H_m + \frac{N_m^2 k_3}{\alpha^5} \int_{-\infty}^{\infty} d\xi e^{-\xi^2} H_m \xi^4 H_m, \quad \alpha \equiv \left( \frac{mw}{\hbar} \right)^{\frac{1}{2}} \\ &= \frac{N_m^2 k_3}{\alpha^5} \int_{-\infty}^{\infty} d\xi e^{-\xi^2} H_m^2 \frac{1}{4} (6m^2 + 6m + 3) \\ &= \frac{k_3}{\alpha^5} \cdot \frac{1}{4} (6m^2 + 6m + 3) \left( \frac{\alpha}{\sqrt{\pi} 2^m m!} \right) \sqrt{\pi} 2^m m! \end{aligned}$$

$$= \frac{k_3}{\alpha^4} \cdot \frac{1}{4} (6m^2 + 6m + 3) \text{----- (3)}$$

In evaluating (3), terms  $\propto$  to  $k_2$  simply do not contribute, since  $\xi^3 H_m$  does not yield any term  $\propto$  to  $H_m$ . For ground state, where  $m=0$ ,  $W_1 = 3k_3 / 4\alpha^4$ , while for the first excited state in which  $m = 1$ ,  $W_1 = 15k_3 / 4\alpha^4$ .

To find the first order modifications in wave function one has to find and evaluate the non-vanishing matrix elements,  $\langle u_k | \hat{H}' | u_m \rangle$  for given  $|u_m\rangle$ .

This can be readily done by noticing from (2a)  $k=m+3, m+1, m-1, m-3$  and from (2b)  $k=m+4, m+2, m-2, m-4$  and evaluate the corresponding elements in a similar manner.

For the ground state ( $m=0$ ), for instance, one can write for  $k=3$

$$\begin{aligned} & \langle u_3 | k_2 x^3 | u_0 \rangle \\ &= \frac{N_3 \cdot N_0}{\alpha^4} \int_{-\infty}^{\infty} d\xi e^{-\xi^2} H_3^2 / 8 \\ &= \frac{1}{8\alpha^4} \cdot \left( \frac{\alpha}{\sqrt{\pi} 2^3 3!} \right)^{\frac{1}{2}} \left( \frac{\alpha}{\sqrt{\pi}} \right)^{\frac{1}{2}} \sqrt{\pi} 2^3 3! \\ &= \frac{\sqrt{3}}{2\alpha^3} \end{aligned}$$

Thus, the modification to the ground state eigenfunction,  $|u_0\rangle$  resulting from  $|u_3\rangle$  is given from (13.19) by

$$\frac{\hat{H}'_{30}}{E_0 - E_3} |u_3\rangle = -\frac{\sqrt{3}}{2\alpha^3} \frac{1}{3\hbar\omega} |u_3\rangle$$

One can likewise find the modifications resulting from other terms.

13.2 (a) Without the perturbing term,  $\hat{H}'$ ,  $\hat{H}$  simply consists of 2D harmonic oscillator with  $k_x, k_y$  spring constants or  $\omega_x, \omega_y$  characteristic frequencies, i.e.

$$\hat{H} = -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + \frac{1}{2} k_x x^2 - \frac{\hbar^2}{2m} \frac{\partial^2}{\partial y^2} + \frac{1}{2} k_y y^2$$

Hence the energy eigenfunction is given by

$$\varphi(x, y) = u_{n_x}(\xi_x) u_{n_y}(\xi_y)$$

with

$$u_{n_x}(\xi_x) = N_{n_x} e^{-\frac{1}{2}\xi_x^2} H_{n_x}(\xi_x), \quad \xi_x = \alpha_x x$$

$$u_{n_y}(\xi_y) = N_{n_y} e^{-\frac{1}{2}\xi_y^2} H_{n_y}(\xi_y), \quad \xi_y = \alpha_y y$$

and

$$\alpha_j = (m\omega_j / \hbar)^{\frac{1}{2}}, \quad \omega_j^2 = k_j / m, \quad j = x, y$$

The eigenenergy reads as

$$E_{n_x, n_y} = \hbar \omega_x \left( n_x + \frac{1}{2} \right) + \hbar \omega_y \left( n_y + \frac{1}{2} \right)$$

with  $n_x, n_y = 0, 1, 2, \dots$

(b) The level shift due to the first order perturbation analysis,

$$W_1 = \left\langle u_{n_x}(\xi_x) u_{n_y}(\xi_y) \mid C_{xy} \mid u_{n_x}(\xi_x) u_{n_y}(\xi_y) \right\rangle$$

yields zero, i.e.  $W_1 = 0$ . This can be seen simply from the parity consideration or from the recurrence relation, (8.32). For instance, the right hand side of

$$x H_{n_x}(\xi) \propto \xi_x H_{n_x} = \frac{1}{2} H_{n_x+1} + n_x H_{n_x-1}$$

does not contain  $H_{n_x}$ , so that  $W_1 = 0$ . However, there is a level shift resulting from the second order perturbation analysis. This shift can be accounted for by the matrix elements considered in (8.51) :

$$\left\langle u_{n_x} \mid x \mid u_{n'_x} \right\rangle = \begin{cases} \frac{\sqrt{n_x+1}}{(2m\omega_x/\hbar)^{1/2}}, n'_x = n_x + 1 \\ \frac{\sqrt{n_x}}{(2m\omega_x/\hbar)^{1/2}}, n'_x = n_x - 1 \\ 0, \text{ otherwise} \end{cases} \text{----- (1)}$$

$$\left\langle u_{n_y} \mid y \mid u_{n'_y} \right\rangle = \begin{cases} \frac{\sqrt{n_y+1}}{(2m\omega_y/\hbar)^{1/2}}, n'_y = n_y + 1 \\ \frac{\sqrt{n_y}}{(2m\omega_y/\hbar)^{1/2}}, n'_y = n_y - 1 \\ 0, \text{ otherwise} \end{cases} \text{----- (2)}$$

Thus, given the state  $|u_{n_x}, u_{n_y}\rangle$  the level shift specified in (13.24) is obtained as

$$E_{n_x n_y}^{(2)} = \hbar \omega_x \left( n_x + \frac{1}{2} \right) + \hbar \omega_y \left( n_y + \frac{1}{2} \right) + \Delta E^{(2)}$$

$$\Delta E^{(2)} = \sum_{\substack{n'_x \neq n_x \\ n'_y \neq n_y}} \frac{\left| \left\langle u_{n'_x} u_{n'_y} \mid C_{xy} \mid u_{n_x, n_y} \right\rangle \right|^2}{[E_{n_x, n_y} - E_{n'_x, n'_y}]^2}$$

Here  $\Delta E^{(2)}$  is contributed by 4 combinations of the eigenfunctions  $|u_{n_x \pm 1}, u_{n_y \pm 1}\rangle$  :

$$\begin{aligned}
\Delta E^{(2)} &= \frac{\left| \langle u_{nx+1,ny+1} | C_{xy} | u_{nx,ny} \rangle \right|^2}{E_{nx,ny} - E_{nx+1,ny+1}} + \frac{\left| \langle u_{nx+1,ny-1} | C_{xy} | u_{nx,ny} \rangle \right|^2}{E_{nx,ny} - E_{nx+1,ny-1}} \\
&+ \frac{\left| \langle u_{nx-1,ny+1} | C_{xy} | u_{nx,ny} \rangle \right|^2}{E_{nx,ny} - E_{nx-1,ny+1}} + \frac{\left| \langle u_{nx-1,ny-1} | C_{xy} | u_{nx,ny} \rangle \right|^2}{E_{nx,ny} - E_{nx-1,ny-1}} \\
&= -\frac{C^2 \frac{n_x+1}{(2m\omega_x/\hbar)} \cdot \frac{n_y+1}{(2m\omega_y/\hbar)}}{\hbar\omega_x + \hbar\omega_y} + \frac{C^2 \frac{n_x+1}{(2m\omega_x/\hbar)} \cdot \frac{n_y}{(2m\omega_y/\hbar)}}{\hbar\omega_y - \hbar\omega_x} \\
&+ \frac{C^2 \frac{n_x}{(2m\omega_x/\hbar)} \cdot \frac{n_y+1}{(2m\omega_y/\hbar)}}{\hbar\omega_x - \hbar\omega_y} + \frac{C^2 \frac{n_x}{(2m\omega_x/\hbar)} \cdot \frac{n_y}{(2m\omega_y/\hbar)}}{\hbar\omega_x + \hbar\omega_y} \\
&= \frac{C^2 \hbar}{4m^2 \omega_x \omega_y} \left[ -\frac{(n_x+1)(n_y+1)}{\omega_x + \omega_y} + \frac{n_x(n_y+1) - (n_x+1)n_y}{\omega_x - \omega_y} + \frac{n_x n_y}{\omega_x + \omega_y} \right]
\end{aligned}$$

For the ground level in which  $n_x = n_y = 0$  there is only one state contributing to  $\Delta E^{(2)}$ , i.e.  $|u_{nx+1,ny+1}\rangle$ , so that one can write

$$\Delta E^{(2)} = -\frac{C^2}{4m^2 \omega_x \omega_y} \frac{1}{(\omega_x + \omega_y)}$$

and up to the second order perturbation analysis

$$E_{00} = \frac{\hbar}{2}(\omega_x + \omega_y) - \frac{C^2}{4m^2 \omega_x \omega_y (\omega_x + \omega_y)} \quad (3)$$

(c) Introduce  $\xi$ ,  $\eta$  as

$$\begin{aligned}\xi &= x + y \\ \eta &= x - y\end{aligned}$$

One can invert the relation, obtaining

$$\begin{aligned}x &= \frac{1}{2}(\xi + \eta) \\ y &= \frac{1}{2}(\xi - \eta)\end{aligned}$$

and write as usual

$$-\frac{\hbar^2}{2m} \left( \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} \right) = -\frac{\hbar^2}{2\mu} \left( \frac{\partial^2}{\partial \xi^2} + \frac{\partial^2}{\partial \eta^2} \right), \quad \mu = m/2 \quad (4)$$

and

$$\begin{aligned}&\frac{1}{2}k_x x^2 + \frac{1}{2}k_y y^2 + Cxy \\ &= \frac{1}{2}k_x \frac{1}{4}(\xi^2 + \eta^2 + 2\xi\eta) + \frac{1}{2}k_y \frac{1}{4}(\xi^2 + \eta^2 - 2\xi\eta) + C \frac{1}{4}(\xi^2 - \eta^2)\end{aligned}$$

$$\simeq \frac{1}{2} \frac{1}{4} (\xi^2 + \eta^2)(k_x + k_y) + \frac{1}{4} C(\xi^2 - \eta^2) \text{----- (5)}$$

where for simplicity an assumption was made, i.e  $k_x \simeq k_y$ , so that  $2\xi\eta(k_x - k_y) \approx 0$ .

With the use of (4),(5) the total Hamiltonian reads as

$$\begin{aligned} \hat{H} &= -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + \frac{1}{2} k_x x^2 - \frac{\hbar^2}{2m} \frac{\partial^2}{\partial y^2} + \frac{1}{2} k_y y^2 + Cxy \\ &= -\frac{\hbar^2}{2\mu} \frac{\partial^2}{\partial \xi^2} + \frac{1}{2} k_+ \xi^2 - \frac{\hbar^2}{2\mu} \frac{\partial^2}{\partial \eta^2} + \frac{1}{2} k_- \eta^2 \text{----- (6a)} \end{aligned}$$

with

$$k_{\pm} = \frac{1}{2} \left[ \frac{1}{2} (k_x + k_y) \pm C \right] \text{----- (6b)}$$

It is therefore clear from (6) that the two coupled harmonic oscillator system becomes decoupled into two independent oscillators with two different effective spring constants,  $k_{\pm}$ .

Hence the energy eigenvalues are given by

$$E_{n_{\xi}, n_{\eta}} = \hbar\omega_+ \left( n_{\xi} + \frac{1}{2} \right) + \hbar\omega_- \left( n_{\eta} + \frac{1}{2} \right)$$

where

$$\begin{aligned} \omega_{\pm} &= (k_{\pm} / \mu)^{\frac{1}{2}} \\ &= \left\{ \frac{\left[ \frac{1}{2} \left[ \frac{1}{2} (k_x + k_y) \pm C \right] \right]}{\mu} \right\}^{1/2} \\ &= \left[ \frac{\frac{1}{2} (k_x + k_y)}{m} \pm \frac{C}{m} \right]^{1/2} \\ &= \left[ \frac{1}{2} (\omega_x^2 + \omega_y^2) \pm \frac{C}{m} \right]^{1/2} \text{----- (7)} \end{aligned}$$

Hence the ground state level is given by

$$E_{00} = \frac{\hbar}{2} (\omega_+ + \omega_-) \text{----- (8)}$$

To compare the above two results (3),(8) one may expand (7) as

$$\begin{aligned} \omega_{\pm} &= \sqrt{\langle \omega^2 \rangle} \left[ 1 \pm \frac{C}{m \langle \omega^2 \rangle} \right]^{1/2} \\ &= \sqrt{\langle \omega^2 \rangle} \left[ 1 \pm \frac{1}{2} \frac{C}{m \langle \omega^2 \rangle} - \frac{1}{4} \frac{C^2}{m^2 \langle \omega^2 \rangle^2} + \dots \right] \end{aligned}$$

with



$$\langle \omega^2 \rangle \equiv \frac{\omega_x^2 + \omega_y^2}{2}$$

Hence

$$E_{00} = \frac{\hbar}{2} \sqrt{\langle \omega^2 \rangle} - \frac{\hbar C^2}{4m^2} \frac{1}{\langle \omega^2 \rangle^{3/2}} \dots \dots \dots (9)$$

and, with the identification

$$\sqrt{\langle \omega^2 \rangle} \approx \omega_x + \omega_y$$

(3) and (9) are in rough agreement, in particular the level shift.

13.3 (a) In the presence of external field, E, the electron is subject to force  $-eE$ . Thus, the corresponding potential energy is given by

$$V = -(-eE) \cdot x = eEx$$

with  $V(x=0) = 0$

(b) The ground state wave function of the infinite potential well is given from (4.8) by

$$u_1(x) = \left(\frac{2}{W}\right)^{\frac{1}{2}} \cos \frac{\pi}{L} x, \quad -\frac{W}{2} \leq x \leq \frac{W}{2}$$

with the energy eigenvalue given from (4.8) by

$$E_1 = \frac{\hbar^2 \pi^2}{2mW^2}$$

Thus, from parity consideration one can write

$$\langle u_0 | eEx | u_0 \rangle = 0,$$

That is, there is no first order level shift.

To obtain the second order level shift one has to consider the matrix element,

$$\langle u_n | eEx | u_1 \rangle$$

where  $|u_n\rangle$  consists of two sets of eigenfunctions,  $\{\cos k_n x\}$  and  $\{\sin k_n x\}$  (see (4.7)).

However, in the light of the parity consideration, only the latter set yields nonzero matrix elements. Thus, consider

$$\begin{aligned} & \langle u_n | eEx | u_1 \rangle \\ &= \frac{2}{W} eE \int_{-W/2}^{W/2} dx \cos\left(\frac{\pi x}{W}\right) \sin\left(\frac{2n\pi}{W} x\right) \cdot x \dots \dots \dots (1) \end{aligned}$$

Now, with the use of the trigonometric identity

$$\sin(a \pm b)x = \sin ax \cos bx \pm \cos ax \sin bx$$

one can write

$$\cos\left(\frac{\pi x}{W}\right) \sin\left(\frac{2n\pi x}{W}\right) = \frac{1}{2} \left[ \sin \frac{\pi}{W} (1+2n)x - \sin \frac{\pi}{W} (1-2n)x \right]$$

and evaluate the integral in (1):

$$\begin{aligned}
& \int_{-W/2}^{W/2} dx \cos\left(\frac{\pi x}{W}\right) \sin\left(\frac{2n\pi x}{W}\right) \cdot x \\
&= \sum_{\pm} \frac{1}{2} \int_{-W/2}^{W/2} dx \sin\left[\frac{\pi}{W}(1 \pm 2n)x\right] \cdot x \\
&= \sum_{\pm} \left\{ \frac{1}{\left[\frac{\pi}{W}(1 \pm 2n)\right]^2} \sin\left[\frac{\pi}{W}(1 \pm 2n)x\right] - \frac{x}{\frac{\pi}{W}(1 \pm 2n)} \cos\left[\frac{\pi}{W}(1 \pm 2n)x\right] \right\}_{-W/2}^{W/2} \\
&= \frac{2W^2}{\pi^2} \left[ \frac{1}{(1+2n)^2} + \frac{1}{(1-2n)^2} \right] \\
&= \frac{4W^2}{\pi^2} \frac{1+4n^2}{(1-4n^2)^2}
\end{aligned}$$

Hence, inserting this result into (1) and using (13.27) in the text,

$$\Delta E^{(2)} = E_1 + \frac{8e^2 E^2 W^2}{\pi^2} \sum_{n \neq 0} \frac{1+4n^2}{(1-4n^2)^2} \cdot \frac{1}{E_0 - E_n}$$

with

$$E_n = \frac{\hbar^2 \pi^2}{2mW^2} n^2$$

For the first excited state,  $u_2$  there is again no first order level shift, i.e.

$$E_1 = \langle u_2 | eEx | u_2 \rangle = 0$$

But, there exists the second order level shift, the analysis of which can be carried out in a way similar to the of the ground state,  $|u_1\rangle$ .

13.4 (a) Given  $|u_{nlm}\rangle$  and the perturbing Hamiltonian  $\hat{H}' \propto z \propto \cos\theta$  one has to find  $|u_{n'l'm'}\rangle$  such that

$$\langle u_{nlm} | \hat{H}' | u_{n'l'm'} \rangle \neq 0$$

The evaluation of this matrix element requires both angular  $(\theta, \varphi)$  and radial  $(r)$  integrations. Here, the angular integration determines whether or not the matrix element becomes zero. Thus, one has to consider

$$\int_0^{2\pi} d\varphi \int_0^\pi \sin\theta d\theta Y_{lm}^* \cos\theta Y_{l'm'} = \int_0^{2\pi} d\varphi \int_{-1}^1 d\mu Y_{lm}^* \mu Y_{l'm'}, \quad \mu = \cos\theta$$

Since  $Y_{lm} \propto \exp\pm im\varphi$ , for the  $\varphi$ -integration not to yield zero one should have  $m = m'$ . Since  $\cos\theta \propto P_1$  and is odd in parity, the product  $P_l P_{l'}$  should also be odd in parity for the  $\theta$ -integration not to yield zero. This requires  $l - l' = \pm 1$ .

Hence the selection rule requires

$$\Delta m = m - m' = 0$$

$$\Delta l = l - l' = \pm 1$$

(b) For the perturbing Hamiltonian

$$\begin{aligned}\hat{H}' &= exE_0 \cos \omega t \\ &= er \sin \theta \cos \phi E_0 \cos \omega t\end{aligned}$$

the selection rule is determined again by the angular integrations:

$$\begin{aligned}\langle u_{nlm} | \hat{H}' | u_{n'l'm'} \rangle \\ \propto \int_0^{2\pi} d\phi \int_{-1}^1 d\mu Y_{lm}^* \sin \theta \cos \phi Y_{l'm'}, \quad \mu = \cos \theta\end{aligned}$$

The integrand of the  $\phi$ -integral reads as

$$\begin{aligned}e^{i(m'-m)\phi} \cdot (e^{i\phi} + e^{-i\phi}) / 2 \\ \propto e^{i(m'-m+1)\phi} + e^{i(m'-m-1)\phi}\end{aligned}$$

and in order for the  $\phi$ -integration not to vanish

$$\Delta m = m' - m = \pm 1.$$

Also, since  $\sin \theta = \sqrt{1 - \cos^2 \theta} = \sqrt{1 - \mu^2}$  the  $\mu$ -integration does not vanish when the product  $P_l^m P_l^{m'}$  possesses an even parity, i.e.

$$\Delta l = l - l' = 0, 2, \dots$$

13.5 (a) In the presence of a harmonic field,

$$E = E_0 \cos \omega t$$

the electron is subject to force,

$$f = qE$$

and the corresponding potential energy or the perturbing Hamiltonian is given by

$$\hat{H}' = \int_0^x (-f) dx = -qEx = -\frac{qE_0 x}{2} (e^{i\omega t} + e^{-i\omega t}) \text{----- (1)}$$

where the potential at  $x=0$  has been taken zero.

(b) The oscillator initially at the state, say  $|u_n\rangle$  can therefore be induced to make a transition to other state by  $\hat{H}'$ . The transition rate can be analyzed using (13.50) in the text:

$$\dot{a}_{n'} = -\frac{i}{\hbar} \hat{H}'_{n'n} e^{i\omega_{n'n} t} \text{----- (2)}$$

where

$$\hat{H}' = \langle u_{n'} | \hat{H}' | u_n \rangle$$

is the transition matrix under consideration and

$$\omega_{n'n} = \frac{1}{\hbar} (E_{n'} - E_n)$$

is the transition frequency between the initial and final states and  $a_{n'}(t)$  is the expansion coefficient of the final state.

Next, using (1) for  $\hat{H}'$  and (8.40) in the text for harmonic oscillator eigenfunctions,  $u_n, u_{n'}$ , one can write

$$\langle u_{n'} | \hat{H}' | u_n \rangle = \langle u_n | \hat{H}' | u_{n'} \rangle$$

$$\begin{aligned}
&= -\frac{qE_0}{2}(e^{i\omega t} + e^{-i\omega t}) \int_{-\infty}^{\infty} dx u_n x u_{n'} \\
&= -\frac{qE_0}{2}(e^{i\omega t} + e^{-i\omega t}) \begin{cases} (n+1)^{1/2} / (2m\omega_c / \hbar)^{1/2}, & n' = n+1 \text{ ----- (3)} \\ n^{1/2} / (2m\omega_c / \hbar)^{1/2} & , n' = n-1 \\ 0 & \text{otherwise} \end{cases}
\end{aligned}$$

where use has been made of the matrix element (8.51) with  $\omega_c$  denoting the characteristic frequency of the oscillator.

Inserting (3) into (2) and performing the time integration, there results

$$a_{n'}(t) = -\frac{qE_0}{2\hbar} \left( \frac{n'}{2m\omega_c / \hbar} \right)^{1/2} \cdot \int_0^t dt' \left[ e^{i(\omega + \omega_{n'n})t'} + e^{-i(\omega - \omega_{n'n})t'} \right] \text{----- (4)}$$

where

$$n' = n \pm 1$$

Thus,

$$\begin{aligned}
\omega_{n'n} &\equiv \frac{1}{\hbar} (E_{n'} - E_n) \\
&= \frac{1}{\hbar} \left[ \hbar\omega_c \left( n' + \frac{1}{2} \right) - \hbar\omega_c \left( n + \frac{1}{2} \right) \right] \\
&= \omega_c (n' - n) \\
&= \pm \omega_c, \quad \omega_c^2 \equiv k/m
\end{aligned}$$

depending on whether  $n' = n+1$  or  $n' = n-1$ .

Now consider the resonant interaction between the field and oscillator, in which the oscillator frequency,  $\omega_c$  and the driving frequency,  $\omega$  are nearly equal to each other.

Then for  $n' = n+1$ ,  $\omega + \omega_c \gg \omega - \omega_c$  and one can neglect the fast oscillating term in (4). By the same token, for  $n' = n-1$ , one can neglect the term,  $\exp -i(\omega - \omega_c)t$ . With this fact in mind, one can perform the integration in (4), obtaining

$$\begin{aligned}
a_{n'}(t) &= -\frac{qE_0}{2} \left( \frac{n'}{2m\omega_c / \hbar} \right)^{1/2} \cdot \frac{1}{(\pm i)(\omega - \omega_c)} \left[ e^{\pm i(\omega - \omega_c)t} - 1 \right] \\
&= -\frac{qE_0}{2} \left( \frac{n'}{2m\omega_c / \hbar} \right)^{1/2} 2e^{\pm i(\omega - \omega_c)t/2} \frac{\sin(\omega - \omega_c)t}{(\omega - \omega_c)} \text{----- (5)}
\end{aligned}$$

Inserting (5) into (4) one finds

$$a_{n'}(t) = -\frac{qE_0}{\hbar} \cdot e^{\pm i(\omega - \omega_c)t/2} \frac{\sin(\omega - \omega_c)t}{(\omega - \omega_c)} \begin{cases} \frac{(n+1)^{1/2}}{(2m\omega_c / \hbar)^{1/2}}, & n' = n+1 \\ \frac{n^{1/2}}{(2m\omega_c / \hbar)^{1/2}}, & n' = n-1 \end{cases}$$

The probability of the oscillator making the transition from  $n$  to  $n'$  states at  $t = \pi / \omega$  is thus obtained by putting  $t = \pi / \omega$ , i.e.  $|a_{n'}(\pi / \omega)|^2$ . For the case of resonant interaction, in which  $\omega - \omega_c = 0$ ,  $\sin[(\omega - \omega_c)t] / (\omega - \omega_c)t = 1$  and one can write

$$|a_{n'}(t)|^2 = \frac{q^2 E_0^2 (\pi / \omega)^2}{2m\omega_c \hbar} \begin{cases} n+1, & n' = n+1 \\ n, & n' = n-1 \end{cases}$$

13.6 Given a circularly polarized light,

$$\underline{E} = E_0 (\hat{x} \cos \omega t + \hat{y} \sin \omega t)$$

the electron is subject to force

$$\underline{f} = -e\underline{E}$$

and the corresponding potential energy or  $\hat{H}'$  is to be found in a manner similar to the problem (13.5). One can thus write

$$\begin{aligned} \hat{H}' &= -eE_0 (x \cos \omega t + y \sin \omega t) \\ &= -eE_0 r \sin \theta (\cos \varphi \cos \omega t + \sin \varphi \sin \omega t) \end{aligned}$$

Given  $\hat{H}'$  one should find  $u_{n'l'm'}$  such that

$$\langle u_{nl0} | \hat{H}' | u_{n'l'm'} \rangle \neq 0 \text{ ----- (1)}$$

Again the condition (1) is determined by the angular integrations. For the case of the first term of  $\hat{H}'$  one should consider

$$\begin{aligned} &\langle u_{nl0} | \sin \theta \cos \varphi | u_{n'l'm'} \rangle \\ &= \int_0^{2\pi} d\varphi \cos \varphi \int_{-1}^1 d\mu \sin \theta Y_{l0}^* Y_{l'm'}, \quad \mu = \cos \theta \end{aligned}$$

Since  $Y_{l0}^*$  is independent of  $\varphi$  and since  $\cos \varphi = (e^{i\varphi} + e^{-i\varphi})/2$  in order for the  $\varphi$ -integration not to yield zero,  $m' = \pm 1$ . That is

$$\Delta m = 0 - m' = \pm 1$$

Also, since  $\sin \theta = (1-u^2)^{1/2}$ , for the  $\theta$ -integration not to vanish,  $P_l \times P_{l'}$  should have an even parity. Hence

$$\Delta l = l - l' = 0, \pm 2, \dots$$

One can similarly find the selection rule for the second term in  $\hat{H}'$ ,  $\propto \sin \theta \sin \varphi$ . That is,

$$\Delta m = 0 - m' = \pm 1$$

$$\Delta l = l - l' = 0, \pm 2, \dots$$

## Chapter 14

14.1 (a) Consider for example the matrix element

$$\begin{aligned} \langle u_{32m} | z | u_{21m'} \rangle &= \langle u_{32m} | r \cos \theta | u_{21m'} \rangle \\ &\propto \int_0^{2\pi} d\varphi \int_{-1}^1 d\mu \mu Y_{2m}^* Y_{1m'} , \quad \mu = \cos \theta \end{aligned}$$

Thus, for the  $\varphi$ -integration to yield non-zero value,  $\Delta m \equiv m - m' = 0$ , and therefore

(i)  $Y_{20}^* Y_{10}$ , (ii)  $Y_{2\pm 1}^* Y_{1\pm 1}$  are the possible contributing combinations.

For the  $\mu$ -integration to give non-zero value the two spherical harmonics should provide odd parity in  $\mu$ . The combinations, (i), (ii) satisfy this condition (see Table 9.1 in the text).

