

Solutions Manual

Fundamentals of Quantum Mechanics:

For Solid State Electronics and Optics

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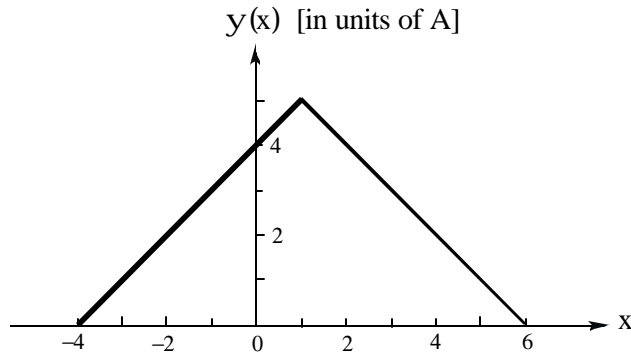
Cambridge University Press

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Chapter 2

2-1.

(a)



(b)

$$1 = \int_{-\infty}^{+\infty} |\Psi(x)|^2 dx = |A|^2 \left[\int_{-4}^1 (4+x)^2 dx + \int_1^6 (6-x)^2 dx \right] = \frac{250}{3} |A|^2$$

$$\therefore A = \frac{1}{5} \sqrt{\frac{3}{10}} \quad .$$

(c) $\langle x \rangle = 1$, by inspection.

Next, find σ^2 first:

$$\sigma^2 = |A|^2 \left[\int_{-4}^1 (x-1)^2 (4+x)^2 dx + \int_1^6 (x-1)^2 (6-x)^2 dx \right] = \frac{5}{2} \quad ;$$

therefore,

$$\langle x^2 \rangle = \sigma^2 + \langle x \rangle^2 = \frac{7}{2} \quad .$$

- (d) The answer to this question is tricky due to the discontinuous change in the slope of the wave function at $x = -4, 1,$ and 6 . Taking this into account ,

$$\langle \text{K. E.} \rangle = -\frac{\hbar^2}{2m} \frac{3}{250} (0 \cdot 1 - 5 \cdot 2 + 0 \cdot 1) = \frac{3\hbar^2}{50m} .$$

2-2. Given

$$\Psi(x) = \begin{cases} \sqrt{\frac{2}{a}} \sin(3\pi x/a), & \text{for } 0 < x < a \\ 0, & \text{for } x \leq 0 \text{ and } x \geq a. \end{cases}$$

(a)

$$\langle H \rangle = -\frac{\hbar^2}{2m} \frac{2}{a} \int_0^a \sin(3\pi x/a) \frac{\partial^2}{\partial x^2} \sin(3\pi x/a) dx = \frac{9\mathbf{p}^2 \hbar^2}{2ma^2} .$$

(b)

$$\hat{H} \sin(3\pi x/a) = \left[-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} \right] \sin(3\pi x/a) = E \sin(3\pi x/a)$$

$$\therefore E = \frac{9\mathbf{p}^2 \hbar^2}{2ma^2} .$$

(c)

$$\Psi(x,t) = \sqrt{\frac{2}{a}} \sin(3\pi x/a) e^{-i \frac{9\pi^2 \hbar}{2ma^2} t} .$$

(d)

$$\Delta H = \left[\langle H^2 \rangle - \langle H \rangle^2 \right]$$

$$= -\frac{\hbar^2}{2m} \frac{2}{a} \int_0^a \sin(3\mathbf{p}x/a) \frac{\partial^4}{\partial x^4} \sin(3\mathbf{p}x/a) dx - \left(\frac{9\mathbf{p}^2 \hbar^2}{2ma^2} \right)^2 = 0 .$$

Yes, it is as expected. Since the given state is an eigen state of the Hamiltonian as shown in (b), the uncertainty in the total energy must be zero as shown in (2.5d).