Hence one can write for the case (i)

$$\begin{aligned} &\langle u_{320} | r \cos \theta | u_{210} \rangle \\ &= N_{320} N_{210} \cdot \int_0^{2\pi} d\varphi \int_{-1}^1 d\mu \mu^2 (3\mu^2 - 1) \int_0^\infty r^2 dr r \left( \frac{r}{a_0} \right)^3 e^{-\frac{r}{a_0} \left( \frac{1}{2} + \frac{1}{3} \right)} \\ &= \left( \frac{1}{a_0} \right)^{3/2} \cdot \frac{1}{(32\pi)^{1/2}} \frac{1}{(a_0)^{3/2}} \frac{1}{81 \cdot (6\pi)^{1/2}} 2\pi \cdot \frac{8}{15} \left( \frac{6a_0}{5} \right)^7 6! \\ &= 0.82 a_0 \end{aligned}$$

Also, for the case (ii)

$$\begin{aligned} &\langle u_{32\pm 1} | r \cos \theta | u_{21\pm 1} \rangle \\ &= N_{32\pm 1} N_{21\pm 1} \cdot \int_0^{2\pi} d\varphi \int_{-1}^1 d\mu \mu^2 (1 - \mu^2) \cdot \int_0^\infty r^2 dr e^{-\frac{r}{a_0} \left( \frac{5}{6} \right)} \left( \frac{r}{a_0} \right)^3 \cdot r \\ &= \left( \frac{1}{a_0} \right)^{3/2} \cdot \frac{1}{(32\pi)^{1/2}} \left( \frac{1}{a_0} \right)^{3/2} \frac{1}{81 \cdot (6\pi)^{1/2}} 2\pi \cdot \frac{4}{15} \left( \frac{6a_0}{5} \right)^7 6! \\ &= 1.78 a_0 \end{aligned}$$

Thus, the average atom dipole moment associated with the transitions from  $|u_{32m}\rangle$  to  $|u_{21m'}\rangle$  is given by

$$\begin{aligned} \tilde{\mu} &= e \frac{1}{3} \left[ \langle u_{320} | r \cos \theta | u_{210} \rangle + \langle u_{321} | r \cos \theta | u_{211} \rangle + \langle u_{32-1} | r \cos \theta | u_{21-1} \rangle \right] \text{----- (1)} \\ &= 1.46 e a_0 \end{aligned}$$

One can evaluate  $\langle u_{32m} | x | u_{21m'} \rangle, \langle u_{32m} | y | u_{21m'} \rangle$  in a similar manner.

Based on the result of (1) one can estimate the spontaneous lifetime as follows. The total spontaneous transition rate is given from (14.58) by

$$W_{sp} = \frac{16\pi^3 \tilde{\mu}^2 \nu_0^3}{\epsilon_0 h c^3}$$

where

$$\nu_0 = \frac{E_3 - E_2}{h} = \frac{13.6eV}{h} \left( \frac{1}{2^2} - \frac{1}{3^2} \right) = 2.87 \times 10^{15} / s$$

is the transition frequency. Inserting  $\tilde{\mu}$  and  $\nu_0$  thus found one can evaluate  $W_{sp}$  :

$$W_{sp} = \frac{64\pi^4 \cdot 8.98 \times 10^9 (1.6 \times 10^{-19})^2 (1.46 \times 0.05 \cdot 10^{-9})^2 (2.87 \times 10^{15})^3}{6.626 \times 10^{-34} \cdot (3 \times 10^8)^3} \\ \cong 1 \times 10^{10} / s$$

where the Coulomb constant ( $=1/4\pi\epsilon_0$ ) has been used.

Hence the spontaneous lifetime of  $|u_{32m}\rangle$  state is  $\sim 1/W_{sp} = 0.1 ns$

(b) For  $n=2$ ,  $\ell=1$ ,  $|p_x\rangle$ ,  $|p_y\rangle$ ,  $|p_z\rangle$  states are given from (10.55), (10.56) and table 10.1 in the text as

$$|p_x\rangle = \left( \frac{3}{4\pi} \right)^{1/2} \sin\theta \cos\phi R_{21}(r)$$

$$|p_y\rangle = \left( \frac{3}{4\pi} \right)^{1/2} \sin\theta \sin\phi R_{21}(r)$$

$$|p_z\rangle = \left( \frac{3}{4\pi} \right)^{1/2} \cos\theta R_{21}(r)$$

$$\text{with } R_{21}(\rho) = \left( \frac{1}{a_0} \right)^{3/2} \left( \frac{1}{24} \right)^{1/2} \rho e^{-\rho/2}, \quad \rho = \frac{2 \cdot r}{a_0 \cdot 2}$$

Consider for example  $|p_z\rangle$  state making a spontaneous transition to the ground state,  $|u_{100}\rangle$ :

$$\langle p_z | z | u_{100} \rangle = \langle p_z | r \cos\theta | u_{100} \rangle \\ = \left( \frac{3}{4\pi} \right)^{1/2} \left( \frac{1}{a_0} \right)^{3/2} \left( \frac{1}{24} \right)^{1/2} \left( \frac{1}{a_0} \right)^{3/2} \frac{1}{\sqrt{\pi}} \int_0^{2\pi} d\phi \int_{-1}^1 d\mu \mu^2 \int_0^\infty dr r^2 \left( \frac{r}{a_0} \right) e^{-\frac{r}{a_0}(1+\frac{1}{2})} r \\ = 0.37 a_0 \approx 0.019 nm$$

The corresponding spontaneous transition rate is given by

$$W_{sp} = \frac{16\pi^3 \tilde{\mu}^2 \nu_0^3}{\epsilon_0 h c^3}$$

where

$$\tilde{\mu} = e \cdot 0.37 a_0$$

and

$$\nu_0 = \frac{E_2 - E_1}{h} = \frac{13.6}{h} \left( 1 - \frac{1}{2^2} \right) eV$$

Inserting these values into  $W_{sp}$  one finds  $W_{sp} \approx 1 \times 10^{11} / s$

Hence, the spontaneous lifetime is about 0.01 ns.

14.2 (a) The Hamiltonian consists of two terms

$$\hat{H} = \hat{H}_0 + \hat{H}'(t) \text{----- (1a)}$$

where the dipole interaction term is given in terms of the electric field with the polarization vector  $\hat{e}_f$  and the electron displacement from the nucleus,  $\underline{r}$ :

$$\hat{H}'(t) = -\hat{\mu}E(t), \quad \hat{\mu} = e(\underline{e}_f \cdot \underline{r}) \text{----- (1b)}$$

The wavefunction is then to be expanded in terms of the two energy eigenstates interacting with the field, i.e.

$$\psi(\underline{r}, t) = a_1(t)e^{-i\omega_1 t} |1\rangle + a_2(t)e^{-i\omega_2 t} |2\rangle \text{----- (2)},$$

The Schrödinger equation reads as

$$\begin{aligned} i\hbar \dot{a}_1(t) e^{-i\omega_1 t} |1\rangle + \hbar\omega_1 a_1(t) e^{-i\omega_1 t} |1\rangle + i\hbar \dot{a}_2(t) e^{-i\omega_2 t} |2\rangle + \hbar\omega_2 a_2(t) e^{-i\omega_2 t} |2\rangle \\ = (\hat{H}_0 + \hat{H}_1) [a_1(t) e^{-i\omega_1 t} |1\rangle + a_2(t) e^{-i\omega_2 t} |2\rangle] \text{----- (3)} \\ = (E_1 + \hat{H}') a_1(t) e^{-i\omega_1 t} |1\rangle + (E_2 + \hat{H}') a_2(t) e^{-i\omega_2 t} |2\rangle \end{aligned}$$

With the identification,  $E_1 = \hbar\omega_1$ ,  $E_2 = \hbar\omega_2$  (3) reduces to

$$\begin{aligned} i\hbar [\dot{a}_1(t) e^{-i\omega_1 t} |1\rangle + \dot{a}_2(t) e^{-i\omega_2 t} |2\rangle] \\ = \hat{H}' [a_1(t) e^{-i\omega_1 t} |1\rangle + a_2(t) e^{-i\omega_2 t} |2\rangle] \text{----- (4)} \end{aligned}$$

Perform the inner product on both sides of (4) w.r.t.  $|1\rangle$  and  $|2\rangle$ , obtaining

$$i\hbar \dot{a}_1(t) e^{-i\omega_1 t} = \langle 1 | \hat{H}' | 2 \rangle a_2(t) e^{-i\omega_2 t} \text{----- (5a)}$$

$$i\hbar \dot{a}_2(t) e^{-i\omega_2 t} = \langle 2 | \hat{H}' | 1 \rangle a_1(t) e^{-i\omega_1 t} \text{----- (5b)}$$

Here use has been made of

$$\langle 1 | 2 \rangle = \langle 2 | 1 \rangle = 0$$

Also one can write

$$\begin{aligned} \langle 1 | \hat{H}' | 2 \rangle &= \langle 2 | \hat{H}' | 1 \rangle \\ &= -\tilde{\mu} E(t) \end{aligned}$$

where

$$\tilde{\mu} \equiv e \langle 1 | \underline{e}_f \cdot \underline{r} | 2 \rangle$$

Thus, (5) can be put into

$$\begin{aligned} \dot{a}_1(t) &= i \frac{\tilde{\mu} E(t)}{\hbar} e^{-i\omega_0 t} a_2(t) \\ \dot{a}_2(t) &= i \frac{\tilde{\mu} E(t)}{\hbar} e^{-i\omega_0 t} a_1(t) \end{aligned} \text{----- (6)}$$

where

$$\omega_0 \equiv \omega_2 - \omega_1$$

represents the atomic transition frequency.

(b) In Schrödinger picture, the wave function is represented by

$$\psi(\underline{r}, t) = a_{1s}(t) |1\rangle + a_{2s}(t) |2\rangle$$



and the Schrödinger equation now reads as

$$\begin{aligned} & i\hbar[\dot{a}_{1s}(t)|1\rangle + \dot{a}_{2s}(t)|2\rangle] \\ & = E_1 a_{1s}(t)|1\rangle + E_2 a_{2s}(t)|2\rangle + \hat{H}'(a_{1s}(t)|1\rangle + a_{2s}(t)|2\rangle) \end{aligned} \quad (7)$$

Performing the inner product on both sides of (7) w.r.t  $|1\rangle$  and  $|2\rangle$ , one obtains

$$\begin{aligned} i\hbar \dot{a}_{1s}(t) &= E_1 a_{1s}(t) - \tilde{\mu} E(t) a_{2s}(t) \\ i\hbar \dot{a}_{2s}(t) &= E_2 a_{2s}(t) - \tilde{\mu} E(t) a_{1s}(t) \end{aligned}$$

Or equivalently,

$$\dot{a}_{1s}(t) = -i\omega_1 a_{1s}(t) + i \frac{\tilde{\mu} E(t)}{\hbar} a_{2s}(t) \quad (8a)$$

$$\dot{a}_{2s}(t) = -i\omega_2 a_{2s}(t) + i \frac{\tilde{\mu} E(t)}{\hbar} a_{1s}(t) \quad (8b)$$

with  $\omega_j = E_j / \hbar$ ,  $j = 1, 2$

Introduce

$$a_{js}(t) = a_j(t) e^{-i\omega_j t} \quad (9)$$

Then

$$\dot{a}_{js}(t) = \dot{a}_j(t) e^{-i\omega_j t} - i\omega_j a_j(t) e^{-i\omega_j t} \quad (10)$$

Inserting (9),(10) into (8) one obtains the coupled equation identical to (6).

(c) Note from (9) that

$$|a_{js}(t)|^2 = |a_j(t)|^2, \quad j = 1, 2$$

which points to the fact that the probability of finding the system in the  $j$ -th state is the same in both Schrödinger and interaction pictures.

Also, the atom dipole moment,  $\tilde{\mu} = e \langle \underline{r} \rangle$  is described by

$$\tilde{\mu} \propto \langle \psi | \underline{r} | \psi \rangle$$

In Schrödinger picture one can write

$$\begin{aligned} \langle \underline{r} \rangle &= \langle (a_{1s}^* u_1 + a_{2s}^* u_2) | \underline{r} | (a_{1s} u_1 + a_{2s} u_2) \rangle \\ &= a_{1s}^* a_{2s} \langle 1 | \underline{r} | 2 \rangle + c.c. \end{aligned} \quad (11)$$

In interaction picture,

$$\begin{aligned} \langle \underline{r} \rangle &= \langle (a_1^* e^{i\omega_1 t} u_1 + a_2^* e^{i\omega_2 t} u_2) | \underline{r} | (a_1 e^{-i\omega_1 t} u_1 + a_2 e^{-i\omega_2 t} u_2) \rangle \\ &= a_1^* a_2 e^{-i\omega_0 t} \langle 1 | \underline{r} | 2 \rangle + c.c. \end{aligned} \quad (12)$$

and in view of (9), (11) and (12) are identical.

14.3 Given the coupled equations

$$\dot{a}'_1 = i\Omega a'_2 e^{i\Lambda t} \quad (1a)$$

$$\dot{a}'_2 = i\Omega a'_1 e^{-i\Lambda t} \quad (1b)$$

with

$$\Omega \equiv \frac{\tilde{\mu}E_0}{2\hbar}, \quad \Lambda \equiv \Delta - i(\gamma_1 - \gamma_2),$$

look for the solution in the form

$$a_1(t) \sim e^{iSt} \text{ ----- (2)}$$

Inserting (2) into (1a)

$$iS e^{iSt} = i\Omega a_2' e^{i\Lambda t}$$

Hence

$$a_2(t) = \frac{S}{\Omega} e^{i(S-\Lambda)t} \text{ ----- (3)}$$

Next inserting (3),(2) into (1b), one can write

$$\frac{S}{\Omega} i(S-\Lambda) e^{i(S-\Lambda)t} = i\Omega e^{iSt-i\Lambda t}$$

Or

$$S^2 - \Lambda S - \Omega^2 = 0 \text{ ----- (4)}$$

This quadratic equation for s can be solved as

$$S_{\pm} = \frac{1}{2} \left( \Lambda \pm \sqrt{\Lambda^2 + 4\Omega^2} \right) \text{ ----- (5)}$$

Therefore,  $a_1'(t)$  is found as

$$a_1' = A_+ e^{iS_+ t} + A_- e^{iS_- t} \text{ ----- (6)}$$

where  $A_{\pm}$  are two constants of integration.

Hence

$$\begin{aligned} a_1 &\equiv a_1' e^{-\gamma_1 t} \\ &= A_+ e^{i\frac{1}{2}[\Delta - i(\gamma_1 - \gamma_2) + \sqrt{\Lambda^2 + 4\Omega^2}]t - \gamma_1 t} + A_- e^{i\frac{1}{2}[\Delta - i(\gamma_1 - \gamma_2) - \sqrt{\Lambda^2 + 4\Omega^2}]t - \gamma_1 t} \text{ ----- (7)} \\ &= A_+ e^{i\frac{1}{2}[\Delta + i\gamma_{12} + \sqrt{\Lambda^2 + 4\Omega^2}]t} + A_- e^{i\frac{1}{2}[\Delta + i\gamma_{12} - \sqrt{\Lambda^2 + 4\Omega^2}]t} \end{aligned}$$

with

$$\gamma_{12} \equiv \gamma_1 + \gamma_2$$

Likewise, one can also find

$$\begin{aligned} a_2'(t) &= \frac{\dot{a}_1'}{i\Omega} e^{-\Lambda t}, \quad \Lambda \equiv \Delta - i(\gamma_1 - \gamma_2) \\ &= \frac{A_+ S_+}{\Omega} e^{i(S_+ - \Lambda)t} + \frac{A_- S_-}{\Omega} e^{i(S_- - \Lambda)t} \\ &= \frac{A_+ S_+}{\Omega} e^{-i\frac{1}{2}[\Delta - i(\gamma_1 - \gamma_2) - \sqrt{\Lambda^2 + 4\Omega^2}]t} + \frac{A_- S_-}{\Omega} e^{-i\frac{1}{2}[\Delta - i(\gamma_1 - \gamma_2) + \sqrt{\Lambda^2 + 4\Omega^2}]t} \end{aligned}$$

Hence

$$\begin{aligned} a_2(t) &= a_2'(t) e^{-\gamma_2 t} \\ &= \frac{A_+ S_+}{\Omega} e^{-i\frac{1}{2}[\Delta + i\gamma_{12} - \sqrt{\Lambda^2 + 4\Omega^2}]t} + \frac{A_- S_-}{\Omega} e^{-i\frac{1}{2}[\Delta - i\gamma_{12} + \sqrt{\Lambda^2 + 4\Omega^2}]t} \text{ ----- (8)} \end{aligned}$$

(b) From the initial conditions given,  $a_1(0)=1$ ,  $a_2(0)=0$ , the constants  $A_{\pm}$  are found.

From (7),(8),

$$\begin{aligned} A_+ + A_- &= 1 \\ S_+ A_+ + S_- A_- &= 0 \end{aligned}$$

so that

$$\begin{aligned} A_+ &= \frac{\begin{vmatrix} 1 & 1 \\ 0 & S_- \end{vmatrix}}{\begin{vmatrix} 1 & 1 \\ S_+ & S_- \end{vmatrix}} = \frac{S_-}{S_- - S_+} \\ A_- &= \frac{S_+}{S_+ - S_-} \end{aligned}$$

Or more explicitly,

$$A_+ = -\frac{1}{\sqrt{\Lambda^2 + 4\Omega^2}} \frac{\Delta - i(\gamma_1 - \gamma_2) - \sqrt{\Lambda^2 + 4\Omega^2}}{2} \text{----- (8a)}$$

$$A_- = \frac{1}{\sqrt{\Lambda^2 + 4\Omega^2}} \frac{\Delta - i(\gamma_1 - \gamma_2) + \sqrt{\Lambda^2 + 4\Omega^2}}{2} \text{----- (8b)}$$

Inserting (8) into (7) one obtains the complete solution,

$$a_1(t) = e^{\frac{1}{2}(i\Delta - \gamma_{12})t} \left\{ -\frac{\Delta - i(\gamma_1 - \gamma_2)}{\sqrt{\Lambda^2 + 4\Omega^2}} i \sin \left[ \frac{1}{2} \sqrt{\Lambda^2 + 4\Omega^2} t \right] + \cos \left[ \frac{1}{2} \sqrt{\Lambda^2 + 4\Omega^2} t \right] \right\} \text{----- (9a)}$$

$$\begin{aligned} a_2(t) &= e^{-\frac{1}{2}(i\Delta + \gamma_{12})t} \frac{1}{\Omega} \left\{ A_+ S_+ e^{i\frac{1}{2}\sqrt{\Lambda^2 + 4\Omega^2}t} + A_- S_- e^{-i\frac{1}{2}\sqrt{\Lambda^2 + 4\Omega^2}t} \right\} \text{----- (9b)} \\ &= \frac{\Omega}{\sqrt{\Lambda^2 + 4\Omega^2}} 2i \sin \left[ \frac{1}{2} \sqrt{\Lambda^2 + 4\Omega^2} t \right] \end{aligned}$$

(c) For  $\gamma_1 = \gamma_2 = \gamma$

$$\begin{aligned} \frac{1}{2}\gamma_{12} &= \frac{1}{2}(\gamma_1 + \gamma_2) = \gamma \\ \Lambda &= \Delta \end{aligned}$$

and (9a), (9b) reduces to (14.70a),(14.70b) in the text, as they should.

For  $\gamma_2 \gg \gamma_1$ , for example,

$$\begin{aligned} \frac{1}{2}\gamma_{12} &\approx \frac{1}{2}\gamma_2 \\ \Lambda &= \Delta + i\gamma_2 \end{aligned}$$

and both  $a_1(t)$ ,  $a_2(t)$  decay at about the same rate,  $\gamma_2/2$ .

14.4(a) with  $a_1(t=0)=1$ , one can write

$$\dot{a}_2 = i\Omega e^{-i\Delta t}, \Delta \equiv \omega - \omega_0, \Omega = \frac{\tilde{\mu}E_0}{2\hbar}$$

Integrating the equation w.r.t.  $t$ , using the initial condition  $a_2(0) = 0$  one finds

$$\begin{aligned} a_2(t) &= i \left( \frac{\Omega}{-i\Delta} \right) (e^{-i\Delta t} - 1) \\ &= i\Omega e^{-i\Delta t/2} 2 \frac{e^{-i\Delta t/2} - e^{i\Delta t/2}}{-2i\Delta} \\ &= i\Omega e^{-i\Delta t/2} \frac{\sin \Delta t / 2}{\Delta / 2} \end{aligned}$$

(b) The probability of the electron making transition from initially given state  $|1\rangle$  to the final state  $|2\rangle$  is given by definition by  $|a_2(t)|^2$ . Because of the finite lifetime, and the distributed nature of levels entailed therein one has to sum over the probabilities:

$$\begin{aligned} |a_2(t)|^2 &= \int d\omega_0 \rho(\omega_0) |a_2(t)|^2 \\ &= \Omega^2 \int d\omega_0 \rho(\omega_0) \frac{\sin^2 \left( \frac{\omega - \omega_0}{2} t \right)}{\left( \frac{\omega - \omega_0}{2} \right)^2} \text{----- (1)} \end{aligned}$$

with  $\rho(\omega)$  denoting the line shape factor. Here, the transition frequency

$$\Omega = \frac{\tilde{\mu}E_0}{2\hbar}, \tilde{\mu} = e \langle 1 | r_2 | 2 \rangle$$

is shown to be exactly identical to the matrix elements of the perturbing or interaction Hamiltonian, i.e.

$$\hat{H}' = e \underline{r} \cdot \underline{E}$$

Thus one may note

$$\hat{H}'_{12} / \hbar = \Omega$$

Therefore, (1) is identical to (13.55) in the text.

(c) Integrating (1) with the use of (13.57) one obtains

$$\begin{aligned} |a_{\{2\}}(t)|^2 &= \frac{2\pi}{\hbar^2} |H'_{12}|^2 \rho(\omega) t \text{----- (2)} \\ &= Rt \end{aligned}$$

where the transition rate,  $R \propto |H'_{12}|^2$  is commensurate with  $|E_0|^2$  or equivalently the light intensity,  $I_v$ :

$$I_v \equiv \frac{\varepsilon E_0^2}{2} \frac{c}{n} = cn\varepsilon_0 \frac{E_0^2}{2} \text{----- (3)}$$

Here,  $2\pi\nu = \omega$ , and the permittivity of the medium,  $\varepsilon$  was specified in terms of vacuum permittivity  $\varepsilon_0$  and index of refraction,  $n$ , i.e.  $\varepsilon = n^2 \varepsilon_0$ .

Inserting (3) into (2), one obtains

$$R = \frac{2\pi}{\hbar^2} \tilde{\mu}^2 \frac{E_0^2}{4} \rho(\omega) = \frac{\tilde{\mu}^2 n \rho(\nu)}{2\hbar^2 c \epsilon} I_\nu \text{----- (4)}$$

where use has been made of

$$\rho(\omega) d\omega = \rho(\omega) 2\pi d\nu \equiv \rho(\nu) d\nu$$

Hence, given an ensemble of atoms all prepared initially in lower level  $|1\rangle$  the incident light is attenuated as it traverses through the medium:

$$I_\nu(z + dz) - I_\nu(z) = \frac{\partial I_\nu}{\partial z} \cdot dz = -N_1 \cdot R h\nu dz \text{----- (5)}$$

where  $N_1$  is the density of atoms in lower level,  $R$  the transition rate thus derived and  $h\nu$  the energy of the photon involved in the transition, i.e. absorption.

One can generalize (5) to the case, in which the densities of atoms in level  $|1\rangle$  and  $|2\rangle$  are given by  $N_1, N_2$ .

Then (5) is generalized as

$$\frac{\partial I_\nu}{\partial z} = -(N_1 - N_2) R h\nu \equiv -\alpha I_\nu \text{----- (6)}$$

Integrating (6) one obtains

$$I_\nu(z) = I_\nu(0) e^{-\alpha z}$$

Hence,  $\alpha$  thus introduced is the linear absorption coefficient and is specified from (6), (4) as

$$\alpha = (N_1 - N_2) \frac{\tilde{\mu}^2 n \rho(\nu)}{2\hbar^2 c \epsilon} h\nu$$

14.5 (a) Given the coupled equation

$$\frac{\partial V}{\partial z} = -L \frac{\partial I}{\partial t} \text{----- (1a)}$$

$$\frac{\partial I}{\partial z} = -C \frac{\partial V}{\partial t} \text{----- (1b)}$$

differentiate (1a) w.r.t.  $z$  and use (1b), obtaining the wave equation

$$\begin{aligned} \frac{\partial^2 V}{\partial z^2} &= -L \frac{\partial}{\partial t} \frac{\partial I}{\partial z} \\ &= -L \frac{\partial}{\partial t} \cdot (-C) \frac{\partial V}{\partial t} \\ &= LC \frac{\partial^2 V}{\partial t^2} \end{aligned}$$

That is,

$$\frac{\partial^2 V}{\partial z^2} - \frac{1}{c^2} \frac{\partial^2 V}{\partial t^2} = 0 \text{----- (2)}$$

where the velocity of propagation is defined in terms of the inductance,  $L$  and capacitance,  $C$  as

$$\frac{1}{c^2} = LC$$

The same wave equation can likewise be derived for I.

(b) The traveling wave representations of the voltage, V and the current, I,

$$V = V_0 \left[ a e^{-i(\omega t - kz)} + a^* e^{i(\omega t - kz)} \right] \text{----- (3a)}$$

$$I = I_0 \left[ a e^{-i(\omega t - kz)} + a^* e^{i(\omega t - kz)} \right] \text{----- (3b)}$$

are the solutions of the wave equation provided  $\omega, k$  satisfy the dispersion relation,

$$k^2 = (\omega / c)^2 = \omega^2 LC$$

To find the relationship between  $V_0, I_0$ , insert (3a),(3b) into (1a), obtaining

$$\begin{aligned} kV_0 &= \omega LI_0 \\ &= \left[ kL / \sqrt{LC} \right] I_0 \\ &= k \sqrt{\frac{L}{C}} I_0 \end{aligned}$$

Hence

$$V_0 = Z_0 I_0$$

with

$$Z_0 = \sqrt{\frac{L}{C}}$$

denoting the line impedance and one may represent  $V_0$  in the form

$$V_0 = \left( \frac{\hbar \omega}{2Cz_0} \right)^{1/2} \text{----- (4)}$$

where  $z_0$  is the length of the transmission line. The  $V_0$  representation in (4) will be made clear in (c).

(c) The energy residing in the transmission line is given by

$$H = \int_0^{z_0=n\lambda} dz \left[ \frac{1}{2} CV^2 + \frac{1}{2} LI^2 \right]$$

where the line length is taken as integer multiple of  $\lambda$ .

One notes from  $V_0 = \sqrt{L/C} \cdot I_0$  that  $CV_0^2 = LI_0^2$ . Hence one can write by using (3)

$$\begin{aligned} H &= \int_0^{z_0=n\lambda} dz CV_0^2 \cdot (aa^* + a^*a) \\ &= \left( \frac{\hbar \omega}{2Cz_0} \right) C (aa^* + a^*a) \cdot z_0 \text{----- (5)} \\ &= \hbar \omega \frac{1}{2} (aa^* + a^*a) \end{aligned}$$

In (5),(4) was used for  $V_0$  and only d.c. components of  $V^2$  contributed to the integral.

(d) If  $a$  and  $a^*$  are defined as

$$a = \frac{1}{\sqrt{2\hbar\omega}}(\omega q + ip) \text{ ----- (6a)}$$

$$a^* = a^+ = \frac{1}{\sqrt{2\hbar\omega}}(\omega q - ip) \text{ ----- (6b)}$$

Then

$$\begin{aligned} aa^* &= \frac{1}{2\hbar\omega}(\omega q + ip)(\omega q - ip) \\ &= \frac{1}{2\hbar\omega}(\omega^2 q^2 + p^2) = a^* a \end{aligned}$$

Hence, (5) reads as

$$H = \frac{1}{2}(p^2 + \omega^2 q^2) \text{ ----- (7)}$$

(e) Consider the Hamilton's equation of motion, using (7). One can write

$$\dot{q} = \frac{\partial H}{\partial p} = p \text{ ----- (8a)}$$

$$\dot{p} = -\frac{\partial H}{\partial q} = -\omega^2 q \text{ ----- (8b)}$$

or equivalently

$$\ddot{p} = -\omega^2 \dot{q} = -\omega^2 p \text{ ----- (9a)}$$

$$\ddot{q} = \dot{p} = -\omega^2 q \text{ ----- (9b)}$$

Thus, these equations of motion are identical to the equation of motion of the harmonic oscillator. Also, (8) explicitly suggests that  $p, q$  are canonically conjugate variables.

(f) If the commutation relation holds true, i.e.  $[q, p] = i\hbar$ , one can write

$$\begin{aligned} [a, a^+] &= aa^+ - a^+ a \\ &= \frac{1}{2\hbar\omega} [(\omega q + ip)(\omega q - ip) - (\omega q - ip)(\omega q + ip)] \\ &= \frac{\omega}{2\hbar\omega} [-iqp + ipq - iqp + ipq] \\ &= \frac{\omega}{2\hbar\omega} \{-i[q, p] + i[p, q]\} \\ &= \frac{\omega}{2\hbar\omega} (2\hbar) \\ &= 1 \end{aligned}$$

Therefore it follows from (5) that

$$\begin{aligned} H &= \hbar\omega \frac{1}{2}(aa^+ - a^+a) \\ &= \hbar\omega \frac{1}{2}(2a^+a + 1) \\ &= \hbar\omega(a^+a + \frac{1}{2}) \end{aligned}$$



## Chapter 15

15.1 (a) In interaction picture, in which the expansion coefficient as a function of time splits into two parts as

$$\psi(t) = a_1(t)e^{-iE_1t/\hbar} |1\rangle + a_2(t)e^{-iE_2t/\hbar} |2\rangle$$

The coupled equation of motion for  $a_1, a_2$  are given from (14.62) by

$$\dot{a}_1 = i\Omega a_2(t)e^{-i\omega_0t} \text{----- (1a)}$$

$$\dot{a}_2 = i\Omega a_1(t)e^{i\omega_0t} \text{----- (1b)}$$

where

$$\Omega = \frac{\tilde{\mu}E(t)}{\hbar}$$

is the atomic transition frequency and

$$\omega_0 = \frac{E_2 - E_1}{\hbar} = \omega_2 - \omega_1$$

is the transition frequency.