2-3. Prove the following commutation relationships:

(a)

$$\begin{aligned} [\hat{A} + \hat{B}, \hat{C}] &= (\hat{A} + \hat{B})\hat{C} - \hat{C}(\hat{A} + \hat{B}) = (\hat{A}\hat{C} - \hat{C}\hat{A}) + (\hat{B}\hat{C} - \hat{C}\hat{B}) \\ &= [\hat{A}, \hat{C}] + [\hat{B}, \hat{C}] \end{aligned} \quad , \text{ Q.E.D.}$$

(b)

$$\begin{aligned} [\hat{A}, \hat{B}\hat{C}] &= \hat{A}\hat{B}\hat{C} - \hat{B}\hat{C}\hat{A} = \hat{A}\hat{B}\hat{C} - (\hat{B}\hat{A}\hat{C} - \hat{B}\hat{A}\hat{C}) - \hat{B}\hat{C}\hat{A} \\ &= (\hat{A}\hat{B}\hat{C} - \hat{B}\hat{A}\hat{C}) + (\hat{B}\hat{A}\hat{C} - \hat{B}\hat{C}\hat{A}) = [\hat{A}, \hat{B}]\hat{C} + \hat{B}[\hat{A}, \hat{C}] \end{aligned} \quad . \quad \text{Q.E.D.}$$

2-4. Prove the following commutation relations:

(a) $[\hat{p}_x, \hat{x}^n] = -i\hbar n \hat{x}^{n-1} .$

Applying the left side to an arbitrary state function $\Psi(x)$ gives:

$$\begin{aligned} [\hat{p}_x, \hat{x}^n] \Psi(x) &= -i\hbar \left(\frac{\partial}{\partial x} x^n - x^n \frac{\partial}{\partial x} \right) \Psi(x) \\ &= -i\hbar n x^{n-1} \Psi(x) \end{aligned} \quad . \quad \text{Q.E.D.}$$

(b) $[\hat{x}, \hat{p}_x^2] = i 2\hbar \hat{p}_x .$

Similar to (a) above:

$$\begin{aligned} [\hat{x}, \hat{p}_x^2] \Psi(x) &= -\hbar^2 \left(x \frac{\partial^2}{\partial x^2} - \frac{\partial^2}{\partial x^2} x \right) \Psi(x) = \hbar^2 \left[2 \frac{\partial}{\partial x} \Psi(x) \right] \\ &= i 2\hbar \hat{p}_x \Psi(x) \end{aligned} \quad . \quad \text{Q.E.D.}$$

(c) Not possible .

2-5. Consider the two-dimensional matrices $\hat{\mathbf{s}}_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$, $\hat{\mathbf{s}}_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$, and $\hat{\mathbf{s}}_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$, whose physical significance will be discussed later in Chapter VI.

(a) The eigen values σ_z of $\hat{\sigma}_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$ are clearly +1 and -1.

For the eigen function corresponding to the eigen value $\sigma_z = +1$:

$$\hat{\sigma}_z \begin{pmatrix} a \\ b \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \begin{pmatrix} a \\ b \end{pmatrix} = +1 \begin{pmatrix} a \\ b \end{pmatrix} ; \therefore \begin{pmatrix} a \\ b \end{pmatrix} = \begin{pmatrix} 1 \\ 0 \end{pmatrix} .$$

For the eigen function corresponding to the eigen value $\sigma_z = -1$:

$$\hat{\sigma}_z \begin{pmatrix} a \\ b \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \begin{pmatrix} a \\ b \end{pmatrix} = -1 \begin{pmatrix} a \\ b \end{pmatrix} ; \therefore \begin{pmatrix} a \\ b \end{pmatrix} = \begin{pmatrix} 0 \\ 1 \end{pmatrix} .$$

The eigen values σ_x of $\hat{\sigma}_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$ are clearly also +1 and -1.

For the eigen function corresponding to the eigen value $\sigma_x = +1$:

$$\hat{\sigma}_x \begin{pmatrix} a \\ b \end{pmatrix} = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} a \\ b \end{pmatrix} = +1 \begin{pmatrix} a \\ b \end{pmatrix} ; \therefore \begin{pmatrix} a \\ b \end{pmatrix} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \end{pmatrix} .$$

For the eigen function corresponding to the eigen value $\sigma_x = -1$:

$$\hat{\sigma}_x \begin{pmatrix} a \\ b \end{pmatrix} = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} a \\ b \end{pmatrix} = -1 \begin{pmatrix} a \\ b \end{pmatrix} ; \therefore \begin{pmatrix} a \\ b \end{pmatrix} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -1 \end{pmatrix} .$$

The eigen values σ_y of $\hat{\sigma}_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$ are clearly also +1 and -1.