Thus, using (1) one can write

$$\begin{aligned} \dot{\rho}_{11} &= \frac{d}{dt} a_1 a_1^* \\ &= \dot{a}_1 a_1^* + a_1 \dot{a}_1^* \text{----- (2a)} \\ &= i\Omega a_2 e^{-i\omega_0t} a_1^* - i\Omega a_2^* e^{i\omega_0t} a_1 \\ &= i\Omega (\rho_{21} e^{-i\omega_0t} - \rho_{12} e^{i\omega_0t}) \end{aligned}$$

$$\begin{aligned} \dot{\rho}_{22} &= \frac{d}{dt} a_2 a_2^* \text{----- (2b)} \\ &= -i\Omega (\rho_{21} e^{-i\omega_0t} - \rho_{12} e^{i\omega_0t}) \end{aligned}$$

$$\begin{aligned} \dot{\rho}_{21} &= \frac{d}{dt} a_1^* a_2 \\ &= \dot{a}_1^* a_2 + a_1^* \dot{a}_2 \\ &= -i\Omega a_2^* e^{i\omega_0t} a_2 + i\Omega a_1 e^{i\omega_0t} a_1^* \text{----- (2c)} \\ &= i\Omega e^{i\omega_0t} (\rho_{11} - \rho_{22}) \\ &= \dot{\rho}_{12}^* \end{aligned}$$

(b) The diagonal elements are identical in both pictures, i.e.

$$\rho_{11}^{(s)} = \rho_{11}^{(i)}, \quad \rho_{22}^{(s)} = \rho_{22}^{(i)}$$

On the other hand, the off diagonal elements differ from each other:

$$\begin{aligned} \rho_{21}^{(s)} &\equiv a_{s2} a_{s1}^* \\ &= a_{i2} e^{-i\omega_2t} a_{i1}^* e^{i\omega_1t} \\ &= \rho_{21}^{(i)} e^{-i\omega_0t} \end{aligned}$$

Thus, the equation of motion for  $\rho_{21}$  in Schrödinger picture appearing in (15.20c) in the text,

$$\dot{\rho}_{21}^{(s)} = -i\omega_0\rho_{21}^{(s)} + i\Omega(\rho_{11} - \rho_{22})$$

can be cast into

$$\frac{d}{dt} \left[ e^{i\omega_0 t} \rho_{21}^{(s)} \right] = i\Omega(\rho_{11} - \rho_{22}) e^{i\omega_0 t}$$

in complete agreement with (2c).

Therefore, the two sets of equations of motion for density matrix are identical.

15.2 (a) With the initial condition  $\rho_{11}(0) = 1, \rho_{22}(0) = 0$ , thus given the equation (15.20) in the text is reduced to

$$\dot{\rho}_{21}^{(s)} = -i\omega_0\rho_{21}^{(s)} + i\Omega, \quad \Omega = \frac{\tilde{\mu}E(t)}{\hbar} \text{----- (1)}$$

Consider a harmonic field,

$$\begin{aligned} E(t) &= E_0 \cos \omega t \\ &= \frac{1}{2} E_0 (e^{i\omega t} + e^{-i\omega t}) \end{aligned}$$

Inserting this harmonic field into (1) and rearranging the terms there results,

$$\frac{d}{dt} \left[ e^{i\omega_0 t} \rho_{21}^{(s)} \right] = i \frac{\tilde{\mu}E_0}{2\hbar} e^{-i(\omega - \omega_0)t} \text{----- (2)}$$

where the term rapidly oscillating in time,  $\exp i(\omega + \omega_0)t$  has been deleted. Integrating (2) with the initial condition  $\rho_{21}(t=0) = 0$ , one obtains

$$e^{-i\omega_0 t} \rho_{21}^{(s)}(t) = i \frac{\tilde{\mu}E_0}{2\hbar} \left[ \frac{1}{-i(\omega - \omega_0)} \right] \left[ e^{-i(\omega - \omega_0)t} - 1 \right]$$

or

$$\rho_{21}^{(s)} = \frac{\tilde{\mu}E_0}{2\hbar} \frac{1}{\omega_0 - \omega} (e^{-i\omega t} - e^{-i\omega_0 t})$$

Hence, the atom dipole moment is given by

$$\begin{aligned} \langle \tilde{\mu} \rangle &= \tilde{\mu} (\rho_{12}^{(s)} + \rho_{21}^{(s)}) \\ &= \frac{\tilde{\mu}^2 E_0}{2\hbar} \frac{1}{\omega_0 - \omega} \left[ e^{-i\omega t} - e^{-i\omega_0 t} + c.c. \right] \text{----- (3)} \\ &= \frac{\tilde{\mu}^2 E_0}{2\hbar} \frac{1}{\omega_0 - \omega} [\cos \omega t - \cos \omega_0 t] \end{aligned}$$

In the short time limit,

$$\begin{aligned} &\cos \omega t - \cos \omega_0 t \\ &= 1 - \frac{\omega^2 t^2}{2} + \dots - \left[ 1 - \frac{\omega_0^2 t^2}{2} + \dots \right] \\ &\simeq \frac{t^2}{2} (\omega_0 + \omega)(\omega_0 - \omega) \end{aligned}$$

and

$$\langle \tilde{\mu} \rangle \approx \frac{\tilde{\mu}^2 E_0}{\hbar} \frac{\omega_0 + \omega}{2} t^2 \text{----- (4)}$$

(c) Using the equation for  $\rho_{21}$  in interaction picture and the same initial condition one can write neglecting the second harmonic component

$$\begin{aligned} \dot{\rho}_{21}^{(i)} &= i \frac{\tilde{\mu} E_0}{2\hbar} (e^{i\omega t} - e^{-i\omega t}) e^{i\omega_0 t} \\ &\approx i \frac{\tilde{\mu} E_0}{2\hbar} e^{-i(\omega - \omega_0)t} \end{aligned}$$

Integrating with the use of the initial condition,  $\rho_{21}(0) = 0$

$$\rho_{21}^{(i)} = \frac{\tilde{\mu} E_0}{2\hbar} \frac{1}{\omega_0 - \omega} (e^{-i(\omega - \omega_0)t} - 1) \text{----- (5)}$$

The atom dipole is thus described with the use of (5) by

$$\begin{aligned} \langle \tilde{\mu} \rangle &\equiv \tilde{\mu} (\rho_{21}^{(s)} + c.c.) \\ &= \tilde{\mu} (\rho_{21}^{(i)} e^{-i(\omega_2 - \omega_1)t} + c.c.) \\ &= \frac{\tilde{\mu}^2 E_0}{2\hbar} \frac{1}{\omega_0 - \omega} (e^{-i\omega t} - e^{-i\omega_0 t} + c.c.) \text{----- (6)} \\ &= \frac{\tilde{\mu}^2 E_0}{\hbar} \frac{1}{\omega_0 - \omega} (\cos \omega t - \cos \omega_0 t) \end{aligned}$$

where  $\omega_2 - \omega_1 = \omega_0$ . Eq (6) is in complete agreement with (3), as it should.

15.3 Start from (15.27a), (15.27b) in the text:

$$\frac{1}{T_2} \sigma_{21}^{(r)} + (\omega - \omega_0) \sigma_{21}^{(i)} = 0 \text{----- (1a)}$$

$$(\omega - \omega_0) \sigma_{21}^{(r)} - \frac{1}{T_2} \sigma_{21}^{(i)} = -\frac{\tilde{\mu} E_0}{2\hbar} (\rho_{11} - \rho_{22}) \text{----- (1b)}$$

Solving  $\sigma_{21}^{(r)}, \sigma_{21}^{(i)}$  in terms of  $(\rho_{11} - \rho_{22})$ , one can write

$$\begin{aligned} \sigma_{21}^{(r)} &= \frac{\begin{vmatrix} 0 & \omega - \omega_0 \\ -\frac{\tilde{\mu} E_0}{2\hbar} (\rho_{11} - \rho_{22}) & \frac{1}{T_2} \end{vmatrix}}{\begin{vmatrix} \frac{1}{T_2} & \omega - \omega_0 \\ \omega - \omega_0 & -\frac{1}{T_2} \end{vmatrix}} \text{----- (2)} \\ &= -\frac{\frac{\tilde{\mu} E_0}{2\hbar} (\omega - \omega_0) (\rho_{11} - \rho_{22})}{(\omega - \omega_0)^2 + 1/T_2^2} \end{aligned}$$

Similarly one obtains

$$\sigma_{21}^{(i)} = \frac{\tilde{\mu}E_0}{2\hbar^2 T_2} (\rho_{11} - \rho_{22}) \text{----- (3)}$$

Inserting (2), (3) into (15.27c) in the text, one finds

$$\rho_{11} - \rho_{22} = (\rho_{11}^{(\sigma)} - \rho_{22}^{(\sigma)}) \frac{1 + (\omega - \omega_0)^2 T_2^2}{1 + (\omega - \omega_0)^2 T_2^2 + 4\Omega^2 T_2 \tau} \text{----- (4)}$$

in agreement with (15.28). Note that

$$\Omega \equiv \frac{\tilde{\mu}E_0}{2\hbar}$$

is the transition frequency. One can in turn use (4) in (2),(3), and obtain (15.29) and (15.30) exactly.

15.4 At steady state, where  $\dot{\rho}_{22} = \dot{\rho}_{11} = 0$  the rate equations (15.41), (15.42) are reduced to

$$\left( \frac{1}{\tau_2} + \frac{1}{\tau_{sp}} + W_i \right) \rho_{22} - W_i \rho_{11} = \lambda_2 \text{----- (1a)}$$

$$-\left( \frac{1}{\tau_{sp}} + W_i \right) \rho_{22} - \left( \frac{1}{\tau_1} + W_i \right) \rho_{11} = \lambda_1 \text{----- (1b)}$$

and one can find  $\rho_{11}, \rho_{22}$  in terms of  $\lambda_1, \lambda_2$ :

$$\rho_{22} = \frac{\begin{vmatrix} \lambda_2 & -W_i \\ \lambda_1 & \frac{1}{\tau_1} + W_i \end{vmatrix}}{\begin{vmatrix} \frac{1}{\tau_2} + \frac{1}{\tau_{sp}} + W_i & -W_i \\ -\left( \frac{1}{\tau_{sp}} + W_i \right) & \frac{1}{\tau_1} + W_i \end{vmatrix}}$$

$$= \frac{\lambda_2 \left( \frac{1}{\tau_1} + W_i \right) + \lambda_1 W_i}{\frac{1}{\tau_1} \left( \frac{1}{\tau_2} + \frac{1}{\tau_{sp}} \right) + W_i \left( \frac{1}{\tau_1} + \frac{1}{\tau_2} \right)}$$

Also

$$\rho_{11} = \frac{\lambda_1 \left( \frac{1}{\tau_2} + \frac{1}{\tau_{sp}} + W_i \right) + \lambda_2 \left( \frac{1}{\tau_{sp}} + W_i \right)}{\frac{1}{\tau_1} \left( \frac{1}{\tau_2} + \frac{1}{\tau_{sp}} \right) + W_i \left( \frac{1}{\tau_1} + \frac{1}{\tau_2} \right)}$$

Hence

$$\begin{aligned}
\rho_{22} - \rho_{11} &= \frac{\frac{\lambda_2}{\tau_1} - \frac{\lambda_1}{\tau_2} - (\lambda_1 + \lambda_2) \frac{1}{\tau_{sp}}}{\frac{1}{\tau_1} \left( \frac{1}{\tau_2} + \frac{1}{\tau_{sp}} \right) + W_i \left( \frac{1}{\tau_1} + \frac{1}{\tau_2} \right)} \\
&= \frac{\lambda_2 \tau_2 - \lambda_1 \tau_1 - (\lambda_1 + \lambda_2) \frac{\tau_1 \tau_2}{\tau_{sp}}}{1 + \frac{\tau_2}{\tau_{sp}} + W_i (\tau_1 + \tau_2)} \\
&\simeq \frac{\lambda_2 \tau_2 - \lambda_1 \tau_1}{1 + W_i (\tau_1 + \tau_2)}
\end{aligned}$$

for  $\tau_{sp} \gg \tau_1, \tau_2$

15.5 (a) Take  $\underline{E}_0 // \hat{z}$ , so that

$$\begin{aligned}
\hat{H}' &= -e \underline{E}_0 \cdot \underline{r} \cos \omega t \\
&= -e E_0 r \cos \theta \cos \omega t
\end{aligned}$$

One has to find  $u_{3lm}$  such that

$$\langle u_{100} | \hat{H}' | u_{3lm} \rangle \neq 0$$

The condition is determined by the angular integration:

$$\langle u_{100} | \hat{H}' | u_{3lm} \rangle \propto \int_0^{2\pi} d\varphi \int_{-1}^1 d\mu \mu Y_{00}^* Y_{lm}$$

It is thus evident from inspection of the integral that

$$\langle u_{100} | \hat{H}' | u_{310} \rangle \neq 0$$

$$\langle u_{100} | \hat{H}' | u_{320} \rangle \neq 0$$

(b) By the same token one can also find the selection rule as

$$\langle u_{310} | \hat{H}' | u_{200} \rangle \neq 0$$

$$\langle u_{320} | \hat{H}' | u_{210} \rangle \neq 0$$

(c) In thermodynamic equilibrium,

$$\frac{N_3}{N_2} = \exp - \frac{E_3 - E_2}{k_B T}$$

where

$$E_3 = -E_0 / 3^2$$

$$E_2 = -E_0 / 2^2$$

$$E_0 = 13.6 \text{ eV}$$

so that

$$\frac{N_3}{N_1} = \exp - \frac{5E_0}{36k_B T}$$

(d) The pumping rate from  $u_{100}$  to  $u_{3lm}$  states is proportional to

$$N_1 W_i$$

where  $N_1$  is the density of atoms in the ground state and

$$W_i = \frac{\tilde{\mu}^2 n g(\nu)}{2\hbar^2 c \epsilon} I_\nu$$

is the transition rate given in terms of light intensity,  $I_\nu$  and the atom dipole moment between the two states involved. If the lifetime of electrons in  $u_{3lm}$  state is  $\tau_3$ , the inversion condition to be met is specified by

$$N_1 W_i \tau_3 \geq N_2$$

or

$$W_i \tau_3 \geq \frac{N_2}{N_1} = \exp - \frac{E_2 - E_1}{k_B T}$$

15.6(a) Given an input  $E_i$  its transmitted component  $E_t$  is given from (15.39) as

$$\frac{E_t}{E_i} = \frac{t_1 t_2 e^{-ikL}}{1-s}, \quad s = r_1 r_2 e^{-2ikL}$$

Hence the transmission coefficient is specified as

$$\begin{aligned} T &\equiv \left| \frac{E_t}{E_i} \right|^2 \\ &= \frac{t_1^2 t_2^2}{(1-r_1 r_2 e^{-2ikL})(1-r_1 r_2 e^{+2ikL})} \\ &= \frac{t_1^2 t_2^2}{1+r_1^2 r_2^2 - 2r_1 r_2 \cos 2kL} \end{aligned}$$

The maximum and minimum T values are therefore given by

$$\begin{aligned} T_{\max} &= \frac{t_1^2 t_2^2}{(1-r_1 r_2)^2}, \quad 2kL = 2n\pi, n = 1, 2, 3, \dots \\ T_{\min} &= \frac{t_1^2 t_2^2}{(1+r_1 r_2)^2}, \quad 2kL = (2n+1)\pi, n = 0, 1, 2, 3, \dots \end{aligned}$$

and the reflection coefficient is given by

$$R = 1 - T$$

(b) The standing wave condition is given by

$$k_\ell \cdot L = \ell \pi, \quad \ell = 1, 2, \dots$$

or

$$\frac{2\pi}{\lambda_\ell} L = \ell \pi$$

that is,

$$\frac{\lambda_\ell}{2} \cdot \ell = L$$

In terms of frequency,  $\nu_\ell (= \frac{c}{\lambda_\ell})$  one can write

$$\nu_\ell = \ell \frac{1}{2L/c}$$

The frequency spacing between two successive modes is therefore given by the inverse cavity round trip time of the wave:

$$\Delta\nu \equiv \nu_{\ell+1} - \nu_\ell = \frac{1}{2L/c} = \frac{1}{\tau_{rt}}$$

L	1m	1cm	100 $\mu$ m	10 $\mu$ m
$\Delta\nu$	$1.5 \times 10^8$	$1.5 \times 10^{10}$	$1.5 \times 10^{12}$	$1.5 \times 10^{13}$

(c) The analysis of (a), (b) can be done exactly in the same way. The only modification required is to replace the velocity of light by  $v = c/n$  with  $n$  denoting the background index of refraction of the medium.

Additionally, due to active lasing, interaction between cavity eigenfrequency and the medium, there is frequency pulling or pushing phenomena, as discussed.

## Chapter 16

16.1 (a) The normalization constant is determined via

$$\begin{aligned}
 1 &= \int d\underline{v} f(\underline{v}) \\
 &= K \int_{-\infty}^{\infty} dv_x \int_{-\infty}^{\infty} dv_y \int_{-\infty}^{\infty} dv_z \cdot e^{-\beta(v_x^2 + v_y^2 + v_z^2)}, \quad \beta = \frac{m}{2k_B T} \\
 &= K \cdot \left( \sqrt{\frac{\pi}{\beta}} \right)^3 = K \left( \frac{2\pi k_B T}{m} \right)^{3/2}
 \end{aligned}$$

Here the formula, (1.20) in the text has been used.

Hence,

$$K = \left( \frac{m}{2\pi k_B T} \right)^{3/2}$$

(b) The phase volume space of  $f(\underline{v})$  in Cartesian coordinate frame is  $dv_x dv_y dv_z$ . In spherical coordinate frame, the corresponding volume space is given by  $v^2 \sin \theta d\phi d\theta dv$ . Thus the probability of finding the particle between  $\underline{v}$  and  $\underline{v} + d\underline{v}$  is described by

$$f(\underline{v}) dv_x dv_y dv_z = f(\underline{v}) v^2 \sin \theta d\phi d\theta dv$$

Hence the reduced probability of the particle having the speed between  $v$  and  $v + dv$  is given by

$$\begin{aligned}
 &\int_0^{2\pi} d\phi \int_0^{\pi} \sin \theta d\theta \cdot v^2 dv f(\underline{v}) \\
 &= \int_0^{2\pi} d\phi \int_0^{\pi} \sin \theta d\theta \cdot v^2 dv \left( \frac{m}{2\pi k_B T} \right)^{3/2} e^{-\frac{mv^2}{2k_B T}} \\
 &= 4\pi \left( \frac{m}{2\pi k_B T} \right)^{3/2} v^2 e^{-\frac{mv^2}{2k_B T}}
 \end{aligned}$$

and the number of such particles is found by multiplying this reduced distribution function by the density of particles,  $N$ :

$$N(v) dv = N \left( \frac{m}{2\pi k_B T} \right)^{3/2} \cdot 4\pi v^2 e^{-\frac{mv^2}{2k_B T}} dv$$

(c) The most probable speed is therefore found from the condition

$$\left. \frac{\partial N(v)}{\partial v} \right|_{v_m} = 0 = 2v_m - \frac{m}{k_B T} v_m^3$$

i.e.

$$v_m^2 = \frac{2k_B T}{m}$$



(d)

$$\begin{aligned}\langle v \rangle &= \frac{\int_0^{\infty} v N(v) dv}{\int_0^{\infty} N(v) dv} \\ &= \frac{\int_0^{\infty} e^{-\beta v^2} v^3 dv}{\int_0^{\infty} e^{-\beta v^2} v^2 dv}\end{aligned}$$

Now,

$$\begin{aligned}\int_0^{\infty} e^{-\beta v^2} v^3 dv, \quad \beta &= \frac{m}{2k_B T} \\ &= \int_0^{\infty} e^{-\beta x} x \frac{1}{2} dx, \quad x = v^2 \\ &= \frac{1}{2} \frac{1}{\beta^2}\end{aligned}$$

$$\begin{aligned}\int_0^{\infty} e^{-\beta v^2} v^2 dv &= -\frac{\partial}{\partial \beta} \int_0^{\infty} e^{-\beta v^2} dv \\ &= -\frac{\partial}{\partial \beta} \cdot \frac{1}{2} \sqrt{\frac{\pi}{\beta}} \\ &= \frac{1}{2} \sqrt{\pi} \cdot \frac{1}{2} \frac{1}{\beta^{3/2}} \\ &= \frac{\sqrt{\pi}}{4\beta^{3/2}}\end{aligned}$$

Hence,

$$\langle v \rangle = \frac{\frac{1}{2\beta^2}}{\frac{\sqrt{\pi}}{4\beta^{3/2}}} = \frac{2}{\sqrt{\pi}} \frac{1}{\beta^{1/2}} = \left( \frac{8k_B T}{\pi m} \right)^{1/2}$$

(e) The number of particles having  $v_x$  and  $v_x + dv_x$  regardless of  $v_y, v_z$  is given by

$$\begin{aligned}
N(v_x) dv_x &= N \int_{-\infty}^{\infty} dv_y \int_{-\infty}^{\infty} dv_z \left( \frac{m}{2\pi k_B T} \right)^{3/2} e^{-\beta(v_x^2 + v_y^2 + v_z^2)} \\
&= N \cdot \left( \frac{m}{2\pi k_B T} \right)^{3/2} \left( \frac{\pi}{\beta} \right) e^{-\beta v_x^2} \\
&= N \cdot \left( \frac{m}{2\pi k_B T} \right)^{1/2} e^{-\frac{mv_x^2}{2k_B T}}
\end{aligned}$$

16.2 (a) The average energy is given in terms of the density of states and the Fermi distribution function as

$$\langle E \rangle = \frac{\int_0^{\infty} dE \cdot E \cdot g(E) f(E)}{\int_0^{\infty} dE \cdot g(E) f(E)}$$

Now, the density of state for electron is given from (4.27) by

$$g_{3D}(E) = \frac{\sqrt{2} m^{3/2} E^{1/2}}{\pi^2 \hbar^3}$$

while the Fermi occupation factor,  $f(E)$  at zero temperature is a step function, i.e.

$$f(E) = \begin{cases} 1, & E \leq E_F \\ 0, & E > E_F \end{cases}$$

Hence

$$\langle E \rangle = \frac{\int_0^{E_F} \frac{\sqrt{2} m^{3/2}}{\pi^2 \hbar^3} E^{3/2} dE}{\int_0^{E_F} \frac{\sqrt{2} m^{3/2}}{\pi^2 \hbar^3} E^{1/2} dE} = \frac{\frac{2}{5} E_F^{5/2}}{\frac{2}{3} E_F^{3/2}} = \frac{3}{5} E_F$$

(b) The evaluation of  $\langle E \rangle$  for arbitrary temperature involves the Fermi 1/2 and 3/2 integrals. This problem offers a good opportunity to get familiar with these important integrals.

16.3 Using the results of the previous problem, one can find the average energy of electrons by

$$\langle E \rangle = \frac{3}{5} E_F = 4.23 eV \quad (1)$$

Now, the thermal energy of electrons is given from the equipartition theorem as

$$\frac{mv_T^2}{2} = \frac{3}{2} k_B T \quad (2)$$

Hence, the equivalent  $T$  is obtained by equating (1) and (2) :

$$T = \frac{2}{3} \cdot 4.23 eV \cdot \frac{1}{8.617 \times 10^{-5} eV/K} = 3.27 \times 10^4 K$$

The corresponding thermal speed is given by

$$\frac{mv_T^2}{2} = \frac{3}{2} k_B T$$

i.e.

$$v_T = \left[ \frac{3 \cdot 1.381 \times 10^{-23} (J/K) \cdot 3.27 \times 10^4 K}{9.1 \times 10^{-31} Kg} \right]^{1/2}$$

$$= 1.22 \times 10^6 \text{ m/s}$$

That is, at this temperature the electron velocity is about one third of the percent of velocity of light.

16.4 For bosons, the distribution function is given from (16.54) by

$$f(E) \propto \frac{1}{e^{E/k_B T} - 1}$$

and the average energy of a boson is therefore specified by

$$\langle E \rangle = \frac{\int_0^\infty dE \cdot \frac{E}{e^{E/k_B T} - 1}}{\int_0^\infty dE \cdot \frac{1}{e^{E/k_B T} - 1}}$$

It will be an interesting exercise to numerically evaluate  $\langle E \rangle$  vs. T and compare the behavior of bosons with those of Fermions and classical particles

16.5 (a) Using the result of (4.9) in the text one can express the energy levels of infinite potential well as

$$E_n - E_c = \frac{\hbar^2 \pi^2}{2m_n W^2} n^2, \quad n = 1, 2, \dots \quad (1)$$

Evidently the reference level of the energy is the bottom of the conduction band in this case. The corresponding energy levels in a quantum well of finite barrier height is lower than those given in (1). This can be easily seen from Fig.4.7 in the text. Here the energy levels are found from the projection of the intersection points onto  $kW/2$  axis

For the ground state energy level, for example,  $E_1$  in an infinite potential well is found from  $kW/2 = \pi/2$  (See Fig. 7.4). In a quantum well of finite barrier height, however, the projected value of the intersection point is less than  $\pi/2$ , so that the corresponding ground state energy is lower.

With this fact in mind and for simplicity of analysis, the potential barrier is taken infinite. Inserting given values of the parameter in (1) one find for  $W = 1nm$

$$E_n = \frac{(1.055 \times 10^{-34})^2 \pi^2}{2 \cdot 0.98 \cdot 9.1 \times 10^{-31} \cdot (10^{-9})^2} \cdot n^2$$

$$\approx 0.38 \cdot n^2 eV$$

Evidently for  $W > 1nm$ ,  $E_1$  is reduced following the power law  $W^2$ .

(b) As a reference first consider the electron concentration,  $n$  in bulk intrinsic semiconductor. In this case  $n$  is given by

$$n = \int_{E_c}^{E_c + \Delta E_c} dE \cdot g_{3D}(E) f(E), \quad (1)$$

where

$$g_{3D}(E) = \frac{\sqrt{2} m_n^{3/2} (E - E_c)^{1/2}}{\pi^2 \hbar^3}$$

is the 3D electron density of states with effective mass  $m_n$  in the conduction band (see 4.25) and

$$f(E) = \frac{1}{1 + \exp\left(\frac{E - E_F}{k_B T}\right)} \approx e^{-\frac{E - E_F}{k_B T}}$$

is the Fermi distribution function or equivalently the electron occupation factor in those quantum states and  $\Delta E_c$  is the width of the conduction band.

The 2D electron concentration in the quantum well is to be obtained in a similar fashion. One can put

$$n_{2D} = \sum_n \Theta(E - E_n) \int_{E_n}^{\infty} dE \cdot g_{2D}(E) f_n(E) \quad (2a)$$

where

$$g_{2D} = \frac{m_n}{\pi \hbar^2} \quad (2b)$$

is the density of states for 2D electrons (see (4.29)) and  $\Theta$  is the heavy side step function,

$$\Theta(x) = \begin{cases} 1 & x \geq 0 \\ 0 & \text{otherwise} \end{cases} \quad (2c)$$

Also  $E_n$  is approximated in this problem by

$$E_n - E_c = E_{on} \cdot n^2 \quad n = 1, 2, \dots$$

with

$$E_{on} = \frac{\hbar^2 \pi^2}{2m_n W^2} \quad (2d)$$

Inserting (2b)-(2d) into (2a) and carrying out the integral there results

$$\begin{aligned} n_{2D} &= \sum_n \frac{m_n k_B T}{\pi \hbar^2} e^{-(E_c - E_F + E_{on} \cdot n^2)/k_B T} \\ &= \frac{m_n k_B T}{\pi \hbar^2} e^{-(E_c - E_F)/k_B T} \cdot \sum_{n=1}^{\infty} e^{-E_{on} \cdot n^2 / k_B T} \end{aligned}$$

(c) For the case of holes one can transcribe the results obtained for electrons. The energy levels of holes in the hole quantum well (see Fig.16.9) are given by

$$E_v - E_n = E_{0p} n^2, \quad E_{0p} = \frac{\hbar^2 \pi^2}{2m_p W^2}, \quad n = 1, 2, \dots \quad (3)$$

where  $m_p$  is now the effective mass of holes in the valence band and the excited energy levels move down the valence band.

The 2D hole density in the valence band is described by

$$p_{2D} = \sum_n \Theta(E_v - E_n) \int_{E_n}^{-\infty} dE \cdot g_{2D}(E_n - E) f_p(E) \quad (4a)$$

where

$$g_{2D}(E_n - E) = \frac{m_p}{\pi \hbar^2} \quad (4b)$$

and the hole occupancy factor is by definition the probability that the state is not occupied by electrons, i.e.

$$\begin{aligned} f_p(E) &= 1 - f_n(E) = 1 - \frac{1}{1 + \exp\left(\frac{E - E_F}{k_B T}\right)} \\ &= \frac{\exp\left(\frac{E - E_F}{k_B T}\right)}{1 + \exp\left(\frac{E - E_F}{k_B T}\right)} \\ &= \frac{1}{1 + \exp\left(\frac{E_F - E}{k_B T}\right)} \approx \exp\left(-\frac{E_F - E}{k_B T}\right), \quad E_F - E > k_B T \end{aligned} \quad (4c)$$

Inserting (4b),(4c),(3) into (4a) one can write

$$\begin{aligned} p_{2D} &= \sum_n \frac{m_p k_B T}{\pi \hbar^2} e^{-(E_F - E_v + E_{0p} n^2)/k_B T} \\ &= \frac{m_p k_B T}{\pi \hbar^2} e^{-(E_F - E_v)/k_B T} \cdot \sum_{n=1}^{\infty} e^{-E_{0p} n^2 / k_B T} \end{aligned}$$

16.6 (a) An electron in a quantum wire enjoys one degree of freedom along, say  $x$ -direction and is confined in  $y$ - and  $z$ -directions respectively. For simplicity of analysis take the barrier heights infinite and the square cross-sectional area,  $W \times W$  of the wire. Then the energy eigenvalue is given from (4.78) as

$$E_{nm} = \frac{\hbar^2 k_x^2}{2m_n} + E_{ym} + E_{zn}$$

with the sublevels given by

$$E_{ym} - E_c = \frac{\hbar^2 \pi^2}{2m_n W^2} m^2 \quad m = 1, 2, \dots$$

$$E_{zn} - E_c = \frac{\hbar^2 \pi^2}{2m_n W^2} n^2 \quad n = 1, 2, \dots$$

For  $W = 1\text{nm}$  and  $m_n = 0.98 m_0$  for instance

$$E_0 = \frac{\hbar^2 \pi^2}{2m_n W^2} \approx 0.38\text{eV}$$

as discussed in (16.5). Hence one can write

$$E_{ym} - E_c = E_0 \cdot m^2$$

$$E_{zn} - E_c = E_0 \cdot n^2$$

Clearly the sublevels of this wire are degenerate in general, the specific examples of which are to be listed as follows:

	m	n	$E_{nm}$ in $W_0$ unit	Degeneracy
Ground level	1	1	2	1
1 <sup>st</sup> excited level	2	1	5	2
	1	2	5	
2 <sup>nd</sup> excited level	2	2	8	1
3 <sup>rd</sup> excited level	2	3	10	2
	3	2	10	

(b) For 1D electrons in quantum wire the 1D density is given by

$$n_{1D} = \sum_{nm} \Theta(E - E_{nm}) \int_{E_{nm}}^{\infty} g_{1D}(E) f_n(E) dE \quad (1a)$$

where

$$E_{nm} = E_c + \Delta E_{nm}, \quad \Delta E_{nm} = E_{on} (n^2 + m^2), \quad E_{on} = \frac{\hbar^2 \pi^2}{2m_n W^2} \quad (1b)$$

and the 1D density of states and Fermi occupation factor are specified by (see 4.31)

$$g_{1D} = \frac{\sqrt{2m_n}^{1/2}}{\pi \hbar^2} \cdot \frac{1}{(E - E_{nm})^{1/2}}$$

$$f_n(E) \approx \exp\left(-\frac{E - E_F}{k_B T}\right)$$

Hence the evaluation of (1a) necessitates the integrations of the form

$$I = \int_{E_{nm}}^{\infty} dE \frac{\sqrt{2m_n}^{1/2}}{\pi \hbar} \cdot \frac{e^{-(E - E_{nm} + E_{nm} - E_F)/k_B T}}{(E - E_{nm})^{1/2}}$$

To evaluate I introduce a dimensionless variable,

$$\frac{E - E_{nm}}{k_B T} = \xi^2$$

Then one can write

$$\begin{aligned}
I &= 2 \cdot \frac{\sqrt{2m_n}^{1/2}}{\pi\hbar} (k_B T)^{1/2} e^{-\frac{E_{nm}-E_F}{k_B T}} \int_0^\infty d\xi \cdot e^{-\xi^2} \\
&= \frac{\sqrt{2m_n}^{1/2} (k_B T)^{1/2}}{\sqrt{\pi\hbar}} e^{-(E_{nm}-E_F)/k_B T}
\end{aligned}$$

Inserting (2) into (1a) there results

$$n_{1D} = \left( \frac{2m_n k_B T}{\pi\hbar^2} \right)^{1/2} \sum_{nm} e^{-(E_c - E_F + \Delta E_{nm})/k_B T}$$

where  $\Delta E_{nm}$  represents the sublevels lying on top of  $E_c$ .

The 1D density of holes can likewise be specified in a similar way. One can write

$$p_{1D} = \sum_{nm} \Theta(E_{nm} - E) \int g_{1D}(E) f_p(E) dE$$

where

$$\begin{aligned}
g_{1D}(E) &= \frac{\sqrt{2m_p}^{1/2}}{\pi\hbar} \frac{1}{(E_{nm} - E)^{1/2}} \\
f_p &\approx \exp\left(-\frac{E_F - E}{k_B T}\right)
\end{aligned}$$

$$E_{nm} = E_V - \Delta E_{nm}, \quad \Delta E_{nm} = E_{op} (n^2 + m^2), \quad E_{op} = \frac{\hbar^2 \pi^2}{2m_p W^2}$$

Hence

$$\begin{aligned}
p_{1D} &= \sum_{nm} \int_{E_{nm}}^{-\infty} dE \frac{\sqrt{2m_p}^{1/2}}{\pi\hbar} \cdot \frac{e^{-\frac{E_F - E_{nm} + E_{nm} - E}{k_B T}}}{(E_{nm} - E)^{1/2}} \\
&= \left( \frac{2m_p k_B T}{\pi\hbar^2} \right)^{1/2} \sum_{nm} e^{-(E_F - E_V + \Delta E_{nm})/k_B T}
\end{aligned}$$

## Chapter 17

17.1 Consider the acceptor impurity atoms incorporated. For the acceptor level  $\varepsilon_s$  and  $g_s$  quantum states associated, the number of distinguishable arrangements of  $P_s$  holes are given by

$$P_s = \frac{g_s(g_s - g_A)(g_s - g_A 2) \dots (g_s - g_A(p_s - 1))}{p_s!}$$

$$= \frac{g_A^{p_s} (g_s / g_A)!}{p_s! (g_s / g_A - p_s)!}$$

Here  $g_A$  is the hole degeneracy factor arising from the valence requirement of the acceptor atom to be satisfied by one hole only.

Hence the total number of distinguishable arrangements is given by

$$P(P_1, P_2, \dots, P_s, \dots) = \prod_{s=1}^{\infty} \frac{g_A^{p_s} (g_s / g_A)!}{p_s! (g_s / g_A - p_s)!} \text{----- (1)}$$

(see(17.15) for electrons, for comparison)

To find the maximum number of arrangements, constrained by (i) the total number of holes to be constant and (ii) the total energy to be conserved, introduce as usual the F function,

$$F[\{p_s\}, \alpha, \beta] = \ln P(\{p_s\}) - \alpha \left[ \sum_s p_s - N \right] - \beta \left[ \sum_s p_s (-\varepsilon_s) \varepsilon_s - E \right] \text{----- (2)}$$

(see (17.16)). Here, the only difference existing between (2) and (17.16) in the text lies in that positive  $\varepsilon_s$  for electrons corresponds to  $-\varepsilon_s$  for holes. This arises from the fact that with increasing energy electrons move up the conduction band, while with increasing energy holes move down the valence band.

The maximum value of  $P(\{p_s\})$  is thus found by putting the derivative of F to zero. In so doing the Stirling's formula for factorials, (16.14) are used, obtaining

$$\frac{\partial F}{\partial p_s} = \frac{\partial}{\partial p_s} [p_s \ln g_A - \ln p_s! - \ln(g_s / g_A - p_s)! - \alpha p_s + \beta \varepsilon_s p_s]$$

$$= \frac{\partial}{\partial p_s} \left\{ p_s \ln g_A - (p_s \ln p_s - p_s) - [(g_s / g_A - p_s) \ln(g_s / g_A - p_s) - (g_s / g_A - p_s)] - \alpha p_s + \beta \varepsilon_s p_s \right\}$$

$$= \ln g_A - \ln p_s + \ln(g_s / g_A - p_s) - \alpha + \beta \varepsilon_s$$

$$= \ln \left[ \frac{g_A (g_s / g_A - p_s)}{p_s} \right] - \alpha + \beta \varepsilon_s$$

$$= 0$$

Hence, one can find

$$p_s = \frac{g_s / g_A}{1 + (1 / g_A) e^{\alpha - \beta \varepsilon_s}} \text{----- (3)}$$

Here the Lagrange undetermined multipliers are to be determined as usual as



$$\alpha = E_F / k_B T$$

$$\beta = 1 / k_B T$$

Now, the number of quantum states,  $g_s$  divided by the degeneracy factor  $g_A$  arising from the valence requirement is by definition the number of acceptor atoms incorporated, i.e.

$$g_s / g_A = N_A,$$

Also,  $\varepsilon_s$  appearing in (3) is the ground state energy of acceptor atoms lying above  $E_V$  by a few  $k_B T$  at room temperature. (see Fig. 17.6)

Thus by identifying

$$\varepsilon_s = E_A, \quad p_s = p_A$$

One can recast (3) as

$$p_A = \frac{N_A}{1 + (1/g_A)e^{(E_F - E_A)/k_B T}}$$

Once  $p_A$  is found the ionized acceptor atoms are given by

$$\begin{aligned} N_A^- &\equiv N_A - p_A \\ &= N_A - \frac{N_A}{1 + (1/g_A)e^{(E_F - E_A)/k_B T}} \\ &= \frac{N_A}{1 + g_A e^{(E_A - E_F)/k_B T}} \end{aligned}$$

Thus, (17.22), (17.23) in the text are derived starting from the basic counting statistics.

17.2 (a) At thermal equilibrium the law of mass action holds true, i.e.

$$np = n_i^2 \text{ ----- (1)}$$

and for nondegenerate case

$$n = n_i \exp \frac{E_F - E_i}{k_B T} \text{ ----- (2a)}$$

$$p = p_i \exp \frac{E_i - E_F}{k_B T} \text{ ----- (2b)}$$

where  $E_i \equiv E_{Fi}$  is the intrinsic Fermi level. At room temperature, for instance, in which  $T=300K$   $n_i = 1.45 \times 10^{10} \text{ cm}^{-3}$  in Si. Thus for given  $p$  one can find  $n$  from (1):

$p$	10	$10^2$	$10^5$	$10^8$	$\text{cm}^{-3}$
$n$	$2.1 \times 10^{19}$	$2.1 \times 10^{18}$	$2.1 \times 10^{15}$	$2.1 \times 10^{12}$	$\text{cm}^{-3}$

One can similarly find  $n$  versus  $T$  using  $n_i(T)$  (see (17.9)).

(b) To find the corresponding  $N_D$  and  $N_D^+$  one has to find the Fermi level first. For simplicity one may first assume the nondegenerate case and find  $E_F$  using (2).

$p$	10	$10^2$	$10^5$	$10^8$	$\text{cm}^{-3}$
$E_F - E_i, \text{ eV}$	0.53	0.47	0.30	0.12	eV

(c) In view of the fact that  $E_C - E_i = 0.56 eV$  at  $T=300K$  nondegenerate statistics holds for  $E_C - E_F \geq 2k_B T$  (see Fig. 17.3). Rvidently, one cannot treat the case of  $p=10 \text{ cm}^{-3}$  by using nondegenerate statistics. In this case one has to use (17.2),(17.6) for  $n, p$ , i.e.

$$n = N_C \frac{2}{\sqrt{\pi}} F_{1/2}(\eta_{Fn}), \eta_{Fn} = (E_F - E_C) / k_B T \text{ ----- (3a)}$$

$$p = N_V \frac{2}{\sqrt{\pi}} F_{1/2}(\eta_{Fp}), \eta_{Fp} = (E_V - E_F) / k_B T \text{ ----- (3b)}$$

and find n from (1) using a numerical analysis.

17.3 With  $T \rightarrow 0$ , the freeze out effect becomes operative. Specifically, the band to band excitation of e-h pairs ceases to occur and this is assured by  $E_F$  approaching  $E_C$  in n-type semiconductors. The resulting large difference between  $E_F$  and  $E_V$  ensures that the valence band is all filled up, by electrons, making it difficult for hole excitation to occur.

Furthermore, the electron emission from the donor level  $E_D$  to the conduction band ceases to occur. This means that the electron should remain bound to the donor impurity atom. This is made possible by  $E_F$  being raised above  $E_D$  level.

By the same token,  $E_F$  in p-type semiconductor is lowered below  $E_A$  level with  $T \rightarrow 0$ .

17.4 (a) With  $E_F - E_C = 0.1 eV$ , n is given at room temperature by

$$n = N_C \frac{2}{\sqrt{\pi}} F_{1/2}\left(\frac{0.1}{0.025}\right), k_B T \cong 0.025 eV$$

With

$$N_C = 4.7 \times 10^{17} \text{ cm}^{-3}$$

at  $T = 300^\circ K$  and

$$F_{1/2}(4) = 6.5115$$

one finds

$$n = 3.45 \times 10^{18} \text{ cm}^{-3}$$

(b) From (17.21) one may write

$$n = N_D^+ = \frac{N_D}{1 + g_D \exp(E_F - E_D) / k_B T}$$

By taking  $g_D = 2$ , and also

$$E_C - E_D \approx 13.6 eV \cdot \frac{m_n}{m_0} \frac{1}{\epsilon_r}$$

$$\epsilon_r = 11.9$$

so that

$$E_C - E_D \approx 0.071 eV$$

Hence

$$\frac{N_D^+}{N_D} = \frac{1}{1 + g_D \exp\left(\frac{0.171}{0.025}\right)}$$

$$\approx 5.36 \times 10^{-4}$$

(c) By the same token one can find  $p$  and  $N_A^- / N_A$  as follows. First, one can write

$$p = N_V \frac{2}{\sqrt{\pi}} F_{1/2}\left(\frac{0.15}{0.025}\right)$$

At room temperature,

$$N_V = 4.7 \times 10^{17} \text{ cm}^{-3}$$

and

$$F_{1/2}(6.0) = 11.447$$

Hence

$$p = 9.04 \times 10^{19} \text{ cm}^{-3}$$

Also, using the result of problem 17.1, one can write

$$p = N_A^- = \frac{N_A}{1 + g_A \exp\left(\frac{E_A - E_F}{k_B T}\right)}$$

By taking  $g_A = 2$ , and

$$E_A - E_V = 13.6 \text{ eV} \cdot \frac{m_p}{m_0} \frac{1}{\epsilon_r}$$

$$= 13.6 \text{ eV} \cdot 0.082 \frac{1}{11.9}$$

$$= 0.087 \text{ eV}$$

Hence

$$\frac{N_A^-}{N_A} = \frac{1}{1 + 2 \cdot \exp\left(\frac{E_A - E_V + E_V - E_F}{k_B T}\right)}$$

$$\cong 7.63 \times 10^{-5}$$

17.5 To plot the hole concentration,  $p$  and the ratio,  $N_A^- / N_A$  versus  $1000/T$  one has to find  $E_F$  for given  $N_A$ . In p-type silicon, the charge neutrality condition reads as

$$n + N_A^- = p \text{ ----- (1)}$$

where

$$n = N_C e^{-\frac{E_c - E_F}{k_B T}} \text{ ----- (2a)}$$

$$p = \begin{cases} N_V \frac{2}{\sqrt{\pi}} F_{1/2}\left(\frac{E_V - E_F}{k_B T}\right), & \text{degenerate} \\ N_V e^{-\frac{E_F - E_V}{k_B T}}, & \text{non degenerate} \end{cases} \quad \text{----- (2b)}$$

$$N_A^- = \frac{N_A}{1 + g_A \exp\left(\frac{E_A - E_F}{k_B T}\right)} \quad \text{----- (2c)}$$

Given  $N_A$  and  $T$ , it will be interesting to find  $E_F$  from (1) and to use  $E_F$  thus found, and plot  $p$ ,  $N_A^- / N_A$  versus  $T$ .

17.6 Choose as an example the n-type silicon for consideration at given temperature, say  $T=300K$  and doping level,  $N_D$ . The Fermi level  $E_F$  is found from

$$n = N_D^+ + p$$

That is,

$$N_C \frac{2}{\sqrt{\pi}} F_{1/2}\left(\frac{E_F - E_C}{k_B T}\right) = \frac{N_D}{1 + g_D \exp\left(\frac{E_F - E_D}{k_B T}\right)} + N_V e^{-\frac{E_F - E_V}{k_B T}}$$

With  $E_F$  thus found for given  $N_D$  and  $T$ , one readily finds the Fermi potential

$$q\phi_{Fn} = E_F - E_i$$

In p-type silicon one can likewise start from

$$p = N_A^- + n$$

and find  $E_F$  therein. The Fermi potential is then readily found from  $E_F$  thus found,

$$q\phi_{Fp} = E_i - E_F.$$

17.7 (a) Approximating the quantum well by the infinite potential well, one can write the subbands therein as

$$E_n = \frac{\hbar^2 \pi^2}{2m_n W^2} n^2, \quad n = 1, 2, 3, \dots$$

(see (4.9)). For  $W=10$  nm the ground state energy level is found as

$$\begin{aligned} E_1 &= \frac{(1.055 \times 10^{-34})^2 (3.14)^2}{0.98 \times 9.1 \times 10^{-31} \cdot (10 \times 10^{-9})^2} J \\ &= 1.231 \times 10^{-21} J \\ &= 7.7 \times 10^{-3} eV \end{aligned}$$

and the first excited subband is given by

$$\begin{aligned} E_2 &= 7.7 \text{ meV} \times 4 \\ &= 31 \text{ meV} \end{aligned}$$

(b) The conduction band of the quantum well consists of discrete subbands and the electron concentration therein is to be specified in terms of the 2D density of states and Fermi occupation factor:

$$n_{2D} = \sum_{s=1}^{\infty} \Delta n_s$$

where

$$\begin{aligned} \Delta n_s &= \int_{E_s}^{\infty} dE g_{2D} f_n(E) \\ &= \int_{E_s}^{\infty} dE \left( \frac{m_n}{\pi \hbar^2} \right) \frac{1}{1 + e^{\frac{E-E_F}{k_B T}}} \\ &= \frac{m_n}{\pi \hbar^2} \int_{E_s}^{\infty} d(E - E_C) \frac{1}{1 + e^{\frac{E-E_C+(E_C-E_F)}{k_B T}}} \\ &\simeq \frac{m_n}{\pi \hbar^2} e^{-\frac{E_C-E_F}{k_B T}} \int_{E_s}^{\infty} d(E - E_C) e^{-\frac{E-E_C}{k_B T}} \\ &= \frac{m_n}{\pi \hbar^2} e^{-\frac{E_C-E_F}{k_B T}} k_B T e^{-\frac{E_s-E_C}{k_B T}} \end{aligned}$$

Hence

$$n_{2D} = \frac{m_n}{\pi \hbar^2} k_B T e^{-\frac{E_C-E_F}{k_B T}} \sum_{s=1}^{\infty} e^{-\frac{E_s-E_C}{k_B T}}$$

where one can represent  $E_s$  as

$$E_s = E_0 s^2, E_0 = \frac{\hbar^2 \pi^2}{2m_n W^2}, s = 1, 2, \dots$$

For  $E_0 \gg k_B T$ ,  $n_{2D}$  electrons reside mainly in the ground state subband.

For  $E_0 \ll k_B T$ , on the other hand, one may approximate the discrete summation by an integral :

$$\begin{aligned} &\sum_{s=1}^{\infty} e^{-\frac{E_0}{k_B T} s^2} \\ &= \int_{(E_0/k_B T)^{1/2}}^{\infty} e^{-\xi^2} d\xi, \quad \xi = \sqrt{\frac{E_0}{k_B T}} \cdot s \\ &= \frac{\sqrt{\pi}}{2} \operatorname{erfc} \sqrt{\frac{E_0}{k_B T}} \end{aligned}$$

Here the complementary error function has been introduced, i.e.

$$\operatorname{erfc} z = \frac{2}{\sqrt{\pi}} \int_z^{\infty} e^{-z^2} dz$$

$n_{2D}$  in this limit is represented by

$$n_{2D} = \frac{m_n k_B T}{2\sqrt{\pi} \hbar^2} \operatorname{erfc} \sqrt{\frac{E_0}{k_B T}} \cdot e^{-\frac{E_C-E_F}{k_B T}}$$

It will be interesting to examine  $n_{2D}$  as a function of well width,  $W$  and temperature,  $T$ .

(c)  $n_{2D}$  consists of two factors :

$$n_{2D} = n_0 \sum_{s=1}^{\infty} e^{-\frac{E_0 s^2}{k_B T}} \text{----- (1)}$$

where the factor

$$n_0 = \frac{m_n k_B T}{\pi \hbar^2} e^{-\frac{E_C - E_F}{k_B T}}$$

corresponds to, for the case of intrinsic silicon,  $n_i^{2/3}$ .

At  $T=300K$ , and for  $m_n \approx m_0$ ,  $m_0$  being the rest mass of electron

$$n_0 \approx 2 \times 10^7 \text{ cm}^{-2}$$

is larger than

$$n_i^{2/3} \approx 5.9 \times 10^6 \text{ cm}^{-2}$$

This suggests that the 2D electron density induced in the conduction band in the well can be higher than that corresponding to the bulk value, provided  $E_0 \ll k_B T$ , i.e. with  $W$  large.

However, with  $W$  decreased to nm range, the second factor in (1) could make  $n_{2D} \ll n_i^{2/3}$ .

(d) The charge neutrality condition for n type silicon reads as

$$N_D^+ + p = n$$

each term of which has already been discussed in detail.

The main result of doping, i.e.  $N_D$  is to raise  $E_F$  toward  $E_C$  in which case  $n_{2D}$  induced in the quantum well also increases exponentially, as detailed in (b).

17.8 (a) The electron in a quantum wire enjoys one degree of freedom and the energy eigenequation reads as

$$\left[ -\frac{\hbar^2}{2m} \nabla^2 + V(x, y) \right] \varphi(x, y, z) = E \varphi(x, y, z)$$

where for simplicity the infinite potential well model is used.

$$V(x, y) = \begin{cases} 0 & -W/2 \leq x, y \leq W/2 \\ \infty & \text{otherwise} \end{cases}$$

One can solve the equation using the separation of variable technique, that is, by putting

$$\varphi(x, y, z) = u(x)u(y)u(z)$$

Using the usual procedure one can find

$$u_n(x) = \left( \frac{2}{W} \right)^{\frac{1}{2}} \begin{cases} \cos k_n x, & k_n = (2n+1)\pi/W, \quad n = 0, 1, 2, \dots \\ \sin k_n x, & k_n = 2n\pi/W, \quad n = 1, 2, \dots \end{cases}$$

$$u_m(y) = \left( \frac{2}{W} \right)^{\frac{1}{2}} \begin{cases} \cos k_m y, & k_m = (2m+1)\pi/W, \quad m = 0, 1, 2, \dots \\ \sin k_m y, & k_m = 2m\pi/W, \quad m = 1, 2, \dots \end{cases}$$

$$u(z) = e^{ikz}$$

with the total energy given by

$$E_T = \frac{\hbar^2 k^2}{2m_n} + E_{nm},$$

$$E_{nm} = E_0 (n^2 + m^2), \quad n, m = 1, 2, \dots, \quad E_0 = \frac{\hbar^2 \pi^2}{2m_n W^2}$$

Hence the ground and first excited state energy levels are

$$E_{1,1} = E_0 \cdot 2 \approx 15 \text{ meV}$$

$$E_{1,2} = E_{2,1} = E_0 \cdot 5 \approx 37.5 \text{ meV}$$

for  $m_n = m_0$ ,  $W = 10 \text{ nm}$ .

(b) The 1D electron density in the conduction band is given in terms of the density of states and Fermi occupation factor:

$$n_{1D} = \sum_{nm} \Delta n_{nm} \text{ ----- (1)}$$

where

$$\begin{aligned} \Delta n_{nm} &= \int_{E_{nm}}^{\infty} dE g_{1D} f_n(E) \\ &= \int_{E_{nm}}^{\infty} dE \left( \frac{\sqrt{2}m_n^{1/2}}{\pi\hbar} \right) \frac{1}{(E - E_{nm})^{1/2}} \frac{1}{1 + e^{(E - E_F)/k_B T}} \\ &= \frac{\sqrt{2}m_n^{1/2}}{\pi\hbar} \int_{E_{nm}}^{\infty} dE \frac{1}{(E - E_{nm})^{1/2}} \frac{1}{1 + e^{(E - E_{nm} + E_{nm} - E_F)/k_B T}} \\ &\approx \frac{\sqrt{2}m_n^{1/2}}{\pi\hbar} e^{-(E_{nm} - E_F)/k_B T} \int_{E_{nm}}^{\infty} \frac{dE e^{-(E - E_{nm})/k_B T}}{(E - E_{nm})^{1/2}} \end{aligned}$$

To perform the integration introduce a new variable,

$$\xi = \left( \frac{E - E_{nm}}{k_B T} \right)^{1/2}$$

Then

$$\begin{aligned} &\int_{E_{nm}}^{\infty} \frac{dE e^{-\frac{E - E_{nm}}{k_B T}}}{(E - E_{nm})^{1/2}} \\ &= 2\sqrt{k_B T} \int_0^{\infty} d\xi e^{-\xi^2} \\ &= \sqrt{k_B T \pi} \end{aligned}$$

Inserting this result into the expression for  $\Delta n$ , one obtains from (1)

$$n_{1D} = \left( \frac{2m_n k_B T}{\pi} \right)^{1/2} \frac{1}{\hbar} e^{\frac{E_C - E_F}{k_B T}} \sum_{nm} g_{nm} e^{\frac{E_0(n^2 + m^2)}{k_B T}} \text{ ----- (2)}$$

where

$$\begin{aligned}
E_{nm} - E_F \\
= E_C + E_0(n^2 + m^2)
\end{aligned}$$

and  $g_{nm}$  denotes the degeneracy for states with  $n, m$  quantum numbers. It will be interesting to perform similar analysis for different  $W$  and  $T$ .

(c) The factor appearing in (2),

$$\left( \frac{2m_n k_B T}{\pi} \right)^{1/2} \frac{1}{\hbar}$$

corresponds to the linear density of electrons, i.e.  $n^{1/3}$ . A main quantum effect consists of the discrete subbands located on top of  $E_C$ . Because of these subbands the bandgap is in effect broadened, the effect of which becomes more prominent with decreasing width of the wire.



## Chapter 18

18.1 (a) The required electron concentration can be found from

$$\rho = \frac{1}{\sigma_n} = \frac{1}{q\mu_n n} = \frac{1}{1.6 \times 10^{-19} \text{ C} \cdot 800 \text{ cm}^2 / \text{Vs} \cdot n \text{ cm}^{-3}} = \frac{1}{1.6 \times 10^{-19} \cdot 800 \cdot n} \cdot \frac{\text{Vs}}{\text{C}} \cdot \text{cm} = 10 \Omega \text{ cm}$$

or

$$n_n = \frac{1}{1.6 \times 10^{-19} \cdot 800 \cdot 10} = 7.8 \times 10^{14} \text{ cm}^{-3}$$

and for  $T = 300\text{K}$

$$p_n = \frac{n_i^2}{n_n} = \frac{(1.45 \times 10^{10})^2}{7.8 \times 10^{14}} = 2.79 \times 10^5 \text{ cm}^{-3}$$

(b) The photogenerated density of  $e - h$  pairs are given by

$$n_{ph} = p_{ph} = g\tau = 10^{21} \cdot 10^{-6} = 10^{15} \text{ cm}^{-3}$$

and the total conductivity,

$$\sigma_T = \sigma_D + \sigma_{ph}$$

is therefore contributed by the dark component,

$$\begin{aligned} \sigma_T &= q\mu_n n + q\mu_p p \\ &\approx q\mu_n n \\ &= 1.6 \times 10^{-19} \text{ C} \cdot 800 \text{ cm}^2 / \text{Vs} \cdot 7.8 \times 10^{14} \text{ cm}^{-3} \\ &= 1.0 \times 10^{-2} \text{ } \Omega \text{ cm}^{-1} \end{aligned}$$

and the photogenerated component

$$\begin{aligned} \sigma_{ph} &= q(\mu_n n_{ph} + \mu_p p_{ph}) \\ &= 1.6 \times 10^{-19} \cdot 10^{15} \text{ cm}^{-3} \cdot (800 + 400) \text{ cm}^2 / \text{Vs} \\ &= 1.92 \times 10^{-1} \text{ } \Omega \text{ cm}^{-1} \end{aligned}$$

(b) The total conductivity is primarily contributed by the photoconductivity and therefore the ratio between electron and hole conductivity is given by that of the mobility:

$$\sigma_n / \sigma_p \approx 2$$

18.2 (a) The light intensity is given in terms of the photon density,  $n_{ph}$ , the quantum of energy,  $h\nu$ , and the photon velocity  $c$  as

$$\begin{aligned} I &= n_{ph} \cdot h \frac{c}{\lambda} \cdot c \\ &= h \frac{c}{\lambda} \cdot F_{ph}, \quad F_{ph} = n_{ph} \cdot c \end{aligned}$$

with  $F_{ph}$  denoting the photon flux.

Thus, for  $I = 10 \text{ Watt/cm}^2$ , one can find

$$F_{ph} = \frac{10 \text{ J/scm}^2 \cdot 500 \times 10^{-9} \text{ m}}{6.626 \times 10^{-34} \text{ Js} \cdot 3 \times 10^8 \text{ m}} = 2.52 \times 10^{19} / \text{cm}^2 \text{ s}$$

(b) The generation rate is given in terms of light intensity and/or photon flux and attenuation coefficient as

$$g = \alpha(I/h\nu) = 2.52 \times 10^{20} / \text{cm}^3 \text{ s}$$

Hence, the photogenerated  $e - p$  pairs at steady state are to be specified, given the respective lifetimes:

$$n_{ph} = g\tau_n$$

$$p_{ph} = g\tau_p$$

(c) Given the rate equation

$$\frac{\partial}{\partial t} p_n = g_L - \frac{p_n - p_{n0}}{\tau_p}; \quad g_L = \alpha I / h\nu \text{ ----- (1)}$$

introduce the excess hole density as

$$\Delta p_n = p_n - p_{n0}$$

and recast (1) into

$$\left( \frac{\partial}{\partial t} + \frac{1}{\tau_p} \right) \Delta p = g_L$$

Equivalently,

$$\frac{\partial}{\partial t} \left( e^{t/\tau_p} \Delta p \right) = g_L e^{t/\tau_p} \text{ ----- (2)}$$

A straightforward integration of (2) yields

$$\Delta p(t) = \Delta p(0) e^{-t/\tau_p} + \tau_p g_L (1 - e^{-t/\tau_p})$$

If initially  $\Delta p(0) \neq 0$ , i.e.

$$p_n(0) - p_{n0} \neq 0$$

it decays away in a few  $\tau_p$ 's, while the photogenerated hole density reaches a steady state value,

$g_L \tau_p$  in the same time frame.

If  $\Delta p(t=0) = 0$ , then

$$p_n(t) = p_{n0} + \tau_p g_L (1 - e^{-t/\tau_p})$$

(d) If light is turned off after  $p_n(t)$  has reached the steady state value,

$$p_n = p_{n0} + \tau_p g_L$$

the rate equation, (2) reduces to

$$\frac{\partial}{\partial t} \left( e^{t/\tau_p} \Delta p \right) = 0$$

and a straightforward integration yields

$$\Delta p(t) = \Delta p(0)e^{-t/\tau_p}$$

i.e.

$$p_n(t) = (p_{n0} + \tau_p g_L)e^{-t/\tau_p} + p_{n0}$$

Thus,  $p_n(t)$  relaxes back to  $p_{n0}$  after a few  $\tau_p$ 's.

18.3 (a) For  $\sigma_n = \sigma_p = \sigma$  the net recombination rate  $U$  in (18.69) reduces to

$$U = \frac{1}{\tau_p} = \frac{p_n \cdot n_n - n_i^2}{n_n + n_i \exp \frac{E_t - E_i}{k_B T} + p_n + n_i \exp \frac{E_i - E_t}{k_B T}}$$

with

$$\sigma v_T N_t \equiv \frac{1}{\tau_p}$$

denoting the hole lifetime as the minority carrier in  $n$ -type semiconductor. For  $n_n, p_n \ll n_i$  in the depletion region and for  $E_t$  at the midgap, i.e.  $E_t - E_i = 0$ ,  $U$  further simplifies as

$$U = -\frac{n_i}{2\tau_p} \equiv -g$$

and describes generation rate,  $g$ .

To evaluate  $\tau_p$ ,  $v_T$  has to be found, which can be done from the equipartition theorem.

For a free electron with rest mass  $m_0$ , one can write

$$\frac{1}{2} m_0 v_T^2 = \frac{3}{2} k_B T$$

so that at room temperature

$$\begin{aligned} v_T &= \left[ \frac{3 \cdot 1.38 \times 10^{-23} \cdot 300}{9.1 \times 10^{-31}} \right]^{1/2} \\ &= 1.16 \times 10^5 \text{ m/s} \\ &= 1.16 \times 10^7 \text{ cm/s} \end{aligned}$$

For holes with effective mass  $m_p$ , one can write

$$v_{Tp} = \left( \frac{m_0}{m_p} \right)^{1/2} v_T = 1.49 v_T$$

Therefore the hole lifetime is to be estimated as

$$\begin{aligned} \frac{1}{\tau_p} &= \sigma N_t v_{Tp} \\ &= 10^{-15} \cdot 10^{15} \cdot 1.49 \times 1.16 \times 10^7 \end{aligned}$$

i.e.

$$\tau_p = 5.8 \times 10^{-8} \text{ s}$$

and the generation rate is given by

$$g = \frac{n_i}{2\tau_p} = \frac{1.45 \times 10^{10}}{2 \cdot 0.059 \mu\text{s}} = 1.25 \times 10^{17} \text{ cm}^{-3}$$

(b) If  $E_t = E_C - 0.25eV$ ,  $E_t$  is above the midgap by

$$\begin{aligned} E_t &= E_i + 0.56 - 0.25 \\ &= E_i + 0.31eV \end{aligned}$$

In this case

$$\begin{aligned} g &= |U| \\ &= \frac{1}{\tau_p} \frac{n_i^2}{n_i \exp \frac{E_t - E_i}{k_B T}} \\ &\simeq \frac{n_i}{\tau_p} e^{\frac{0.31}{0.025}}, \quad T = 300K \\ &= 2.5 \times 10^{17} / cm^3 s \cdot 4.12 \times 10^{-6} \\ &= 1.03 \times 10^{12} / cm^3 s \end{aligned}$$

For  $E_t = E_V + 0.25 eV$ , so that  $E_t = E_i - 0.56 + 0.25 = E_i - 0.31eV$ .

Hence the generation rate is the same as the case already considered above.

18.4 (a) At steady state, in which  $\dot{p}_n = 0$ , the rate equation reads as

$$D_p p_n'' + g_L - \frac{p_n - p_{n0}}{\tau_p} = 0$$

where primes denote differentiation w.r.t  $x$ . Dividing the equation by  $D_p$ , one can write

$$\Delta p_n'' - \frac{\Delta p_n}{L_p^2} = -\frac{g_L}{D_p} \quad (1)$$

where

$$\begin{aligned} \Delta p_n &\equiv p_n - p_{n0}, \\ L_p^2 &\equiv D_p \tau_p \end{aligned}$$

The homogeneous solution of (1) has two branches,  $\exp -x/L_p$  and  $\exp +x/L_p$ , the latter of which has to be discarded out of physical considerations. The particular solution is given by

$$\Delta p_n = g_L \cdot \frac{L_p^2}{D_p} = g_L \tau_p$$

Therefore the solution is given by

$$\begin{aligned} \Delta p_n &= p_n(x) - p_{n0} \\ &= A e^{-x/L_p} + g_L \tau_p \end{aligned} \quad (2)$$

The constant  $A$  is determined from the boundary condition,

$$D_p p_n'(0) = v_R (p_n(0) - p_{n0}) \quad (3)$$

Inserting (2) to (3)

$$D_p A \left( -\frac{1}{L_p} \right) = v_R (A + g_L \tau_p)$$

Hence

$$\begin{aligned} A &= -g_L \tau_p \cdot \frac{v_R}{v_R + L_p / \tau_p} \\ &= -g_L \tau_p \cdot \frac{v_R \cdot \tau_p / L_p}{1 + v_R \cdot \tau_p / L_p} \end{aligned} \quad \text{----- (4)}$$

When  $A$  is inserted into (2) there results

$$p_n(x) = p_{n0} + g_L \tau_p - g_L \tau_p \cdot \frac{v_R \cdot \tau_p / L_p}{1 + v_R \cdot \tau_p / L_p} e^{-x/L_p}$$

(b) It will be instructive to plot  $p_n(x)$  for different values of  $g_L$ ,  $\tau_p$ ,  $L_p$  and see the roles of these parameters on  $p_n(x)$ .

18.5 (a) The recombination rate of minority carriers is given from (18.73) or (18.74) by

$$U = \frac{p_n - p_{n0}}{\tau_p} \quad \text{----- (1)}$$

Also, the photogenerated hole density which constitutes the excess hole density is given by

$$p_{ph} = p_n = g\tau_p = 10^{18} \cdot 10 \cdot 10^{-6} = 10^{11} \text{ cm}^{-3} \quad \text{----- (2)}$$

On the other hand, the background concentration,  $p_{n0}$  is to be found from the given resistivity:

$$\begin{aligned} \rho &\approx \frac{1}{q \cdot \mu_n \cdot n_{n0}} \\ &= \frac{1}{1.6 \times 10^{-19} \text{ C} \cdot 800 \text{ cm}^2 / \text{Vs} \cdot n_{n0} \text{ cm}^{-3}} \\ &= 0.6 \Omega \text{ cm} \end{aligned}$$

so that one can find using  $\mu_n = 800 \text{ cm}^2 / \text{Vs}$

$$\begin{aligned} n_{n0} &= \frac{1}{1.6 \times 10^{-19} \cdot 800 \cdot 0.6} \\ &= 1.3 \times 10^{16} \text{ cm}^{-3} \end{aligned}$$

Therefore  $p_{n0}$  at room temperature is given by

$$p_{n0} = \frac{n_i^2}{n_{n0}} = \frac{(1.45 \times 10^{10})^2}{1.3 \times 10^{16}} = 1.62 \times 10^4 \text{ cm}^{-3} \quad \text{----- (3)}$$

Inserting (2), (3) into (1), the recombination rate is found as

$$U \cong \frac{10^{11}}{10^{-5}} = 10^{16} / \text{cm}^3 \text{ s}$$

(b) To estimate the total recombination near the surface, recall the recombination velocity which is given by

$$v_R = \sigma v_T N_t t_s$$

$$= \frac{t_s}{\tau_p}$$

with  $t_s$  denoting the effective surface layer. Thus,  $t_s$  is found from

$$t_s = v_R \cdot \tau_p$$

$$= 100 \text{ cm} / \text{s} \cdot 10 \times 10^{-6} \text{ s}$$

$$= 10^{-3} \text{ cm}$$

Therefore, the total number of recombination near the surface is given by

$$U_T = U \cdot t_s = 10^{13} \text{ cm}^{-2}$$

18.6 (a) With the simplification,  $\sigma_n = \sigma_p = \sigma$  the recombination rate for the case of single level traps at the level  $E_j$  is given from (18.69) as

$$U_j = \frac{\sigma v_T N_t(E_j)(np - n_i^2)}{n + p + 2n_i \cosh\left(\frac{E_j - E_i}{k_B T}\right)}$$

For multilevel traps one can generalize the recombination rates as

$$U = \sum_j U_j$$

$$= \sum_j \frac{\sigma v_T N_t(E_j)(np - n_i^2)}{n + p + 2n_i \cosh\left(\frac{E_j - E_i}{k_B T}\right)}$$

One can in general represent the trap profile in terms of a distribution function,

$$N_t(E_j) = f_t(E)$$

and express  $U$  in terms of distributed traps:

$$U = \sigma v_T (np - n_i^2) \int_{-E_G/2}^{E_G/2} \frac{f_t(E)}{n + p + 2n_i \cosh\left(\frac{E - E_i}{k_B T}\right)} dE$$

where  $E$  is taken zero at the midgap.

For a flat trap level profile,

$$f_t(E) = D_{ss}$$

$U$  reduces to

$$U = \frac{1}{\tau} (np - n_i^2) \int_{-E_G/2}^{E_G/2} \frac{dE}{n + p + 2n_i \cosh\left(\frac{E - E_i}{k_B T}\right)} \text{----- (1)}$$

where

$$\frac{1}{\tau} = \sigma v_T D_{ss}$$

(b) In the depletion depth, for instance, where  $n, p \ll n_i$ ,  $U$  is turned into a generation rate as

$$g = |U| = \frac{n_i}{2\tau_{eff}}$$

Here the effective lifetime is represented by

$$\frac{1}{\tau_{eff}} = \sigma V_T D_{ss} \int_{-E_G/2}^{E_G/2} \frac{dE}{\cosh\left(\frac{E - E_i}{k_B T}\right)} \dots\dots (2)$$

Now,

$$\begin{aligned} \int_{-E_G/2}^{E_G/2} \frac{dE}{\cosh\left(\frac{E - E_i}{k_B T}\right)} &= k_B T \int_0^{E_G/2k_B T} \frac{d\xi}{\cosh \xi}, \quad \xi = \frac{E - E_i}{k_B T} \\ &= k_B T \tan^{-1}(e^\xi) \Big|_0^{E_G/2k_B T} \\ &= k_B T \left[ \tan^{-1}(e^{E_G/2k_B T}) - \tan^{-1}(1) \right] \\ &= k_B T (\pi/2 - \pi/4) \\ &= k_B T \cdot (\pi/4) \end{aligned}$$

Here use was made of the fact that  $E_G \gg 2k_B T$  and  $\tan^{-1}(e^{E_G/2k_B T}) \simeq \pi/2$ .

Hence, the effective lifetime

$$\frac{1}{\tau_{eff}} = \sigma V_T D_{ss} \cdot k_B T \cdot (\pi/4)$$

is approximately determined by  $D_{ss} k_B T$  traps located near the midgap.

(c) For the trap distribution

$$f(E) = N_t \exp\left(-\frac{(E - E_{tc})^2}{2\sigma^2}\right)$$

one can insert the distribution function in (1) and (2) and carry out a similar analysis.

## Chapter 19

19.1 (a) The operational principle of the junction diode is to raise or lower the junction band bending by applying biases and to utilize the restoring force of the junction to reach the equilibrium configuration. To examine the carrier fluxes one has to consider the profile of carrier concentrations, which for the case of  $n(x)$ , for example, is given by (see Fig. (19.3))

$$n(x) = \begin{cases} n_{n0}, & x > x_n \\ n_{n0} e^{-\frac{q\phi(x)}{k_B T}}, & x_n > x > -x_p \\ n_{p0}, & x < -x_p \end{cases}$$

The concentration decreases exponentially in the junction depletion depth from  $n_{n0}$  in the n bulk to  $n_{p0}$  in the p bulk. Thus, the diffusion flux in the junction depletion depth is given by

$$\begin{aligned} F_{n,diff} &\equiv -D_n \frac{\partial n(x)}{\partial x} \\ &= -D_n n_{n0} e^{-\frac{q\phi(x)}{k_B T}} \cdot \left( -\frac{q}{k_B T} \frac{\partial \phi(x)}{\partial x} \right) \\ &= -D_n n(x) \left( \frac{q}{k_B T} \right) \left( -\frac{\partial \phi(x)}{\partial x} \right) \quad \text{----- (1)} \\ &= -\mu_n n(x) E \\ &= -F_{n,drift} \end{aligned}$$

Here the Einstein relation

$$qD_n = k_B T \mu_n$$

has been used, and the space charge field is expressed in term of the space charge potential,  $E = -\partial\phi/\partial x$ . Clearly, (1) states that the electron diffusion flux from right to left in Fig.19.3, for example, in equilibrium is balanced by the drift flux from left to right. By the same token the hole diffusion flux from left to right in the same figure is balanced by the drift flux from right to left:

$$\begin{aligned} F_{p,diff} &\equiv -D_p \frac{\partial p(x)}{\partial x} \\ &= -\mu_p p(x) E \\ &= -F_{p,drift} \end{aligned}$$

Under bias, however, the junction barrier potential decreases or increases depending on whether the junction is forward biased or reverse biased:

$$\phi_{bi} \rightarrow \phi_{bi} - V \quad \text{----- (1)}$$

and the junction depletion depth changes accordingly, i.e.

$$W(V) = W(V=0) \cdot \left( 1 - \frac{V}{\phi_{bi}} \right)^{1/2} \quad \text{----- (2)}$$



where

$$W_0 = \left[ \frac{2\varepsilon(N_A + N_D)}{qN_A N_D} \varphi_{bi} \right]^{1/2}$$

denotes the equilibrium depletion depth. Therefore, under bias the detailed balancing between the drift and diffusion fluxes for both electrons and holes are broken. This can be generally seen as follows.

(b) Consider the hole diffusion from left to right in Fig. 19.3, which can be roughly expressed as

$$\begin{aligned} F_{p,diff} &\approx -D_p \frac{P_{n0} - P_{p0}}{W(V)} \\ &\approx D_p \frac{P_{p0}}{W_0(1 - V/\varphi_{bi})^{1/2}} \end{aligned} \quad \text{----- (3)}$$

Thus, under forward bias,  $V > 0$   $W(V) < W_0$ , and  $F_{p,diff}$  increases from its equilibrium value.

On the other hand, the hole drift flux from right to left can be roughly represented

$$\begin{aligned} F_{p,drift} &\approx p_{n0} \mu_p E \\ &\approx -p_{n0} \mu_p \frac{\varphi_{bi} - V}{W_0(1 - V/\varphi_{bi})^{1/2}} \\ &= -p_{n0} \mu_p \varphi_{bi} \cdot \frac{1}{W_0} (1 - V/\varphi_{bi})^{1/2} \end{aligned} \quad \text{----- (4)}$$

and is shown to decrease from the equilibrium value. In this manner the diffusion flux becomes larger than the drift flux and there ensues a net hole flux from left to right under a forward bias.

Under reverse bias, in which  $V < 0$ , the opposite situation prevails, i.e. drift flux from right to left becomes larger than the diffusion flux from left to right and there is a net flux from right to left.

The same kind of analysis can be made to the case of diffusion and drift fluxes of electrons. In this case there ensues a net electron flux from right to left under forward bias and from left to right under reverse bias.

19.2 In completely depleted approximation, the space charge field is linear in  $x$ , i.e.

$$E(x) = \begin{cases} \frac{qN_D}{\varepsilon_s} (x - x_n), & 0 \leq x \leq x_n \\ -\frac{qN_A}{\varepsilon_s} (x + x_p), & -x_p \leq x \leq 0 \end{cases} \quad \text{----- (1)}$$

(See (19.2) and Fig. 19.3).

The space charge potential,  $\varphi(x)$  can be obtained by integrating  $E(x)$ :

$$\begin{aligned}
\varphi(x) &= -\int_{-x_p}^x dx E(x) \quad , \quad -x_p \leq x \leq 0 \\
&= \int_{-x_p}^x \frac{qN_A}{\epsilon_s} (x+x_p) dx \\
&= \frac{qN_A}{2\epsilon_s} (x+x_p)^2 \text{ ----- (2)}
\end{aligned}$$

where  $\varphi(x)$  has been taken zero at  $x = -x_p$  and  $\varphi(x)$  is quadratic in  $x$ , as expected.

Continuing on in the range  $0 \leq x \leq x_n$ , one can write

$$\begin{aligned}
\varphi(x) &= \frac{qN_A}{2\epsilon_s} x_p^2 + \int_0^x dx \left( -\frac{qN_D}{\epsilon_s} \right) (x-x_n) \\
&= \frac{qN_A}{2\epsilon_s} x_p^2 + \frac{qN_D}{\epsilon_s} \left( x_n x - \frac{1}{2} x^2 \right) \text{ ----- (3)}
\end{aligned}$$

To examine the behavior of  $\varphi(x)$ , near edge of the junction on n-side,  $x_n$ , introduce a variable

$$\Delta x = x_n - x$$

and express  $\varphi(x)$  in terms of  $\Delta x$ :

$$\begin{aligned}
\varphi(x) &= \frac{qN_A}{2\epsilon_s} x_p^2 + \frac{qN_D}{2\epsilon_s} x_n^2 - \frac{qN_D}{2\epsilon_s} \Delta x^2 \\
&= \varphi_{bi} - \frac{qN_D}{2\epsilon_s} \Delta x^2 \text{ ----- (4)}
\end{aligned}$$

Note here that the intrinsic band bending is given by definition by

$$\varphi_{bi} \equiv \frac{qN_A}{2\epsilon_s} x_p^2 + \frac{qN_D}{2\epsilon_s} x_n^2$$

Thus, near the edge of the junction depletion region,  $x \approx x_n$ , the electron concentration decreases exponentially as the junction edge is approached from the n bulk (see Fig. (19.2) and (19.6) and one can write from (4)

$$\begin{aligned}
n(x) &= n_{n0} \exp - \frac{q^2 N_D \Delta x^2}{2\epsilon_s k_B T} \\
&= n_{n0} e^{-\xi^2}, \quad \xi \equiv \left( \frac{q^2 N_D}{2\epsilon_s k_B T} \right)^{1/2} \cdot \Delta x \text{ ----- (5)}
\end{aligned}$$

Thus, the validity of the completely depleted approximation depends on how fast  $n(x)$  reduces to become negligible, compared with  $N_D$  near the edge of the depletion region:

$$\begin{aligned}
g[N_D - n(x)] &= g[N_D - n_{n0} e^{-\xi^2}] \\
&\approx gN_D
\end{aligned}$$

To be specific, take  $\xi=2$  at which  $n_{n0} \exp - \xi^2 = 0.018n_{n0}$  is to be neglected, compared with  $N_D$ , The condition defines the spatial width in which the electron concentration is reduced from  $n_{n0}$  to the nearly depleted level:

$$2 = \xi$$

$$= \sqrt{\frac{q^2 N_D}{2\varepsilon_s k_B T}} \Delta \tilde{x}_n$$

That is

$$\Delta \tilde{x}_n = 2 / \sqrt{\frac{q^2 N_D}{2\varepsilon_s k_B T}} \text{----- (6)}$$

To assess (6) more explicitly, consider the  $p - n$  junction doped with  $N_A = 10^{17} \text{ cm}^{-3}$  and  $N_D = 10^{16} \text{ cm}^{-3}$ , respectively. Then one finds

$$\left[ \frac{q^2 N_D}{2\varepsilon_s k_B T} \right]^{1/2} = \left[ \frac{(1.6 \times 10^{-19})^2 \cdot 10^{16+6} 4\pi 8.988 \times 10^9}{2 \cdot 11.9 \cdot 1.381 \times 10^{-23} \cdot 300} \right]^{1/2}$$

$$\approx 1.71 \times 10^7 / \text{m} \text{----- (7)}$$

$$\approx 1.71 \times 10 / \mu\text{m}$$

where the Coulomb constant,

$$\frac{1}{4\pi\varepsilon_0} = 8.988 \times 10^9 \text{ Nm}^2 / \text{C}^2$$

was used, together with  $\varepsilon_r = 11.9$ , and  $T = 300\text{K}$ .

Hence, one finds

$$\Delta \tilde{x}_n = \frac{2}{\sqrt{\frac{q^2 N_D}{2\varepsilon_s k_B T}}} \approx 0.12 \mu\text{m}$$

One can likewise find near  $-x_p$

$$\Delta \tilde{x}_p = \frac{2}{\sqrt{\frac{q^2 N_A}{2\varepsilon_s k_B T}}} \approx 0.04 \mu\text{m}$$

For  $N_A, N_D$  thus given

$$\varphi_{bi} = \frac{k_B T}{q} \ln \frac{N_A N_D}{n_i^2} \approx 0.525 \text{ V}$$

while the depletion depth is given by

$$W = \left[ \frac{2\varepsilon_s (N_A + N_D)}{q N_A N_D} \varphi_{bi} \right]^{1/2}$$

$$\approx 11 \mu\text{m}$$

(see (19.9),(19.8)). Using (19.7) one can in turn split  $W$  into  $x_n, x_p$  as

$$x_n = W / (1 + N_D / N_A) \approx 10 \mu\text{m}$$

$$x_p = W / (1 + N_A / N_D) \approx 1 \mu\text{m}$$

Hence

$$\Delta \tilde{x}_n / x_n \approx 0.01$$

$$\Delta \tilde{x}_p / x_p \approx 0.035$$

and therefore the completely depleted approximation for specifying the space charge is shown accurate in most of the depletion region,  $W$ .

19.3 (a) Given the linearly graded space charge

$$\rho = \begin{cases} q(N_A - N_D) = ax, & -W/2 \leq x \leq W/2 \\ 0, & \text{otherwise} \end{cases}$$

one can find the space charge field from the poisson's equation:

$$\frac{\partial E}{\partial x} = -\frac{a}{\epsilon_s} x$$

Integrating, there results

$$E(x) = -\frac{a}{2\epsilon_s} x^2 + A$$

The constant of integration is determined by the boundary condition

$$\begin{aligned} E(\pm W/2) &= 0 \\ &= -\frac{a}{2\epsilon_s} (W/2)^2 + A \end{aligned}$$

so that one can write

$$E(x) = -\frac{a}{2\epsilon_s} \left[ \left( \frac{W}{2} \right)^2 - x^2 \right] \text{----- (1)}$$

Once the electric field is known, the space charge potential can be readily found using

$$-\frac{\partial \phi(x)}{\partial x} = E(x)$$

Integrating both sides with the use of (1)

$$\phi = -\frac{a}{2\epsilon_s} \left[ \left( \frac{W}{2} \right)^2 x - \frac{1}{3} x^3 \right] + B$$

Here, the constant of integration is determined from the boundary condition,

$$\begin{aligned} \phi(-W/2) &= 0 \\ &= -\frac{a}{2\epsilon_s} \left[ \left( \frac{W}{2} \right)^2 \left( -\frac{W}{2} \right) - \frac{1}{3} \left( -\frac{W}{2} \right)^3 \right] + B \end{aligned}$$

Hence

$$\begin{aligned} \phi(x) &= -\frac{2}{3} \frac{a}{2\epsilon_s} \left( \frac{W}{2} \right)^3 - \frac{a}{2\epsilon_s} \left[ \left( \frac{W}{2} \right)^2 x - \frac{1}{3} x^3 \right] \\ &= \frac{a}{2\epsilon_s} \left( \frac{W}{2} \right)^3 \left[ \frac{1}{3} \xi^3 - \xi - \frac{2}{3} \right], \quad \xi = \frac{x}{W/2} \end{aligned}$$

(b) The built-in potential,  $\phi_{bi} = \phi(W/2) - \phi(-W/2)$ , is specified in terms of the doping level

in the two bulk regions. Since  $\varphi(-W/2)$  was taken zero in this case, one can write

$$\begin{aligned}\varphi_{bi} &= \varphi(W/2) \\ &= -\frac{2a}{\epsilon_s} \left(\frac{W}{2}\right)^3, \quad a = q(N_A - N_D) < 0 \\ &= \frac{k_B T}{q} \ln\left(\frac{N_A N_D}{n_i^2}\right)\end{aligned}$$

Given  $N_A, N_D, \varphi_{bi}$  and  $W$  are determined in a manner similar to the p-n step junction, together with space charge field and potential. The  $I - V$  behavior can then be modeled in steps identical to the case of the step junction diode.

19.4 Under bias the system is pushed away from equilibrium into nonequilibrium and current flows. The current is generally specified in terms of quasi-Fermi levels as

$$J_n = \mu_n n \frac{d}{dx} E_{Fn} \quad \text{----- (1a)}$$

$$J_p = \mu_p p \frac{d}{dx} E_{Fp} \quad \text{----- (1b)}$$

(see (18.51) in the text) Also, the forward current in the  $p - n$  junction is specified from (19.27), (19.28) by

$$J_n \approx \frac{qD_n n_{p0}}{L_n} e^{qV/k_B T}, \quad x = -x_p \quad \text{----- (2a)}$$

$$J_p \approx \frac{qD_p p_{n0}}{L_p} e^{qV/k_B T}, \quad x = x_n \quad \text{----- (2a)}$$

By inserting (2) into (1) one can specify the slope of the quasi-Fermi levels in  $W$  :

$$\frac{dE_{Fn}}{dx} = \frac{(qD_n n_{p0} / L_n) e^{qV/k_B T}}{\mu_n n_{n0}} \quad \text{----- (3a)}$$

$$\frac{dE_{Fp}}{dx} = \frac{(qD_p / L_p) e^{qV/k_B T}}{\mu_p p_{p0}} \quad \text{----- (3b)}$$

Note in (3) that  $n, p$  appearing in (1) should be identified to  $n_{n0}, p_{p0}$  when applied to the junction depletion region. Take a specific case in which the p-n junction is doped with  $N_A = 10^{17} \text{ cm}^{-3}, N_D = 10^{16} \text{ cm}^{-3}$ , respectively and consider the slope of  $E_{Fn}$  in  $W$ . Using the Einstein relation one can write from (3a)

$$\begin{aligned}\frac{dE_{Fn}}{dx} &= \frac{k_B T \mu_n n_{p0} e^{qV/k_B T}}{L_n \mu_n n_{n0}} \\ &= \frac{k_B T}{L_n} \frac{n_i^2}{p_{p0} n_{n0}} e^{qV/k_B T}\end{aligned} \quad \text{----- (4)}$$

Now, with the use of  $\mu_n = 800 \text{ cm}^2 / V \cdot s$  and lifetime  $\tau_n$  of  $0.1 \mu s$  in Si, for example, one can estimate the diffusion length:

$$\begin{aligned}
L_n &= (D_n \tau_n)^{\frac{1}{2}} \\
&= \left( \frac{k_B T \mu_n \tau_n}{q} \right)^{\frac{1}{2}} \\
&= \left( \frac{1.381 \times 10^{-23} \cdot 300 \cdot 800 \cdot 10^{-4} \cdot 10^{-7}}{1.6 \times 10^{-19}} \right)^{\frac{1}{2}} \\
&\approx 1.46 \times 10^{-5} \text{ m} \\
&= 14.6 \mu\text{m}
\end{aligned}$$

Using this estimation of  $L_n$  in (4), together with  $p_{p0} = 10^{17} \text{ cm}^{-3}$ ,  $n_{n0} = 10^{16} \text{ cm}^{-3}$  one can estimate the slope of  $E_{Fn}$  at 300K:

$$\begin{aligned}
\frac{dE_{Fn}}{dx} &= \frac{1.381 \times 10^{-23} \cdot 300 (1.45 \times 10^{10})^2}{1.46 \times 10^{-5}} \cdot \frac{10^{17} 10^{16}}{10^{17} 10^{16}} \cdot e^{qV/k_B T} \\
&\approx 6 \times 10^{-29} e^{qV/k_B T} \quad \text{J / m} \\
&= 3.7 \times 10^{-16} e^{qV/k_B T} \quad \text{eV / } \mu\text{m}
\end{aligned}$$

Thus, for the forward voltage,  $V = 0.6V$ , for example,

$$e^{\frac{qV}{k_B T}} \approx 1.2 \times 10^{10}$$

and

$$\frac{dE_{Fn}}{dx} \approx 4.8 \times 10^{-6} \text{ eV / } \mu\text{m}$$

Hence, in the junction depletion depth corresponding to  $N_A = 10^{17} \text{ cm}^{-3}$ ,  $N_D = 10^{16} \text{ cm}^{-3}$ , and  $W \approx 11 \mu\text{m}$  the total change of  $E_{Fn}$  therein is less than  $\sim 5 \times 10^{-5} \text{ eV}$ .

This means that the quasi equilibrium approximation of taking  $E_{Fn}$  flat in  $W$  is indeed a good approximation. However, with the forward voltage further increasing, the approximation ceases to be valid. For the case of reverse bias,

$$J_n \approx \frac{q D_n n_{p0}}{L_n} = \frac{k_B T \mu_n n_{p0}}{L_n}$$

and therefore the approximation is valid in general for any reverse bias.

One can examine the validity of flat  $E_{Fp}$  in  $W$  in a similar fashion.

19.5 (a) The junction band bending is determined by the sum of two Fermi levels operative in n- and p-bulks, i.e.

$$\phi_{bi} = \phi_{Fn} + \phi_{Fp}$$

Hence, if  $E_{Fn}$  is located above  $E_C$  in n-bulk and  $E_{Fp}$  below  $E_V$  in p- bulk,  $\phi_{bi}$  can be larger than  $E_G / q$ .

(b) The condition  $q\phi_{bi} = E_G$  can be achieved, if  $E_F = E_C$  and  $E_F = E_V$  in n- and p-bulks, for example. In this case one can write

$$\begin{aligned}
n &= N_D^+ = \frac{N_D}{1 + g_D e^{(E_F - E_D)/k_B T}} \\
&= \frac{2}{\sqrt{\pi}} N_C F_{1/2}(0), \quad E_C = E_F
\end{aligned}
\tag{1}$$

Also

$$\begin{aligned}
p &= N_A^- = \frac{N_A}{1 + g_A e^{(E_A - E_F)/k_B T}} \\
&= \frac{2}{\sqrt{\pi}} N_V F_{1/2}(0), \quad E_V = E_F
\end{aligned}
\tag{2}$$

Inserting the values of  $N_C, N_V$  and the ionization energies,  $E_C - E_D, E_A - E_F$  in (1), (2) for Si, Ge,  $N_A, N_D$  can be estimated.

19.6 (a) The overlap between conduction and valence bands by 0.2eV can be realized by raising  $E_F$  above  $E_C$  by 0.1eV, for example, and lowering  $E_F$  below  $E_V$  by 0.1eV, respectively. Thus one can write

$$\begin{aligned}
n &= N_D^+ \\
&= \frac{N_D}{1 + g_D e^{(E_F - E_D)/k_B T}} \\
&= \frac{2}{\sqrt{\pi}} N_C F_{1/2} \left( \frac{E_F - E_C}{k_B T} \right)
\end{aligned}
\tag{1}$$

with

$$E_F - E_C = 0.1eV$$

Also,

$$\begin{aligned}
p &= N_A^- \\
&= \frac{N_A}{1 + g_A e^{(E_A - E_F)/k_B T}} \\
&= \frac{2}{\sqrt{\pi}} N_V F_{1/2} \left( \frac{E_V - E_F}{k_B T} \right)
\end{aligned}
\tag{2}$$

with

$$E_V - E_F = 0.1eV$$

Inserting the respective values of  $N_C, N_V$  in (1),(2) at say 300K one can find the required doping levels,  $N_D, N_A$  in Si, GaAs.

(b) The flux of electrons under a forward bias is given from(19.28) by

$$\begin{aligned}
F_n &= J_n/q \\
&= \frac{D_n n_{p0}}{L_p} e^{qV/k_B T} \quad \text{----- (3a)} \\
&= \frac{k_B T \cdot \mu_n}{q \cdot L_p} \cdot \frac{n_i^2}{p_{p0}} e^{qV/k_B T}
\end{aligned}$$

where under this degeneration case

$$p_{p0} = \frac{2}{\sqrt{\pi}} N_V F_{1/2} \left( \frac{0.1}{k_B T (eV)} \right) \text{----- (3b)}$$

Likewise one can express the hole flux as

$$\begin{aligned}
F_p &= J_p/q \\
&= \frac{D_p p_{n0}}{L_p} e^{qV/k_B T} \\
&= \frac{k_B T \cdot \mu_p}{q \cdot L_p} \cdot \frac{n_i^2}{n_{n0}} e^{qV/k_B T} \quad \text{----- (4a)}
\end{aligned}$$

where

$$n_{n0} = \frac{2}{\sqrt{\pi}} N_C F_{1/2} \left( \frac{0.1}{k_B T (eV)} \right) \text{----- (4b)}$$

Inserting the respective values of  $N_C, N_V$  from *Si, GaAs*, together with the respective typical values of  $\mu_n, \mu_p$ , one can readily estimate the fluxes in the degenerate semiconductor systems.

19.7 (a) Recall from (19.6) – (19.9) that

$$\begin{aligned}
\phi_{bi} &= \frac{k_B T}{q} \ln \left( \frac{N_A N_D}{n_i^2} \right) \\
&= \frac{q}{2\epsilon_s} \cdot \frac{N_A N_D}{N_A + N_D} \cdot W^2 \\
&= \frac{1}{2} E_{\max} W \quad \text{----- (1)}
\end{aligned}$$

Also,

$$\begin{aligned}
x_n &= W / (1 + N_D / N_A) \\
x_p &= W / (1 + N_A / N_D)
\end{aligned}$$

Thus for given doping level,  $N_A, N_D$ , the junction parameters,  $\phi_{bi}, E_{\max}, W, x_n, -x_p$  can be readily evaluated.

(b) The application of reverse bias,  $-V_R$  induces the following changes or modifications :

$$\begin{aligned}
\phi_{bi} &\rightarrow \phi_{bi} + |V_R| \\
W(V_R) &= \left[ \frac{2\epsilon_s (N_A + N_D)}{q \cdot N_A N_D} (\phi_{bi} + |V_R|) \right]^{1/2}
\end{aligned}$$

(see(19.14)). Hence, from (1)



$$E_{\max} = \frac{2(\varphi_{bi} + |V_R|)}{\left[ \frac{2\epsilon_s (N_A + N_D)}{q \cdot N_A N_D} (\varphi_{bi} + |V_R|) \right]^{1/2}}$$

$$= \frac{2(\varphi_{bi} + |V_R|)^{1/2}}{\left[ \frac{2\epsilon_s (N_A + N_D)}{q \cdot N_A N_D} \right]^{1/2}} \text{----- (2)}$$

Hence one can find the breakdown voltage  $V_{BR}$  from (2) for given breakdown field,  $E_{\max} = 3 \times 10^5 \text{ V/cm}$ . It is important to note that  $V_{BR}$  depends sensitively on the doping levels,  $N_A, N_D$ . For example, at  $N_A = 2 \times 10^{18} \text{ cm}^{-3}$ ,  $N_D = 10^{15} \text{ cm}^{-3}$ ,  $\varphi_{bi} \approx 0.78 \text{ V}$  and  $V_{BR} \approx 17 \text{ V}$ . At the same  $N_A$  but for  $N_D = 2 \times 10^{17} \text{ cm}^{-3}$ , the built in potential is about the same, i.e.  $\varphi_{bi} \approx 0.9 \text{ V}$  but the breakdown voltage is reduced by a factor of about 10, i.e.  $V_{BR} \approx 1.2 \text{ V}$ .

19.8 The Zener breakdown is mainly dictated by the tunneling probability, in particular the Fowler-Nordheim tunneling, which is given from (6.12) by

$$T \sim \exp \left( - \frac{4(2m_n)^{1/2}}{3qE\hbar} E_G^{3/2} \right) \quad (1)$$

Here  $E_G$  is the bandgap and  $E$  the electric field operative in the junction. Under a reverse bias,  $-V_R$   $E$  is enhanced, the maximum value of which is given by

$$E_{\max} \sim \frac{2(\varphi_{bi} + |V_R|)^{1/2}}{\left[ \frac{2\epsilon_s (N_A + N_D)}{q \cdot N_A N_D} \right]^{1/2}} \quad (2)$$

as discussed in problem (19.7).

The critical electric field for the onset of Zener breakdown is determined by the fact that the critical electric field provides a triangular potential barrier for valence band electrons in the p region to undergo F-N tunneling into the conduction band in the n region, as shown in Fig.19.12 in the text. The thickness,  $d$  of the barrier as determined by the condition

$$qE \cdot d = E_G$$

i.e.

$$d = E_G / qE$$

is the critical factor of the F-N tunneling probability as clear from (1). This means that the bandgap,  $E_G$  is a key parameter dictating the onset of Zener breakdown. The larger the bandgap, the larger critical field is required.

Once  $E$  exceeds the critical value any farther increase of  $|V_R|$  enhances  $T$  exponentially, giving rise to exponential increase of junction reverse current.

In addition to the tunneling probability the incident flux of valence band electrons on the triangular potential barrier is an important parameter as well. The flux is commensurate with electron density therein and the thermal speed :

$$F_n \propto N_V v_T$$

$$\propto m_n^{3/2} \cdot m_n = m_n^{5/2}$$

Hence the effective mass of electrons constitutes another key parameter affecting the breakdown current.

19.9 (a) The diffusion equation of excess holes in the quasi-neutral region on the n-side is given by

$$p_n'' - \frac{p_n - p_{n0}}{L_n^2} = 0 \text{ ----- (1)}$$

Since the distance,  $d$  between the edge of the depletion region  $x_n$  and metal contact (see Fig.19.8) is shorter than  $L_n$ , the second term in (1) is to be neglected. In this case the excess holes depend linearly on  $x$ , i.e.

$$p_n(x) = A(x - x_n) + B \quad x \geq x_n \text{ ----- (2)}$$

Here, the two constants of integration are determined from the boundary conditions,

$$p_n(x = x_n) = p_{no} e^{qV/k_B T} \text{ ----- (3a)}$$

$$p_n(x = x_n + d) = p_{no} \text{ ----- (3b)}$$

Inserting (2) into (3), one can write

$$B = p_{no} e^{qV/k_B T}$$

$$A \cdot d + B = p_{no}$$

and by inserting A, B thus determined in (2) one can write

$$p_n(x) = p_{no} - p_{no} \left( e^{qV/k_B T} - 1 \right) x / d \text{ ----- (4a)}$$

(b) Therefore the hole diffusion current is given in this case by

$$\begin{aligned} J_p &= qD_p \left( -\frac{\partial p_n}{\partial x} \right) \\ &= \frac{qD_p p_{no}}{d} \left( e^{qV/k_B T} - 1 \right) \end{aligned}$$

while  $J_n$  is to be obtained in the same way as was done in the text.

19.10 (a) Consider the diffusion equation for excess holes,

$$p_n'' - \frac{p_n - p_{n0}}{L_p^2} + \frac{\tilde{g}_D}{D_p} = 0 \text{ ----- (1)}$$

with built in boundary conditions

$$p_n(x_n) = 0 \text{ ----- (2a)}$$

$$p_n(x \rightarrow \infty) = p_{no} + \tilde{g}_D \tau_p \text{ ----- (2b)}$$

(1) is a standard inhomogeneous linear differential equation,

$$p_n'' - \frac{p_n}{L_p^2} = - \left( \frac{p_{n0}}{L_p^2} + \frac{\tilde{g}_D}{D_p} \right)$$

The homogeneous solution is first obtained by putting the right hand side zero, in which case one finds

$$p_n = A e^{-(x-x_n)/L_p}$$

Here the term,  $\exp(x-x_n)/L_p$  is not included out of physical considerations. The particular solution is readily obtained from inspection as

$$p_n = p_{no} + \tilde{g}_0 \tau_p,$$

where

$$L_p^2 / D_p = \tau_p$$

Hence the solution reads

$$p_n(x) = A e^{-(x-x_n)/L_p} + p_{no} + \tilde{g}_D \tau_p \text{ ----- (3)}$$

Using (3) in (2a), one determines the constant of integration,

$$A = -(p_{no} + \tilde{g}_D \tau_p)$$

Thus the complete solution reads as

$$p_n(x) = (p_{no} + \tilde{g}_D \tau_p) (1 - e^{-(x-x_n)/L_p})$$

in agreement with (19.51) and the solution automatically satisfies the boundary condition (2b).

(b) The load voltage and current are given by

$$V_L = V - I_L R_s \text{ ----- (1)}$$

$$I_L = I_l - I_s (e^{qV/k_B T} - 1) \text{ ----- (2)}$$

Inverting (2) one can write

$$V = \frac{k_B T}{q} \left[ \ln \left( \frac{I_l - I_L}{I_s} \right) + 1 \right]$$

Therefore the load power is given by

$$\begin{aligned} P_L &= V_L I_L \\ &\approx V_L \left[ I_l - I_s \left( e^{\frac{qV}{k_B T}} - 1 \right) \right] \text{ ----- (3)} \end{aligned}$$

where for simplicity the series resistance  $R_s$  has been neglected and  $V_L$  is taken same as  $V$ . Hence the maximum power is obtained from

$$\begin{aligned} 0 &= \frac{\partial P_L}{\partial V_L} \Big|_{V_{Lm}} \\ &= I_l - I_s (e^{qV_{Lm}/k_B T} - 1) - V_L I_s e^{qV_{Lm}/k_B T} \cdot \frac{q}{k_B T} \\ &= I_l + I_s - I_s e^{qV_{Lm}/k_B T} \left( 1 + \frac{qV_{Lm}}{k_B T} \right) \end{aligned}$$

That is,

$$e^{qV_{Lm}/k_B T} = \frac{I_l + I_s}{I_s \left( 1 + \frac{qV_{Lm}}{k_B T} \right)}$$

$$= \frac{1 + I_l/I_s}{1 + qV_{Lm}/k_B T}$$

Equivalently

$$V_{Lm} = \frac{k_B T}{q} \ln \left( 1 + \frac{I_l}{I_s} \right) - \frac{k_B T}{q} \ln \left( 1 + \frac{qV_{Lm}}{k_B T} \right)$$

in which the first term is identical to  $V_{OC}$  which was derived in (19.57a).

Also, one can find the load current at which the maximum power is attained as follows.

$$\begin{aligned} I_{Lm} &= I_l - I_s \left( e^{qV_{Lm}/k_B T} - 1 \right) \\ &= I_l - I_s \frac{1 + I_l/I_s}{1 + qV_{Lm}/k_B T} \\ &\approx I_l - \frac{I_l}{qV_{Lm}/k_B T} = I_l \left( 1 - \frac{k_B T}{qV_{Lm}} \right) \end{aligned}$$

19.11 (a) It will be interesting to include the effect of series resistance  $R_s$  in the power expression,

$$\begin{aligned} P_L &= V_L I_L \\ &= (V - I_L R_s) \left[ I_l - I_s \left( e^{q(V - I_L R_s)/k_B T} - 1 \right) \right] \text{----- (4)} \end{aligned}$$

and analyze the maximum  $P_L$  in (4) by means of perturbation or numerical scheme.

(b) For extracting the maximum power one has to consider two key factors, i.e. the open circuit voltage,  $V_{OC}$  and the short circuit current  $I_{sc} = -I_l$ . Evidently maximizing these two quantities are the key issues. These two parameters are interrelated with each other by

$$V_{OC} = \frac{k_B T}{q} \ln \left( \frac{I_l}{I_s} \right) \text{----- (1)}$$

(see 19.57a) and  $V_{OC}$  is shown to increase with increasing  $I_l$ . Also, the photocurrent,  $I_l$  is critically dependent on the linear cell attenuation coefficient  $\alpha$ :

$$\begin{aligned} I_l &\propto g \\ &= \alpha I \end{aligned}$$

where

$$\alpha = A^* (\hbar\omega - E_G)^{1/2}$$

is critically dependent on the bandgap of the material (see(19.47)).

Naturally, enhancing  $I_l$  is a most important factor for the maximum power extraction. This in turn requires large linear attenuation coefficient,  $\alpha$  or equivalently small cell bandgap,  $E_G$ , so that larger fraction of solar radiation can be absorbed and utilized.

Increased  $I_l$  also increases  $V_{OC}$ , as pointed out but  $V_{OC}$  is also increased via reducing the saturation current  $I_s$ , as clear from (1). However, since

$$I_s \propto n_i^2$$

(see(19.26b)), the reduction of  $I_s$  necessitates smaller intrinsic concentration,  $n_i$  and since  $n_i \propto \exp - E_G/2k_B T$  it requires large bandgap.

In view of these an optimal compromise is needed for the maximum power extraction.

## Chapter 20

20.1 Refer to Fig. 20.2 in the text.

The band bending in pnp transistor provides quantum well for electrons in conduction band in the base region. When an electron approaches the base edges the potential hill near the edges pushes it back toward the bulk base.

When a hole approaches the edge, however, it rolls up the potential hill of the valence band to be pushed out of the base region. A potential hill pushing back electron should obviously push a hole upward the hill.

Thus, an electron rolls down the hill, while a hole roll up the hill pushed by corresponding forces. It is therefore obvious that the quantum well for holes in the valence band in npn transistor confines holes while electrons are pushed out of potential plateau in the conduction band near the base edges.

20. 2 (a) To derive the linking current in pnp transistor, note that electrons are confined by the quantum well in the base and there is no electron current:

$$J_n = q\mu_n nE + qD_n \frac{dn}{dx} = 0$$

Hence E is given with the use of Einstein relation by

$$\begin{aligned} E &= -\frac{D_n}{\mu_n} \frac{1}{n} \frac{dn}{dx} \\ &= -\frac{k_B T}{q} \frac{1}{n} \frac{dn}{dx} \end{aligned} \quad \text{----- (1)}$$

Inserting (1) into the expression for hole current density one can write

$$\begin{aligned} J_p &= q\mu_p pE - qD_p \frac{dp}{dx} \\ &= q \left[ \mu_p p \left( -\frac{k_B T}{q} \right) \frac{1}{n} \frac{dn}{dx} - D_p \frac{dp}{dx} \right] \text{----- (2)} \\ &= -qD_p \frac{1}{n} \left( p \frac{dn}{dx} + n \frac{dp}{dx} \right) \\ &= -qD_p \frac{1}{n} \frac{d}{dx} (pn) \\ \text{i.e. } -\frac{J_p n}{qD_p} &= \frac{d}{dx} (pn) \end{aligned}$$

where the Einstein relation

$$qD_p = k_B T \cdot \mu_p$$

has again been used.

Integrating (2) w.r.t. x over the base region one obtains from the left band side

$$\frac{J_p}{q^2} \int_0^{W_B} dx \frac{qn(x)}{D_p} = \frac{J_p}{q^2} \cdot \frac{1}{\tilde{D}_p} Q_B \text{----- (3a)}$$

where  $J_p$  is taken out of the integral since it should be constant,  $\tilde{D}_p$  is the effective hole diffusion constant which is again taken out of the integral via the mean value theorem and

$$Q_B = q \int_0^{W_B} dx n_n(x) = q \int_0^{W_B} dx N_{DB}(x)$$

is the Gummel number.

The right hand side yields

$$\begin{aligned} \int_0^{W_B} d(np) &= np \Big|_0^{W_B} \\ &= p_{p0} \left( n_{n0} e^{qV_{CB}/k_B T} - n_{n0} e^{qV_{EB}/k_B T} \right) \text{----- (3b)} \end{aligned}$$

where  $V_{CB}$ ,  $V_{EB}$  are the voltages applied at the p-type collector and p-type emitter, respectively w.r.t. the n-type base. Note that the bias is always referred to the voltage applied to the p side w.r.t. the n side, so that if the voltage is positive it is automatically taken as forward bias.

Equating (3a), (3b) one finds the linking current in pnp transistor:

$$I_p = -I_S (e^{qV_{CB}/k_B T} - e^{qV_{EB}/k_B T}) \text{----- (4a)}$$

where

$$I_S = \frac{A_E q^2 p_{n0}}{Q_B} = \frac{A_E q n_i^2}{N_{DB} W_B} \text{----- (4b)}$$

is given in terms of cross-sectional area,  $A_E$  and base donor doping level.

(b) Under a forward active bias,  $V_{EB} > 0$ ,  $V_{CB} < 0$  and  $p_n(x=0) = p_{n0} \exp(qV_{EB}/k_B T)$  while  $p_n(W) = p_{n0} \exp(-qV_{CB}/k_B T) \approx 0$ .

The diffusion equation for excess holes in the base region is given by

$$p_n'' - \frac{p_n - p_{n0}}{L_p^2} = 0, \quad L_p^2 = D_p \tau_p$$

Since  $W_B < L_p$ , one may neglect the second term, in which case  $p_n(x)$  is linear in  $x$ , i.e.

$$p_n(x) = p_{n0} e^{qV_{EB}/k_B T} \left( 1 - \frac{x}{W_B} \right) + p_{n0} e^{qV_{CB}/k_B T} \frac{x}{W_B} \text{----- (5)}$$

Note that  $p_n(x)$  satisfies the boundary conditions at  $x = 0$ ,  $x = W_B$ , respectively.

With  $p_n(x)$  thus found the collector current is specified as

$$I_C = A_E q D_p \left( -\frac{dp_n}{dx} \right) = I_S (e^{qV_{EB}/k_B T} - e^{qV_{CB}/k_B T}) \text{----- (6)}$$

with

$$I_S = \frac{A_E q D_p n_i^2}{N_{DB} W_B}, \quad p_{n0} = \frac{n_i^2}{N_{DB}}$$

(6) is in agreement with the expression of the linking current, (4a) as it should.

(c) The recombination of  $p_n$  as occurs in the base is to be described by

$$I_{rB} = qA_E \int_0^{W_B} \frac{p - p_{n0}}{\tau_p} dx \text{ ----- (7)}$$

Using (5) in (7) and performing the integration one finds

$$I_{rB} = \frac{qA_E n_i^2 W_B}{2N_{DB} \tau_p} e^{qV_{EB}/k_B T} \text{ ----- (8)}$$

Hence the base transport factor reads as

$$\alpha_T = \frac{|I_C|}{|I_{pE}|} = \frac{|I_{pE}| - |I_{rB}|}{|I_{pE}|} = 1 - \frac{|I_{rB}|}{|I_{pE}|} = 1 - \frac{W_B^2}{2L_{pB}^2} \text{ ----- (9)}$$

where

$$I_{pE} = \tilde{I}_{pE} (e^{qV_{EB}/k_B T} - 1) \approx \tilde{I}_{pE} e^{qV_{EB}/k_B T}, \quad \tilde{I}_{pE} = \frac{A_E q D_{pB} n_i^2}{N_{DB} W_B} \text{ ----- (10)}$$

The hole current,  $I_{pE}$  injected from the emitter to base under a forward bias is accompanied by the electron current injected in the opposite direction from base to emitter:

$$I_{nE} = \tilde{I}_{nE} e^{qV_{EB}/k_B T}, \quad \tilde{I}_{nE} = \frac{A_E q D_{nE} n_i^2}{N_{AE} \tilde{l}_{nE}}$$

with  $\tilde{l}_{nE}$  denoting the lesser of the emitter width  $W_E$  and the electron diffusion length,  $L_n$ .

Hence the emitter injection efficiency is given by

$$\gamma = \frac{I_{pE}}{I_{pE} + I_{nE}} = \frac{1}{1 + \frac{I_{nE}}{I_{pE}}} = \frac{1}{1 + \frac{GN_B D_{nE}}{GN_E D_{pB}}}$$

where  $GN$  denotes the respective Gummel numbers.

The net current gain is therefore

$$\alpha_F = \frac{|I_C|}{|I_E|} = \frac{|I_{pE}|}{|I_{pE}| + |I_{nE}|} \cdot \frac{|I_C|}{|I_{pE}|} = \gamma \alpha_T$$

and the amplification factor is given from the Kirchhoff's law by

$$\beta_F = \frac{|I_C|}{|I_B|} = \frac{\alpha_F}{1 - \alpha_F}$$

(see (20.18))

20.3 The collector current is contributed by the diffusing minority carriers in the base. In the npn transistor  $I_C$  is due to the diffusion flux of electrons in the p-type case, while in pnp transistor  $I_C$  is due to the diffusion flux of holes in n – type base. In either case the injected minority carriers are described by  $\exp(qV_{BE}/k_B T)$  or  $\exp(qV_{EB}/k_B T)$ . The resulting diffusion currents are always accompanied by the respective recombination currents  $\propto \exp(qV_{BE}/2k_B T)$  or  $\exp(qV_{EB}/2k_B T)$ . However, the latter current is not connected to the output collector terminal as clear from Fig. 20.5 and  $I_C$  is therefore solely contributed by the diffusion fluxes of carriers and is therefore characterized by  $I_C \propto \exp(qV_{BE}/k_B T)$  or  $\exp(qV_{EB}/k_B T)$ .

20.4 To set up the Ebers Moll equations in pnp transistor recall that the emitter current is contributed



by holes in the base and electrons in the emitter:

$$I_E = I_S (e^{qV_{EB}/k_B T} - e^{qV_{CB}/k_B T}) + \tilde{I}_{nE} (e^{qV_{EB}/k_B T} - 1) \text{----- (1)}$$

where

$$I_S = \frac{A_E q D_p n_i^2}{N_{DB} W_B}, \quad \tilde{I}_{nE} = \frac{A_E q D_{nE} n_i^2}{N_{AE} \tilde{l}_{nE}}$$

with

$$\tilde{l}_{nE} = W_E \text{ or } L_n$$

denoting the lesser of  $W_E, L_n$ . It is important to note in (1) that the current flow is taken positive when it flows into the device through the terminal in this case the emitter, as clearly sketched in Fig. 20.5 The voltage applied to the collector  $V_{CB}$  also induces the electron current in the collector and is given by

$$I_{nC} = \tilde{I}_{nC} (e^{qV_{CB}/k_B T} - 1), \quad \tilde{I}_{nC} = -\frac{q A_C D_{nC} n_i^2}{N_{AC} \tilde{l}_{nC}} \text{----- (2)}$$

with

$$\tilde{l}_{nC} = W_C \text{ or } L_n$$

again denoting the lesser of the two. Note in (2) that the current flowing into the device through the collector terminal is taken positive.

The emitter and collector currents can be reexpressed from (1), (2) by regrouping the terms as

$$I_E = I_{ES} (e^{qV_{EB}/k_B T} - 1) - \alpha_R I_{CS} (e^{qV_{CB}/k_B T} - 1) \text{----- (3)}$$

$$I_C = I_{CS} (e^{qV_{CB}/k_B T} - 1) - \alpha_F I_{ES} (e^{qV_{EB}/k_B T} - 1) \text{----- (4)}$$

where

$$I_{ES} \equiv I_S + \tilde{I}_{nE}, \quad I_{CS} \equiv I_S + \tilde{I}_{nC}$$

$$\alpha_R \equiv \frac{I_S}{I_S + \tilde{I}_{nC}}, \quad \alpha_F \equiv \frac{I_S}{I_S + \tilde{I}_{nE}}$$

(3), (4) are the Ebers-Moll equations for pnp transistor. These equations can be cast into the forward active and reverse active currents as

$$I_E = I_F - \alpha_R I_R$$

$$I_C = I_R - \alpha_F I_F$$

where

$$I_F \equiv I_{ES} (e^{qV_{EB}/k_B T} - 1)$$

$$I_R \equiv I_{CS} (e^{qV_{CB}/k_B T} - 1)$$

and from Kirchhoff's law the base current can be expressed in terms of the collector and emitter currents, i.e.

$$I_B = -I_C - I_E$$

The equivalent circuit of pnp transistor is identical to that of npn transistor shown in Fig. 20.6 in the text. The only modification required is,  $I_F, I_R$  are directed in the opposite directions from the case of npn transistor.

20.5 (a) To model  $I_E, I_C$  in terms of the time constants involved, consider first the excess hole charge in the base as the minority carrier in pnp transistor. One can write

$$Q_B = \int_0^{W_B} qA_E(p_n(x) - p_{n0})dx \text{ ----- (1)}$$

Under a forward active bias,

$$\begin{aligned} p_n(x) &= p_{n0}e^{qV_{EB}/k_B T} \left(1 - \frac{x}{W_B}\right) + p_{n0}e^{qV_{CB}/k_B T} \frac{x}{W_B} \text{ ----- (2)} \\ &\approx p_{n0}e^{qV_{EB}/k_B T} \left(1 - \frac{x}{W_B}\right) \end{aligned}$$

Inserting (2) into (1) and performing the integration one finds

$$\begin{aligned} Q_{pB} &= A_E q \frac{1}{2} p_{n0} (e^{qV_{EB}/k_B T} - 1) W_B \\ &\approx A_E q \frac{1}{2} p_{n0} e^{qV_{EB}/k_B T} W_B \end{aligned}$$

Hence the base transit time of holes is given by definition by

$$\tau_{trB} = \left| \frac{Q_{pB}}{I_C} \right| = \frac{W_B^2}{2D_p}$$

since under forward active bias the collector current is given by

$$|I_C| \cong \frac{A_E q D_p n_i^2}{N_{DB} W_B} e^{qV_{EB}/k_B T}$$

In addition, the hole injection into the base  $|Q_{pB}|$  is accompanied by the electron injection into the emitter  $|Q_{nE}|$ , both of which are proportional to the diode factor:

$$\begin{aligned} Q_F &= |Q_{pB}| + |Q_{nE}| \\ &= Q_{F0} (e^{qV_{EB}/k_B T} - 1) \end{aligned}$$

Thus given  $Q_F, I_C, I_B$  are to be expressed in terms of the time constants:

$$\begin{aligned} I_C &= \frac{Q_F}{\tau_F} \\ I_B &= \frac{Q_F}{\tau_{BF}} \end{aligned}$$

Since  $Q_F$  is primarily contributed by  $Q_{pB}$  one can write

$$\begin{aligned} I_C &= \frac{Q_F}{\tau_F} \\ &\approx \frac{Q_{pB}}{\tau_{trB}}, \quad \tau_{trB} = \frac{W_B^2}{2D_p} \end{aligned}$$

Hence

$$\tau_F \approx \tau_{trB}$$

Also,  $\tau_{BF}$  is well approximated by the recombination time of holes in the base,  $\tau_p, \tau_{BF} \approx \tau_p$ .

(b) Therefore, the gain factor is to be represented by the time constants as

$$\beta_F = \left| \frac{I_C}{I_B} \right| \approx \frac{\tau_p}{\tau_{trB}} = \frac{\tau_p}{W_B^2 / 2D_p} = \frac{2L_p^2}{W_B^2}$$

Clearly the smaller base width, the larger the gain.

(c) The terminal currents can thus be expressed in terms of charges stored and time constants involved. The base current is given under forward active bias by

$$I_B = \frac{Q_F}{\tau_{BF}} + \frac{dQ_F}{dt} + \frac{dQ_{VE}}{dt} + \frac{dQ_{VC}}{dt}$$

where the first two terms represent the steady state and transient contribution of  $Q_F$ , while the remaining two terms account for the transient change of  $I_B$  due to decreased uncompensated dopant charge in the base emitter junction and increased uncompensated dopant charge at the base collector junction, respectively. Naturally this is associated with the reduction or extension of the junction depletion depth under bias. Likewise one can write

$$I_C = \frac{Q_F}{\tau_F} - \frac{dQ_{VC}}{dt}$$

$$I_E = -I_B - I_C$$

20.6 Compare first  $n^{++} - p^+ - n$  transistor with npn transistor. The amplitudes of  $I_E$ ,  $I_C$  and base recombination currents are dependent on  $N_{AB}$  in the base as

$$I_E \sim I_C \sim I_S \sim \frac{A_E q D_n n_i^2}{N_{AB} W_B}$$

$$I_{rB} \sim \frac{q A_E n_i^2 W_B}{N_{AB} \tau_n}$$

and the emitter injection efficiency is specified by

$$\gamma \sim \frac{1}{1 + \frac{W_B N_{AB} D_{pE}}{W_E N_{DE} D_{nB}}}$$

Thus, disregarding the degenerate statistics of carrier concentrations for now,  $I_E$ ,  $I_C$  are shown to decrease with increasing doping level  $N_{AB}$ .

$I_{rB}$  also decreases with  $N_{AB}$  but the minority carrier lifetime, in this case,  $\tau_n$  could also decrease to off-set the decrease of  $I_{rB}$ . Clearly, the emitter injection efficiency could approach unity for  $N_{DE} \gg N_{AB}$ . It would be interesting to examine the effect of degenerate statistics, replacing  $N_{AB}$ ,  $N_{DE}$  by  $p_{p0}$ ,  $n_{n0}$ , respectively and examine the currents involved.

It should also be noted that with  $p^+$  doping in the base, the base width  $W_B$  can be shortened to enhance the current gain,  $\beta$  while preserving the neutral base.

Comparing  $p^{++} - n^+ - p$  transistor with the usual pnp transistor is to be carried out in similar fashion. The only modification required in this case is to interchange the roles of electron and holes and  $N_{AB} \rightarrow N_{DE}$ ,  $N_{DE} \rightarrow N_{AE}$ .

## Chapter 21

21. 1 (a) The problem consists of replacing the role of electrons with that of holes.

In n - substrate for PMOS the charge is generally specified by

$$\rho(x) = q[N_D^+ - n_n(x) + p_n(x)] \text{----- (1)}$$

Also, the charge neutrality in the n – bulk reads as

$$N_D^+ + p_{n0} = n_{n0} \text{----- (2)}$$

The surface band bending involved in this analysis is to be constructed as the mirror image of Fig. 21.4 in the text. Here one should introduce the Fermi potential for electrons above  $E_i$ ,  $q\phi_{Fn}$  and the band bends up as the surface is approached from the bulk for hole inversion.

Drawing the energy band diagram will be an interesting exercise.

If the space charge potential,  $\phi(x)$  increases as the surface is approached from the bulk, i.e.  $\phi(x) > 0$ , the electron potential energy,  $-q\phi(x)$  bends down, the spacing between  $E_C$  and  $E_F$  reduces. Consequently  $n_n(x)$  increases:

$$n_n(x) = n_{n0} e^{\beta\phi(x)}, \quad \beta = q / k_B T \text{----- (3)}$$

By the same token,  $p_n(x)$  decreases as

$$p_n(x) = p_{n0} e^{-\beta\phi(x)} \text{----- (4)}$$

If  $\phi(x)$  decreases on the other hand, the opposite situation prevails, i.e.  $p_n(x)$  increases while  $n_n(x)$  decreasing.

Combining (1) – (4) the Poisson equation reads as

$$\begin{aligned} \frac{d^2}{dx^2} \phi(x) &= -\frac{\rho}{\epsilon_S} \\ &= \frac{q}{\epsilon_S} \left[ n_{n0} (e^{\beta\phi} - 1) - p_{n0} (e^{-\beta\phi} - 1) \right], \quad \beta = q / k_B T \text{----- (5)} \\ &= \frac{qn_{n0}}{\epsilon_S} \left[ (e^{\beta\phi} - 1) - \frac{p_{n0}}{n_{n0}} (e^{-\beta\phi} - 1) \right] \end{aligned}$$

The first integration of (5) can be carried out by multiplying both sides with  $d\phi$ , as detailed in the text:

$$\begin{aligned} \int_0^\phi d\phi \frac{d^2\phi}{dx^2} &\equiv \int_0^\phi \frac{d\phi}{dx} d\phi \left( \frac{d\phi}{dx} \right) \\ &= \int_0^{-E} (-E) d(-E) \\ &= \frac{1}{2} E^2 \end{aligned}$$

while

$$\begin{aligned} \frac{qn_{n0}}{\epsilon_S} \int_0^\phi d\phi \left[ (e^{\beta\phi} - 1) - \frac{p_{n0}}{n_{n0}} (e^{-\beta\phi} - 1) \right] \\ = \frac{qn_{n0}}{\epsilon_S \beta} \left[ (e^{\beta\phi} - \beta\phi - 1) + \frac{p_{n0}}{n_{n0}} (e^{-\beta\phi} + \beta\phi - 1) \right] \end{aligned}$$

where one can put

$$\frac{qn_{n0}}{\epsilon_s \beta} \equiv \left( \frac{k_B T}{q} \right)^2 \frac{1}{L_D^2}$$

with the Debye screening distance specified by

$$L_D = \left( \frac{k_B T}{q^2} \frac{\epsilon_s}{n_{n0}} \right)^{1/2}$$

Hence, equating both sides there results

$$\begin{aligned} E(x) &= -\frac{d\varphi}{dx} \\ &= \mp \sqrt{2} \frac{k_B T}{q L_D} F\left(\beta\varphi_s, \frac{p_{n0}}{n_{n0}}\right) \end{aligned} \quad \text{----- (6)}$$

where

$$F\left(\beta\varphi_s, \frac{p_{n0}}{n_{n0}}\right) = \left[ (e^{\beta\varphi} - \beta\varphi - 1) + \frac{p_{n0}}{n_{n0}} (e^{-\beta\varphi} + \beta\varphi - 1) \right]^{1/2} \quad (7)$$

Now that the space charge field has been expressed in terms of the potential one can specify the surface charge density with the well known identity:

$$\begin{aligned} Q_s &= -\epsilon_s E_s, \\ &= \pm \sqrt{2} \frac{k_B T}{q L_D} F\left(\beta\varphi_s, \frac{p_{n0}}{n_{n0}}\right) \end{aligned} \quad \text{----- (8)}$$

with

$$\begin{aligned} E_s &\equiv E(x=0) \\ \varphi_s &\equiv \varphi(x=0) \end{aligned}$$

denoting the surface field and potential, respectively. Note that (8) for PMOS is similar in contents with (21.14) for NMOS. The obvious differences between the two consist of

$$\begin{aligned} \varphi_s &\leftrightarrow -\varphi_s \\ p_{p0} &\leftrightarrow n_{n0} \\ n_{p0} &\leftrightarrow p_{n0} \end{aligned}$$

(b) This differences imply in turn that the electron accumulation ensues for  $\varphi(x) > 0$  and hole inversion occurs for  $\varphi(x) < 0$  in PMOS. Also the surface depletion occurs for  $0 \leq \varphi(x) \leq 2\varphi_{Fn}$ .

(c) As discussed in the text, the capacitor consists of  $C_{ox}$  and  $C_s$  connected in series:

$$\frac{1}{C} = \frac{1}{C_{ox}} + \frac{1}{C_s}$$

where

$$C_{ox} \equiv \epsilon_{ox} / t_{ox}$$

is the oxide capacitance per unit area and

$$C_s \equiv \frac{\partial |Q_s|}{d\varphi_s}$$

accounts for the changes in the surface charge w.r.t.  $\varphi_s$ .

With the use of (8), one can write

$$C_S = \frac{\epsilon_S}{\sqrt{2}L_D} \frac{\left| 1 - e^{\beta\varphi_s} + \frac{p_{n0}}{n_{n0}} (e^{-\beta\varphi_s} - 1) \right|}{F(\beta\varphi_s, \frac{p_{n0}}{n_{n0}})} \text{----- (9)}$$

(9) is identical with (21.20) in context except for the polarity of  $\varphi_s$ .

In accumulation for  $\varphi(x) > 0$ ,

$$C_S \sim \frac{\epsilon_S}{\sqrt{2}L_D} e^{\beta|\varphi_s|/2}, \quad \beta = \frac{q}{k_B T}$$

while in inversion for  $\varphi(x) < 0$  and  $|\varphi_s| > 2\varphi_{Fn}$ ,

$$C_S \sim \frac{\epsilon_S}{\sqrt{2}L_D} \sqrt{\frac{p_{n0}}{n_{n0}}} e^{\beta|\varphi_s|/2}$$

In the depletion region in which  $0 \leq \varphi_s \leq 2\varphi_{Fn}$

$$C_S \sim \frac{\epsilon_S}{\sqrt{2}L_D} \frac{1}{\sqrt{\beta\varphi_s}} \approx \frac{\epsilon_S}{W_D}$$

(d) With the channel inversion well specified via  $\varphi_s$ , one can use the variable depletion approximation and derive  $I-V$  curve in the same way as detailed in the text.

The main difference consists of the polarity of  $V_G$ ,  $V_T$  and  $V_D$ .

$$I_D = \frac{W}{L} \mu_p C_{OX} (|V_G| - |V_T| - \frac{1}{2}|V_D|) |V_D|$$

21.2 As already discussed,

$$I_D \propto C_{OX} (V_G - V_T)$$

in NMOS and

$$I_D \propto C_{OX} (|V_G| - |V_T|)$$

in PMOS. In these devices, the quantum well is induced by applying  $V_G$  and mobile charge carriers are capacitively coupled into the well for conduction.

In contrast in bipolar junction transistor, the output collector current

$$I_C \propto \exp(qV_{BE} / k_B T)$$

in npn transistor and

$$I_C \propto \exp(qV_{EB} / k_B T)$$

in pnp transistor and these currents are driven by the diffusive spilling in of charge carriers across the lowered junction potential barriers. Thus, the difference consists of capacitive coupling of charges and diffusive exponential spilling in of charge carriers across the lowered potential barrier.

21.3 (i) Consider first the  $n^+$  polygate NMOS. As clear from Fig. 21.2 the  $n^+$  polygate has the workfunction of  $q\varphi_{poly} \approx 4.05eV$ . To find the work function of the p substrate one has to find  $p_{p0}$ . This can be done from the given resistivity data:

$$\rho \equiv \frac{1}{q\mu_p p_{p0}} = 1\Omega cm$$

or

$$P_{p0} = \frac{1}{1.6 \times 10^{-19} C 400 \text{ cm}^2 / Vs 1 \Omega \text{ cm}}$$

$$= 1.56 \times 10^{16} \text{ cm}^{-3}$$

Hence from (17.30)

$$\varphi_{Fp} = \frac{k_B T}{q} \cdot \ln \left( \frac{P_{p0}}{n_i} \right)$$

$$= 25.8 \text{ mV} \cdot \ln \left( \frac{1.56 \times 10^{16}}{1.45 \times 10^{10}} \right)$$

$$= 0.36 \text{ V}$$

Hence the work function of the p substrate is given by

$$q\varphi_{sc} = q\chi + E_G / 2 + q\varphi_{Fp}$$

$$= (4.05 + 0.56 + 0.36) \text{ eV}$$

$$= 4.97 \text{ eV}$$

Hence the flat band voltage is given by

$$V_{FB} = \varphi_{poly} - \varphi_{sc}$$

$$= -0.92 \text{ V}$$

(ii) For p<sup>+</sup> polygate and n substrate PMOS, one find n from the data

$$\rho = \frac{1}{q\mu_n n} = 1 \Omega \text{ cm}$$

so that

$$n_{n0} = 7.8 \times 10^{15} \text{ cm}^{-3}$$

and

$$\varphi_{Fn} = \frac{k_B T}{q} \cdot \ln \left( \frac{n_{n0}}{n_i} \right) = 0.34 \text{ V}$$

Hence,

$$V_{FB} = \varphi_{poly} - \varphi_{sc}$$

$$= (4.05 + 1.12) - [4.05 + (0.56 - 0.34)]$$

$$= 0.9 \text{ V}$$

Therefore, for the case of NMOS the band bends down by  $0.92 \text{ eV}$  as the surface is approached from the p bulk (see Figs. 21.2 and 21.3). For the case of PMOS the band bends up by  $0.9 \text{ eV}$ . To flatten out the band bending the flat band voltages are required. It will be instructive to sketch these energy levels, together with the flat band configuration.

21.4 (a) To find the inverted electron density, introduce the variable resistor associated with NMOS:

$$I_D = \frac{W}{L} C_{OX} \mu_n (V_G - V_T - \frac{1}{2} V_D) V_D$$

$$\equiv \frac{V_D}{R}$$

where the  $V_G$  controlled channel resistor is given by

$$\frac{1}{R} = \frac{W}{L} C_{OX} \mu_n (V_G - V_T - \frac{1}{2} V_D)$$

$$\equiv \frac{1}{\rho \cdot \frac{L}{W \cdot t_{ch}}} \quad \text{----- (1)}$$

$$\equiv \frac{W \cdot t_{ch}}{L} q \mu_n n$$

where  $\rho$  is the resistivity and  $t_{ch}$  the effective thickness of the inverted channel.

Thus,  $W \cdot t_{ch}$  represent the effective cross-sectional area of the channel. Also, use has been made of

$$\rho = 1/\sigma = 1/q\mu_n n$$

Now, consider the case where

$$R = 5K\Omega$$

for example. Then for  $W/L = 5$  one can write from (1)

$$5 \times 10^3 \Omega = \frac{1}{5} \cdot \frac{1}{1.6 \times 10^{-19} C \cdot 600 cm^2 / Vs \cdot 1 \Omega cm \cdot n \cdot t_{ch}}$$

from which one finds

$$n \cdot t_{ch} = 6.7 \times 10^{11} cm^{-2}$$

For the channel thickness of about 10nm,

$$n \sim 6.7 \times 10^{17} cm^{-3}$$

(b) The gate voltage required is found from (1) as

$$C_{OX} (V_G - V_T - \frac{1}{2} V_D) = q \cdot n \cdot t_{ch}$$

or

$$q \cdot n \cdot t_{ch} = q \cdot 6.7 \times 10^{11} cm^{-2} = q \cdot 6.7 \times 10^{15} m^{-2}$$

$$= \frac{\epsilon_{OX}}{50 \cdot 10^{-9} m} (V_G - V_T - 0.05)$$

Hence

$$V_G - V_T \approx \frac{1.6 \times 10^{-19} \cdot 6.7 \times 10^{15} \cdot 50 \times 10^{-9} \cdot 4\pi \cdot 8.988 \times 10^9}{3.9}$$

$$= 1.6V$$

Here the Coulomb constant

$$\frac{1}{4\pi\epsilon_0} = 8.988 \times 10^9 Nm^2 / C^2$$

was used together with the oxide dielectric constant of  $\epsilon_r = 3.9$ .



One can carry out similar analyses for other resistor values.

21.5 (a) Given the device  $I-V$  curve

$$I_D = \frac{W}{L} C_{OX} \mu_n (V_G - V_T - \frac{1}{2} V_D) V_D, \quad V_{DSAT} = V_G - V_T \text{ ----- (1)}$$

one can formally express the same  $I_D$  in terms of the channel voltage  $V(y)$  at  $y$  distance from the source, i.e.

$$I_D = \frac{W}{y} C_{OX} \mu_n \left[ V_G - V_T - \frac{1}{2} V(y) \right] V(y) \text{ ----- (2)}$$

Equating (1), (2) one can write

$$\frac{1}{L} (V_G' - \frac{1}{2} V_D) V_D = \frac{1}{y} \left[ V_G' - \frac{1}{2} V(y) \right] V(y)$$

with

$$V_G' \equiv V_G - V_T$$

or after rearranging the terms one can write

$$V(y)^2 - 2V_G' V(y) + \frac{2y}{L} (V_G' - \frac{1}{2} V_D) V_D = 0$$

One can thus solve this quadratic equation for the channel voltage as a function of  $y$ , obtaining

$$V(y) = V_G' \pm \left[ V_G'^2 - \frac{2y}{L} (V_G' - \frac{1}{2} V_D) V_D \right]^{1/2} \text{ ----- (3)}$$

Since by definition

$$V(y=0) = 0$$

the solution is given by the negative branch of (3).

(b) Next, the longitudinal channel field is given in terms of  $V(y)$  as

$$\begin{aligned} E(y) &\equiv -\frac{\partial V(y)}{\partial y} \\ &= -\frac{(V_G' - \frac{1}{2} V_D) V_D}{L \left[ V_G'^2 - \frac{2y}{L} (V_G' - \frac{1}{2} V_D) V_D \right]^{1/2}} \text{ ----- (4a)} \\ &= -\frac{V_D}{L} \cdot \frac{1}{(\gamma - \alpha \frac{y}{L})^{1/2}} \end{aligned}$$

where

$$\gamma \equiv \frac{V_G'^2}{(V_G' - \frac{1}{2} V_D)^2} \text{ ----- (4b)}$$

$$\alpha \equiv 2 \frac{V_D}{V_G' - \frac{1}{2}V_D} \text{ ----- (4c)}$$

Note that in device saturation, i.e. for  $V_D = V_G'$ ,  $\gamma = 4$ ,  $\alpha = 4$ , so that the channel field E diverges at  $y = L$ , as expected

(c) With the use of (4), the electron transit time from source to drain is specified as,

$$\begin{aligned} \tau_{tr} &= \int_0^L \frac{dy}{v_d} \\ &= \int_0^L \frac{dy}{\mu_n |E(y)|} \\ &= \frac{L}{\mu_n V_D} \int_0^L dy \left(\gamma - \alpha \frac{y}{L}\right)^{1/2} \text{ ----- (5)} \\ &= \frac{L}{\mu_n V_D} \cdot \left(\frac{-2L}{3\alpha}\right) \left(\gamma - \alpha \frac{y}{L}\right)^{1/2} \Big|_0^L \\ &= \frac{2L^2}{3\mu_n V_D \alpha} \left[\gamma^{3/2} - (\gamma - \alpha)^{3/2}\right] \end{aligned}$$

(5) represents the general expression of the transit time of electrons as a function of  $V_G$ ,  $V_D$ . Note that the transit time,  $\tau_{tr}$  is given in essence by

$$\frac{L^2}{\mu_n V_D} = \frac{L}{\mu_n (V_D / L)} = \frac{L}{v_d}$$

as it should be. In device saturation where  $V_{DSAT} = V_G'$ ,  $\gamma = \alpha = 4$ , so that

$$\tau_{tr} = \frac{4}{3} \frac{L^2}{\mu_n V_{DSAT}}$$

21.6 (a) Consider first NMOS with n<sup>+</sup> polygate and substrate doping  $N_A = 10^{17} \text{ cm}^{-3}$ . The threshold voltage is given from (21.37) in terms of flat band voltage, Fermi potential and body effect coefficient as

$$V_T = V_{FB} + 2\phi_{Fp} + \gamma(\phi_{Fp} - V_B)^{1/2} \text{ ----- (1)}$$

The Fermi potential in p substrate is given from (17.30) at 300K by

$$\begin{aligned} \phi_{Fp} &= \frac{k_B T}{q} \ln \left( \frac{N_A}{n_i} \right) \\ &= 0.41V \end{aligned}$$

Hence the flat band voltage is given in terms of the work function difference between n<sup>+</sup> poly gate and p substrate as

$$\begin{aligned} V_{FB} &= 4.05 - (4.05 + 0.56 + \phi_{Fp}) \\ &= -0.97V \end{aligned}$$

The oxide capacitance at  $t_{OX} = 10\text{nm}$  is

$$\begin{aligned}
C_{ox} &= \frac{\epsilon_{ox}}{t_{ox}} \\
&= \frac{1}{10 \cdot 10^{-9}} \cdot \frac{3.9}{4\pi \cdot 8.988 \times 10^9} \\
&= 3.5 \times 10^{-3} \text{ C}^2 / \text{Nm}^3
\end{aligned}$$

Hence, the body effect coefficient at  $N_A = 10^{17} \text{ cm}^{-3}$  is given by

$$\begin{aligned}
\gamma &= \frac{(2\epsilon_s q N_A)^{1/2}}{C_{ox}} \\
&= \frac{1}{C_{ox}} \left[ \frac{2 \cdot 11.9 \cdot 1.6 \times 10^{-19} \cdot 10^{17+6}}{4\pi \cdot 8.988 \times 10^9} \right]^{1/2} \\
&= 0.53 \text{ V}^{1/2}
\end{aligned}$$

Therefore at zero bulk bias,  $V_B = 0$

$$\begin{aligned}
V_T &\approx -0.97 + 2 \cdot 0.41 + 0.53(2 \times 0.41)^{1/2} \\
&\approx 0.33 \text{ V}
\end{aligned}$$

Likewise, for PMOS with  $p^+$  poly gate and n substrate doping,  $N_D = 10^{17} \text{ cm}^{-3}$ ,

$$\begin{aligned}
V_T &= 0.97 - 2 \cdot 0.41 - 0.53(2 \times 0.41)^{1/2} \\
&= -0.33 \text{ V}
\end{aligned}$$

One can carry out similar analyses for other substrate doping levels.

(b) If a positive charge sheet  $Q_f$  is present at the interface between oxide and substrate, a negative charge sheet,  $-Q_f$  is required at the interface between the polygate electrode and oxide to achieve the flat band configuration.

The resulting voltage developed across the oxide is by definition the additional flat band voltage required. Thus, one can write

$$\Delta V_{FB} \cdot C_{ox} = -Q_f, \quad Q_f = q \cdot 10^{11} \text{ cm}^{-2}$$

and

$$\begin{aligned}
\Delta V_{FB} &= -\frac{Q_f}{C_{ox}} \\
&= -\frac{1.6 \times 10^{-19} \text{ C} \cdot 10^{11+4} / \text{m}^2}{3.5 \times 10^{-3} \text{ C} / \text{V}} \\
&= -0.05 \text{ V}
\end{aligned}$$

Here,  $C_{ox}$  obtained in (a) has been used. With the use of this new flat band voltage,  $V_T$  analysis can be carried out in the same way as in (a).

21.7 (a) The lifetime of electrons in the quantum well is determined by the condition,

$$NT \approx 1 \text{ ----- (1)}$$

where  $T$  is the tunneling probability and  $N$  the total average number the electron encounters the barrier before tunneling out of the well.

The barrier potential on the left of the well has the width thicker than that of the potential barrier on the right. Hence one needs to consider  $T$  across the barrier on the right hand side, which is given from (6.5), (6.6) by

$$T = \frac{1}{1 + \Lambda} \text{----- (1a)}$$

$$\Lambda = \frac{V^2}{4E(V-E)} \sinh^2 d \sqrt{\frac{2m}{\hbar^2}(V-E)} \text{----- (1b)}$$

where  $V = 3.1eV$  is the barrier height,  $E$  is the kinetic energy of electrons and  $d = 8nm$  is the barrier width. For well width  $W > 80nm$  the ground state energy of the quantum well is much smaller than thermal energy,  $k_B T / 2 = 25.8meV$  at 300K.

Hence we have to put  $E = k_B T / 2 \ll V$ .

Thus, (1b) simplifies as

$$\Lambda = \frac{V}{2k_B T} \frac{1}{4} \exp 2d \left( \frac{2m}{\hbar^2} V \right)^{1/2}$$

Hence, inserting given values of the parameter, one can write

$$\Lambda = \frac{3.1}{2 \cdot (0.0258)} \cdot e^\chi$$

where

$$\begin{aligned} \chi &= 2 \cdot 8 \times 10^{-9} \left[ \frac{2 \times 9.1 \times 10^{-31} \times 3.1 \times 1.6 \times 10^{-19}}{(1.055 \times 10^{-34})^2} \right]^{1/2} \\ &= 144 \end{aligned}$$

so that

$$T = \Lambda^{-1} \approx 1.93 \times 10^{-64}$$

Thus to satisfy the condition (1) N should be specified by

$$N \approx \frac{1}{T} \sim 5.2 \times 10^{63}$$

Now, the thermal speed of electron is given from the equipartition theorem as

$$\frac{1}{2} m v_T^2 = \frac{1}{2} k_B T$$

so that at 300K,

$$v_T \approx 6.8 \times 10^4 m/s$$

Therefore the lifetime of electron is given for  $W = 80nm$ , for example, by the round trap time of electron times  $N$ , i.e.

$$\begin{aligned} \tau &= \frac{2 \times 80 \times 10^{-9}}{6.8 \times 10^4} \cdot 5.2 \times 10^{63} \\ &\approx 1.2 \times 10^{52} \end{aligned}$$

and is shown nearly infinite. Naturally the lifetime increases with increasing well width,  $W$ .

(b) Evidently, reducing the lifetime to  $1\mu s$  necessitates enhancing tunneling probability to a sufficient extent. This can be done by applying electric field,  $E$ , so that the barrier potential on the right with smaller thickness  $d (= 8nm)$  transforms into a triangular shape. The resulting F – N tunneling is given from (6.12) by

$$T \approx \exp - \frac{4\sqrt{2m}}{3q|E|\hbar} (V - E)^{3/2}$$

$$\approx \exp - \frac{4\sqrt{2m}}{3q|E|\hbar} V^{3/2}, \quad V = 3.1eV$$

where the kinetic energy of electron is much smaller than barrier height and is neglected. As discussed in (a), the lifetime is thus given by the product of the round trip time times  $N(=1/T)$ , i.e.

$$\tau = \frac{2W}{v_T} \frac{1}{T}$$

$$= \frac{2 \times 80 \times 10^{-9}}{6.8 \times 10^4} \cdot \exp - \frac{4\sqrt{2m}V^{3/2}}{3q|E|\hbar}$$

Hence, by putting  $\tau = 10^{-6} s$ , the required E is found as

$$|E| = \frac{4\sqrt{2m}V^{3/2}}{3q\hbar} \frac{1}{\ln[10^6 \cdot (6.8/1.6)]}$$

$$= \frac{4 \cdot (2 \cdot 9.1 \times 10^{-31})^{1/2} (3.1 \times 1.6 \times 10^{-19})^{3/2}}{3 \cdot 1.6 \times 10^{-19} \cdot 1.055 \times 10^{-34} \cdot 17.6}$$

$$= 2.1 \times 10^9 V / m$$

$$= 2.1V / nm$$

(c) The ground state energy of the quantum well is approximately given from (4.9) by

$$E_1 = \frac{\hbar^2 \pi^2}{2mW^2}$$

and represents the 1D kinetic energy of electron, i.e.

$$\frac{1}{2} m v_z^2 = \frac{\hbar^2 \pi^2}{2mW^2}$$

Next, scale  $W$  in terms of  $nm$ ,

$$W = n \cdot 10^{-9}, \quad n = 1, 2, \dots$$

Then  $v_z$  as a function of  $W$  is given by

$$v_z = \left( \frac{\hbar \pi}{m 10^{-9}} \right) \frac{1}{n}$$

$$= \left( \frac{1.055 \times 10^{-34} \cdot 3.14}{9.1 \times 10^{-31} \cdot 10^{-9}} \right) \cdot \frac{1}{n}$$

$$= 3.6 \times 10^5 \cdot \frac{1}{n} m/s$$

(d) Hence, the width of the well in which  $v_z$  is equal to the thermal speed of free 1D electron is given by

$$6.8 \times 10^4 = 3.6 \times 10^5 \cdot \frac{1}{n}$$

i.e.

$$n = \frac{36}{6.8} = 5.3$$

That is, the well width is

$$W = 5.3 \text{ nm}$$

(e) For  $W$  ranging from 10 to 100nm the electron kinetic energy in the ground state is less than the thermal energy at room temperature. This suggests that for this range of  $W$ , the electron in the well can be viewed as classical particle moving with thermal speed, and the lifetime analysis carried out in (a) needs no modification resulting from discrete quantized energy level.

21.8 The excess electrons present in the floating gate screen the gate field lines applied to invert the channel. As a result the threshold voltage in the programmed cell is larger than that of the erased cell, as clearly illustrated in Fig. 21.18:

$$V_{TCGP} = V_{TCGE} + \frac{|Q_{FG}|}{C_{ONO}}$$

Here  $|Q_{FG}|$  is the excess electron charge stored in the floating gate and  $C_{ONO}$  is the oxide capacitance between floating and control gates.

Thus, at the oxide thickness of 15nm,

$$\begin{aligned} C_{ONO} &= \frac{\epsilon_{OX}}{t_{OX}} = \frac{\epsilon_r \cdot \epsilon_0}{t_{OX}} \\ &= \frac{3.9}{15 \times 10^{-9} \cdot 4\pi \cdot 8.988 \times 10^9} \\ &= 2.3 \times 10^{-3} \text{ C/Vm}^2 \end{aligned}$$

Thus, the threshold shift, for example, of 5V,

$$V_{TCGP} - V_{TCGE} = 5V$$

is caused by  $|Q_{FG}|$  which is given by

$$\begin{aligned} 5 \cdot C_{ONO} &= |Q_{FG}| \\ &= q \cdot N \end{aligned}$$

with  $N$  denoting the number of excess electrons. Hence one finds

$$\begin{aligned} N &= \frac{5 \cdot 2.3 \times 10^{-3}}{1.9 \times 10^{-19}} \\ &= 6 \times 10^{16} / \text{m}^2 \\ &= 6 \times 10^{12} / \text{cm}^2 \end{aligned}$$

For the floating gate with  $100 \times 100 \text{ nm}$  cross-sectional area for instance

$$N \approx 600$$

## Chapter 22

22.1 In the bulk MOSFET the channel inversion is formed in the quantum well, which is induced by  $V_G$ . In the quantum wire FET on the other hand the channel is built in during the device fabrication. Thus there is no need for the voltage induced channel. In addition, in the quantum wire FET the possible leakage path through the substrate is minimized, e.g. the punch through, hot hole induced forward biasing of the source junction, etc. Thus, the quantum wire devices are compatible with the downscaling the device dimensions. Furthermore, the vertical wire structure holds up the promise of higher degree of device integration.

However, the fabrication steps of the quantum wire devices are complicated, compared with bulk MOSFETs. Also, because of the scattering of charge carriers with rough oxide interface, the mobility in quantum wire FET could be lower than in bulk MOSFETs.

22.2 (a) The energy eigenequation of an electron in the quantum wire is given by

$$-\frac{\hbar^2}{2m_n} \left( \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} \right) \varphi(x, y, z) = E\varphi(x, y, z) \text{----- (1)}$$

Here the electron is confined in  $x, y$  directions, while it moves along the  $z$  – direction as a free particle. For simplicity of analysis, the potential barrier confining the electron is taken infinite. Then (1) readily reduces to two infinite potential well problems in  $x, y$  directions and the free particle motion in the  $z$  – direction. Thus one can write the wavefunction from chapter 4 as

$$\varphi(x, y, z) = u_n(x)u_m(y)e^{ikz} \text{----- (2a)}$$

where

$$u_n(x) = \left( \frac{2}{W} \right)^{1/2} \begin{cases} \cos k_n x & k_n = (2n+1)\pi/W & n = 0, 1, \dots \\ \sin k_n x & k_n = 2n\pi/W & n = 1, 2, \dots \end{cases} \text{----- (2b)}$$

$$u_m(y) = \left( \frac{2}{W} \right)^{1/2} \begin{cases} \cos k_m y & k_m = (2m+1)\pi/W & n = 0, 1, \dots \\ \sin k_m y & k_m = 2m\pi/W & n = 1, 2, \dots \end{cases} \text{----- (2c)}$$

The corresponding energy eigenvalues are given by

$$E = E_{nm} + \frac{\hbar^2 k^2}{2m_n} \text{----- (3a)}$$

$$E_{nm} = W_0(n^2 + m^2), \quad W_0 \equiv \frac{\hbar^2 \pi^2}{2mW^2} \text{----- (3b)}$$

(see (4.9)). The ground state and a few excited states are listed as follows, together with the degree of degeneracy.

	m	n	$E_{nm}$ in $W_0$ unit	Degeneracy
Ground level	1	1	2	1
1 <sup>st</sup> excited level	2	1	5	2
	1	2	5	
2 <sup>nd</sup> excited level	2	2	8	1
3 <sup>rd</sup> excited level	2	3	10	2
	3	2	10	

(b) The density of 1D electrons in the wire can be obtained in a way similar to what has been discussed in problem 16.6. The density is given by

$$n_{1D} = \sum_{nm} \Theta(E - E_{nm}) \int_{E_{nm}}^{\infty} g_{1D}(E) f_n(E) dE \text{ ----- (4a)}$$

where  $\Theta$  is the heavy side step function, and

$$g_{1D}(E) = \frac{\sqrt{2}m_n^{1/2}}{\pi\hbar^2} \frac{1}{(E - E_{nm})^{1/2}} \text{ ----- (4b)}$$

is the 1D density of state (see (4.31)) and

$$f_n(E) = e^{-(E-E_F)/k_B T}$$

is the Fermi occupation factor (see (17.1c))

Next, consider the integral

$$I = \int_{E_{nm}}^{\infty} dE \frac{\sqrt{2}m_n^{1/2}}{\pi\hbar} \frac{e^{-(E-E_{nm}+E_{nm}-E_F)/k_B T}}{(E - E_{nm})^{1/2}} \text{ ----- (5)}$$

where the sublevels in the quantum wire are defined w.r.t.  $E_C$ , i.e.

$$E_{nm} \equiv E_C + W_0(n^2 + m^2)$$

Introduce a dimensionless variable of integration,

$$\xi^2 \equiv \frac{E - E_{nm}}{k_B T}$$

Then  $I$  transforms as

$$\begin{aligned} I &= \frac{2\sqrt{2}m_n^{1/2}}{\pi\hbar} (k_B T)^{1/2} e^{-\frac{E_{nm}-E_F}{k_B T}} \int_0^{\infty} d\xi e^{-\xi^2} \\ &= \frac{\sqrt{2}m_n^{1/2}}{\pi\hbar} (k_B T)^{1/2} e^{-\frac{E_C-E_F+\Delta E_{nm}}{k_B T}} \end{aligned} \text{ ----- (6a)}$$

where the formula (1.24) in the text has been used and

$$\Delta E_{nm} \equiv W_0(n^2 + m^2) \text{ ----- (6b)}$$

Inserting (6) into (4a) there results

$$n_{1D} = \left( \frac{2m_n k_B T}{\pi\hbar^2} \right)^{1/2} e^{-\frac{E_C-E_F}{k_B T}} \sum_{nm} e^{-\frac{\Delta E_{nm}}{k_B T}}$$

(c) This problem remains an open ended question. In view of the channel formed physically in device fabrication the accumulation, depletion and inversion regions of capacitive coupling of electrons could be different from those of bulk MOSFET.

(d) In view of the lack of precise formulation of channel inversion the comparison between classical and quantum mechanical descriptions cannot be clearly made. However, one can point out a few general features distinguishing the two descriptions.

The first concerns with the issue of surface versus bulk channel inversion. Classically, the concentration profile of inverted electrons is sharply peaked at the oxide interface, as clearly shown in Fig. 21.10. Quantum mechanically, however, the profile is pushed away from the



interface due to the wave nature of electrons. This has a significant bearing on the  $C - V$  characteristics, as shown in Fig. 21.10.

The second concerns with the discrete energy levels operative in quantum description. This effect is clearly exhibited in (6) in terms of  $\Delta E_{nm}$ . The effect will be insignificant if  $\Delta E_{nm} \ll k_B T$  for large  $W$ . However, with decreasing  $W$   $\Delta E_{nm}$  could be larger than  $k_B T$ , which could lead to exponential reduction of inverted electrons.

22.3 Fig. 22.12 provides a convenient platform on which to analyze the problem. The Schottky barrier is defined as the difference between the energy level of  $E_V$  and  $E_{Fm}$  in this case:

$$\begin{aligned} q\phi_{Bp} &\equiv q\chi + E_G - q\phi_m \\ &= 4.05 + 1.12 - 4.75 \\ &= 0.42eV \end{aligned}$$

The built in barrier potential is determined as usual by the difference between two Fermi levels, i.e.

$$\begin{aligned} q\phi_{bi} &= E_{Fs} - E_{Fm} \\ &= q\chi + E_G - qV_p - q\phi_m \end{aligned}$$

Now, for  $N_A = 10^{18} \text{ cm}^{-3}$  for example

$$\begin{aligned} qV_p &\equiv E_G / 2 - q\phi_{Fp} \\ &= E_G / 2 - k_B T \ln \left( \frac{N_A}{n_i} \right) \\ &= 0.56 - 0.0258 \cdot \ln \left( \frac{10^{18}}{1.45 \times 10^{10}} \right) \\ &= 0.09eV \end{aligned}$$

Hence

$$\begin{aligned} q\phi_{bi} &= 4.05 + 1.12 - 0.09 - 4.75 \\ &= 0.33eV \end{aligned}$$

(b) Fig. 22.12 provides a typical band bending for p-type semiconductor in which  $E_{Fm} > E_{Fs}$ , in the absence of surface states.

One can readily introduce the surface states and surface layer in a manner similar to Fig. 22.13. The only difference consists of bending down of energy levels rather than bending up as the interface is approached from the semiconductor bulk.

Consider for simplicity a uniform distribution of surface state with density  $D_s$ . Prior to contacting the metal, surface states lying below  $E_F$  is occupied by electrons and as a result the band bends up at the surface as in Fig. 22.13.

When a contact is made with Au, however, electrons are transferred from metal to semiconductor, since  $E_{Fm} > E_{Fs}$  in this case. Consequently, the space charge similar to Fig. 22.12 is formed and band bends down as shown in the figure.

As a result of which, some of the electrons trapped at the surface states prior to contact is

released.

Now the difference between two Fermi levels,  $E_{Fm} - E_{Fs}$  or the corresponding work functions is partitioned between the built in potential and the surface layer potential, i.e.

$$(q\chi + E_G - qV_p) - q\phi_m = q\phi_{sl} + q\phi_{bi} \text{----- (1)}$$

Also, the positive charge sheet,  $Q_m$  on the metal surface is balanced by the surface charge of trapped electrons and space charge of dopant ions:

$$Q_m = |Q_{ss}| + |Q_{sc}| \text{----- (2)}$$

where

$$\begin{aligned} |Q_{sc}| &= qW \\ &= (2q\epsilon_S N_A \phi_{bi})^{1/2} \text{----- (3)} \end{aligned}$$

and

$$|Q_{ss}| = qD_s(qV_p + q\phi_{bi}) \text{----- (4)}$$

Here the depletion depth  $W$  in (3) corresponds to the case where  $N_D \gg N_A$  in (19.8b) and  $Q_{ss}$  in (4) is provided by electrons trapped in states below  $E_{Fs}$  in Fig. 22.12.

Finally,  $\phi_{sl}$  is specified by definition as

$$\phi_{sl} = \frac{Q_m}{\epsilon_i} \delta \text{----- (5)}$$

with  $\epsilon_i$  denoting the permittivity in the surface layer and  $\delta$  its thickness.

Inserting (2) – (5) into (1) one can write

$$\Lambda = \phi_{bi} + \frac{\delta}{\epsilon_i} \left[ qD_s(qV_p + q\phi_{bi}) + (2q\epsilon_S N_A \phi_{bi})^{1/2} \right] \text{----- (6a)}$$

where

$$\Lambda \equiv \chi + E_G / q - V_p - \phi_m \text{----- (6b)}$$

Regrouping the terms I (6a), one can write

$$a\phi_{bi} + b\phi_{bi}^{1/2} + c = 0 \text{----- (7)}$$

where

$$\begin{aligned} a &= 1 + \frac{q^2 D_s \delta}{\epsilon_i} \\ b &= \frac{(2q\epsilon_S N_A)^{1/2} \delta}{\epsilon_i} \\ c &= \frac{q^2 D_s V_p \delta}{\epsilon_i} - \Lambda \end{aligned}$$

The quadratic equation for  $\phi_{bi}^{1/2}$  can be readily solved, but in the limit of small  $\delta$  one can disregard the second term in (7) and obtain

$$\phi_{bi} = \frac{\Lambda - q^2 D_s V_p \delta / \epsilon_i}{1 + q^2 D_s \delta / \epsilon_i} \text{----- (8)}$$

Eq. (8) is the counterpart of (22-18), as applied to the p – substrate interfaced with Au. In the limit of no surface states,  $D_s = 0$ , the built in potential is strictly determined by  $\Lambda$ , that is, the difference between two Fermi levels (see (6b)).

In the other limit of large surface state, i.e.  $D_s \rightarrow \infty$  it follows from (8) that

$$\phi_{bi} = -V_p \text{ ----- (9)}$$

This specifically points to Fermi level pinning by surface states. As discussed earlier, when the surface state near  $E_V$  are filled with electrons the band bends up in a manner similar to Fig. 22.13. However, if  $E_V$  at the interface is raised up by an amount  $V_p$ , it hits the large interface density  $D_s$  and the band bending is pinned, regardless of Au contacting the substrate.

22.4 The I – V behavior of the Schottky diode made up of Au contacted silicon p substrate can be derived, following steps detailed in the text for the case of n-substrate. Evidently, the only modification required is to replace the role of electrons with that of holes. For this purpose one should sketch band bending corresponding to Fig. 22.14. In the present case the band bends down with  $E_{Fs}$  located on top of  $E_V$ .

To derive I-V curve due to the thermionic emission theory one should first consider the emission of holes from semiconductor to metal at thermodynamic equilibrium, i.e. at  $V = 0$  :

$$J_{sm}(V = 0) = q \int_{E_B}^{-\infty} dE g_{3D}(E) [1 - f(E)] v_x \text{ ----- (1)}$$

(see (22.19) in the text). Here

$$g_{3D} = \frac{\sqrt{2} m_p^{3/2}}{\pi^2 \hbar^3} (E_V - E) \text{ ----- (2a)}$$

is the 3D density of states for holes and the kinetic energy of holes is given by

$$E_V - E = \frac{1}{2} m_p v^2 \text{ ----- (2b)}$$

Also,

$$1 - f(E)$$

is the probability that the state is not occupied by the electron or hole occupation factor with  $f(E)$  denoting Fermi distribution function. Thus one can write

$$\begin{aligned} 1 - f(E) &= 1 - \frac{1}{1 - e^{E - E_F / k_B T}} \\ &= \frac{1}{1 + e^{E_F - E / k_B T}} \text{ ----- (2c)} \\ &\simeq e^{-(E_F - E) / k_B T} \\ &= e^{-(E_V + qV_p - E) / k_B T} \end{aligned}$$

since  $E < E_F$ . Inserting (2a) – (2c) into (1) one can write

$$J_{sm}(V = 0) = \frac{q m_p^3}{4\pi^2 \hbar^3} e^{\frac{-qV_p}{k_B T}} \int_{-\infty}^{\infty} dv_y e^{-\beta v_y^2} \int_{-\infty}^{\infty} dv_z e^{-\beta v_z^2} \int_{v_B}^{\infty} dv_x e^{-\beta v_x^2} v_x, \quad \beta = \frac{m_p}{2k_B T} \text{ ----- (3)}$$

where  $v_B$  represents the minimum hole velocity for overcoming the barrier,

$$\frac{1}{2} m_p v_B^2 = q\phi_{bi}$$

One can readily evaluate (3), using (1.24) in the text, obtaining

$$\begin{aligned} J_{sm}(V=0) &= A_p^* T^2 e^{\frac{-qV_p}{k_B T}} e^{\frac{-q\phi_{bi}}{k_B T}} \\ &= A_p^* T^2 e^{\frac{-q\phi_{Bp}}{k_B T}}, \quad A_p^* = \frac{qm_p k_B^2}{2\pi^2 \hbar^3} \end{aligned} \quad \text{----- (4)}$$

where

$$\phi_{Bp} \equiv \phi_{bi} + V_p \quad \text{----- (5)}$$

denotes the Schottky barrier given in terms of  $\phi_{bi}$  and  $qV_p = E_{Fs} - E_V$  (see Fig. 22.12). At equilibrium detailed balancing prevails, so that

$$J_{sm}(V=0) = J_{ms}(V=0) \quad \text{----- (6)}$$

Under bias,  $E_{Fs}$ ,  $E_{Fm}$  split to accommodate the voltage applied, while the Schottky barrier remains the same, since  $\phi_{Bp}$  is determined solely by the difference between the two work functions involved. Therefore, with  $V$  applied at the semiconductor,  $\phi_{bi}(V)$  should increase or decrease such that

$$\begin{aligned} q\phi_{Bp} &\equiv q\phi_{bi} + qV_p \\ &= qV + q\phi_{bi}(V) + qV_p \end{aligned} \quad \text{----- (7)}$$

remains fixed, regardless of  $V$ .

Therefore

$$\begin{aligned} q\phi_{bi}(V) &= q\phi_{Bp} - qV_p - qV \\ &= q\phi_{bi} - qV \end{aligned} \quad \text{----- (8)}$$

Inserting (8) into (4) one finds

$$\begin{aligned} J_{sm}(V) &= A_p^* T^2 e^{\frac{-qV_p}{k_B T}} e^{\frac{-q\phi_{bi}(V)}{k_B T}} \\ &= A_p^* T^2 e^{\frac{-qV_p}{k_B T}} e^{\frac{-q[\phi_{bi} - qV]}{k_B T}} \\ &= A_p^* T^2 e^{\frac{-q\phi_{Bp}}{k_B T}} e^{\frac{qV}{k_B T}} \end{aligned}$$

Hence under bias the detailed balancing is destroyed and current flows from the semiconductor to metal, i.e.  $-J_p$ ,

$$\begin{aligned} -J_p &= J_{sm}(V) - J_{sm}(V=0) \\ &= A_p^* T^2 e^{-q\phi_{Bp}/k_B T} (e^{qV/k_B T} - 1) \end{aligned} \quad \text{----- (9)}$$

Note in (9) that  $V$  is applied at semiconductor w.r.t. metal (see (7)). (9) indicates therefore that the forward current flows when a negative bias is applied at the metal.

Next, to derive I-V curves due to the drift diffusion theory, one has to start with

$$J_p = qp\mu_p E - qD_p \frac{\partial p}{\partial x} \text{----- (10)}$$

(see (22.58)) and the well known relationship,

$$D_p / \mu_p = k_B T / q \text{----- (11a)}$$

$$E = -\frac{\partial \phi}{\partial x} \text{----- (11b)}$$

Inserting (11) into (10)  $J_p$  can be recast into

$$J_p e^{\beta\phi(x)} = -qD_p \frac{\partial}{\partial x} [e^{\beta\phi(x)} p(x)] \text{----- (12)}$$

with  $\beta = q / k_B T$ . Integrating both sides of (12) there results

$$-J_p = \frac{qD_p e^{\beta\phi(x)} p(x) \Big|_0^W}{\int_0^W dx e^{\beta\phi(x)}} \text{----- (13)}$$

To evaluate  $J_p$  one has to consider the space charge field  $E(x)$  and potential,  $\phi(x)$ .  $E(x)$  in this case is identical to that in  $n^{++} - p$  junction, as can be clearly seen from Fig. 22.12. Thus, one can write

$$E(x) = E_{\max}(V) \left[1 - \frac{x}{W(V)}\right], \quad E_{\max} = \frac{qN_A W(V)}{\epsilon_S}$$

and

$$\phi(x) = -E_{\max}(V) \left[x - \frac{x^2}{2W(V)}\right] + \phi_{Bp} \text{----- (14)}$$

Note in (14) that at the interface  $\phi(0)$  should account for the Schottky barrier, i.e.  $-q\phi(0) = -q\phi_{Bp}$

With the use of (14) one can evaluate the numerator in (13):

$$\begin{aligned} p(0)e^{\beta\phi(0)} &= N_V e^{\frac{E_F - E_V(0)}{k_B T}} e^{\beta\phi_{Bp}}, \quad \beta = \frac{q}{k_B T} \\ &= N_V \\ p(W)e^{\beta\phi(W)} &= N_V e^{\frac{E_F - E_V(W)}{k_B T}} e^{\beta(V_p + V)} \\ &= N_V e^{\beta V} \end{aligned}$$

where as clearly shown in Fig.22.12

$$\begin{aligned} E_F - E_V(0) &= q\phi_{Bp} \\ E_F - E_V(W) &= qV_p \end{aligned}$$

Hence

$$qD_p e^{\beta\phi(x)} p(x) \Big|_0^W = qD_p N_V (e^{\beta V} - 1) \text{----- (15)}$$

Also, using (14) the denominator of (13) can be evaluated:

$$\begin{aligned}
& \int_0^W dx e^{\beta\varphi(x)} \\
&= e^{\beta\varphi_{bp}} \int_0^W dx \exp \left\{ \frac{\beta q N_A}{2\varepsilon_S} [x^2 - 2xW(V)] \right\} \\
&= e^{\beta\varphi_{bp}} \int_0^W dx \exp \left\{ \frac{\beta q N_A}{2\varepsilon_S} [(x - W(V))^2 - W(V)^2] \right\} \text{----- (16)} \\
&= e^{\beta\varphi_{bp}} \left( \frac{2\varepsilon_S}{q N_A \beta} \right)^{1/2} D(\zeta)
\end{aligned}$$

where the function,

$$D(\zeta) \equiv e^{-\zeta^2} \int_0^\zeta ds e^{s^2}, \quad \zeta \equiv (\beta q N_A / 2\varepsilon_S)^{1/2} W(V), \quad s = (\beta q N_A / 2\varepsilon_S)^{1/2} [W(V) - x]$$

thus introduced is called the Dawson integral (see (22.34b)). In the asymptotic limit

$$D(\zeta) \approx 1/2\zeta$$

Hence inserting (15), (16) into (13) one can derive the drift diffusion expression of the current of Schottky diode consisting of Au contacted p type silicon substrate.

$$-J_p = J_{SD} e^{\beta\varphi_{bp}} (e^{\beta V} - 1), \quad \beta = q / k_B T$$

where

$$\begin{aligned}
J_{SD} &= \frac{q^2 D_p N_V N_A \beta W(V)}{\varepsilon_S} \\
&= \frac{q^2 D_p N_V}{k_B T} \left[ \frac{2q N_A \varphi_{bi}(V)}{\varepsilon_S} \right]^{1/2}, \\
\varphi_{bi}(V) &= \varphi_{bi}(V=0) - V
\end{aligned}$$

Note holes are transferred from semiconductor to the metal so that the polarity of current density should be negative.

22.5 Given the Cu work function,  $q\varphi_m = 4.5eV$ , the silicon band near the interface bends up or down depending on doping conditions.

(a) For n-type Si, the work function for  $E_{Fs}$  is given by

$$\begin{aligned}
q\varphi_s &= q\chi + E_G / 2 - q\varphi_{Fn} \\
&= 4.05 + 0.56 - k_B T \ln \left( \frac{N_D}{n_i} \right) \\
&= 4.61 - k_B T \ln \left( \frac{N_D}{n_i} \right)
\end{aligned}$$

Hence if  $q\varphi_{Fn} = k_B T \ln(N_D / n_i) > 4.61 - 4.5eV$   $q\varphi_m > q\varphi_s$  and bands bends up, providing

potential barrier to electrons, as clearly shown in Fig. 22.11. The effect of  $Q_{ss}$  on band bending can be seen clearly from Fig. 22.13.

If  $q\phi_{Fn} < 4.61 - 4.5eV$ , on the other hand the band bends down and resulting consequences can be discussed together with the case of p type silicon. For p type Si, the work function for  $E_{Fs}$  is given by

$$\begin{aligned} q\phi_s &= q\chi + E_G / 2 + q\phi_{Fp} \\ &= 4.05 + 0.56 + k_B T \ln \left( \frac{N_A}{n_i} \right) \end{aligned}$$

Therefore

$$q\phi_s > q\phi_m (= 4.5eV)$$

regardless of doping level of  $N_A$  and the band bends down, creating barriers for holes (see Fig. 22.12). The effect of  $Q_{ss}$  on band bending has been discussed in problem 22.3

(b) If band bends up as in n-type Si (Fig. 22.11), photogenerated electrons roll down the potential hill from the interface toward Si bulk. On the other hand photogenerated holes roll up the hill. The resulting direction of photocurrent is opposite to the forward current of Schottky diode.

If the band bends down as in the case of p – type Si (see Fig. 22.12) photogenerated electrons roll down the hill toward the interface, while holes in the valence band roll up the hill toward the silicon bulk.

The resulting direction of the photocurrent is again opposite to the forward current of Schottky diode.

(c) In both case one can write

$$I = I_S (e^{\beta V} - 1) - I_l, \quad \beta = q / k_B T \text{ ----- (1)}$$

where

$$I_S = \begin{cases} A_n^* T^2 e^{-q\phi_{Bn}/k_B T} & \text{for n - type} \\ A_p^* T^2 e^{-q\phi_{Bp}/k_B T} & \text{for p - type} \end{cases}$$

and  $I_l$  is the photogenerated current.

Hence the open circuit voltage is found by putting  $I$  in (1) zero:

$$V_{OC} = \frac{q}{k_B T} \ln \left( \frac{I_l}{I_S} \right)$$

22.6 (a) The work function of intrinsic Si is given by

$$\begin{aligned} q\phi_{Si} &= q\chi + E_G / 2 \\ &= 4.05 + 0.56 \\ &= 4.61eV \end{aligned}$$

Thus, if the work function of metal is less than  $4.61eV$ , i.e.

$$q\phi_m < 4.61eV$$

the band bends down in the interface and electron concentration at the surface becomes larger than  $n_i$  in the bulk and Schottky Ohmic contact for electrons can be realized.

If

$$q\phi_m > 4.61eV$$

on the other hand, band bends up and surface hole concentration becomes larger than  $n_i$  in the bulk. Thus Schottky Ohmic contact for holes results.

(b) The Debye length of electrons is given from (22.44b) by

$$L_D = \left( \frac{\epsilon_s k_B T}{q^2 n_s} \right)^{1/2}$$

where the surface electron concentration

$$n_s = n_i e^{\beta\phi_s}, \quad \beta = q / k_B T, \quad q\phi_s \equiv q\phi_{Si} - q\phi_m$$

is given in terms of the difference in work functions involved.

Thus, for  $L_D$  of  $10nm$  for example the corresponding  $\phi_s$  is found at  $300K$  from

$$10 \times 10^{-9} = \left[ \frac{11.9 \cdot 1.381 \times 10^{-23} \cdot 300}{4\pi \cdot 8.988 \times 10^9 \cdot (1.6 \times 10^{-19})^2 \cdot 1.45 \times 10^{10+6} \cdot e^{\beta\phi_s}} \right]$$

or

$$e^{\beta\phi_s/2} = 3.4 \times 10^3$$

Hence,

$$\begin{aligned} \phi_s &= \frac{2k_B T}{q} \ln(3.4 \times 10^3) \\ &= 0.42V \end{aligned}$$

and therefore the metal work function required is

$$\begin{aligned} q\phi_m &= q\phi_{Si} - 0.42 \\ &= 4.61 - 0.42 \\ &= 4.19eV \end{aligned}$$

By the same token the metal work function required for  $L_D = 10nm$  for holes at  $300K$  is

$$\begin{aligned} q\phi_m &= 4.61 + 0.42 \\ &= 5.03eV \end{aligned}$$