For the eigen function corresponding to the eigen value $\sigma_x = +1$:

$$\hat{\sigma}_y \begin{pmatrix} a \\ b \end{pmatrix} = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \begin{pmatrix} a \\ b \end{pmatrix} = +1 \begin{pmatrix} a \\ b \end{pmatrix} ; \therefore \begin{pmatrix} a \\ b \end{pmatrix} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ i \end{pmatrix} .$$

For the eigen function corresponding to the eigen value $\sigma_x = -1$:

$$\hat{\sigma}_y \begin{pmatrix} a \\ b \end{pmatrix} = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \begin{pmatrix} a \\ b \end{pmatrix} = -1 \begin{pmatrix} a \\ b \end{pmatrix} ; \quad \therefore \begin{pmatrix} a \\ b \end{pmatrix} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -i \end{pmatrix} .$$

(b) These eigen states in the Dirac notation in the representation in which $\hat{\sigma}_z$ is diagonal are as follows:

The eigen functions corresponding to the eigen values $\sigma_z = +1$ and -1 are, respectively

$$\begin{pmatrix} |\sigma_z = 1, +\rangle \\ |\sigma_z = 1, -\rangle \end{pmatrix} = \begin{pmatrix} 1 \\ 0 \end{pmatrix} , \text{ and } \begin{pmatrix} |\sigma_z = -1, +\rangle \\ |\sigma_z = -1, -\rangle \end{pmatrix} = \begin{pmatrix} 0 \\ 1 \end{pmatrix} .$$

The eigen functions corresponding to the eigen values $\sigma_x = +1$ and -1 are, respectively

$$\begin{pmatrix} |\sigma_x = 1, +\rangle \\ |\sigma_x = 1, -\rangle \end{pmatrix} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \end{pmatrix} , \text{ and } \begin{pmatrix} |\sigma_x = -1, +\rangle \\ |\sigma_x = -1, -\rangle \end{pmatrix} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -1 \end{pmatrix} .$$

The eigen functions corresponding to the eigen values $\sigma_y = +1$ and -1 are, respectively

$$\begin{pmatrix} |\sigma_y = 1, +\rangle \\ |\sigma_y = 1, -\rangle \end{pmatrix} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ i \end{pmatrix} , \text{ and } \begin{pmatrix} |\sigma_y = -1, +\rangle \\ |\sigma_y = -1, -\rangle \end{pmatrix} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -i \end{pmatrix} .$$

Note: The + and – signs in the Dirac notation for the eigen states of the Pauli spin-matrices refer to the spin-up and spin-down states, respectively, in the representation in which $\hat{\sigma}_z$ is diagonal.

2-6. Consider the Hamiltonian operator \hat{H} with discrete eigen values. Suppose the Hamiltonian is a Hermitian operator which by definition satisfies the condition:

$$\int \Psi^*(x) \hat{H} \Phi(x) dx = \left(\int \Phi^*(x) \hat{H} \Psi(x) dx \right)^* .$$

- (a) The eigen values of the Hamiltonian are all real:

Let $\Psi(x)$ and $\Phi(x)$ in the definition of a Hermitian operator be an eigen state of the Hamiltonian \hat{H} corresponding to the eigen value E_i .

$$\int \Psi^*(x) \hat{H} \Phi(x) dx = \int \Psi_{E_i}^*(x) \hat{H} \Psi_{E_i}(x) dx = E_i .$$

Similarly,

$$\left(\int \Phi^*(x) \hat{H} \Psi(x) dx \right)^* = \left(\int \Psi_{E_i}^*(x) \hat{H} \Psi_{E_i}(x) dx \right)^* = E_i^* .$$

The condition of Hermiticity of the Hamiltonian leads to: $E_i = E_i^*$.

- (b) Let $\Psi(x)$ and $\Phi(x)$ in the definition of a Hermitian operator be an eigen state of the Hamiltonian \hat{H} corresponding to the eigen value E_i and E_j , respectively. The Hermiticity condition gives:

$$(E_i - E_j) \int \Psi_{E_i}^*(x) \Psi_{E_j}(x) dx = 0 .$$

Therefore, if $(E_i - E_j) \neq 0$, then $\int \Psi_{E_i}^*(x) \Psi_{E_j}(x) dx = 0$, or the eigen functions corresponding to different eigen values are necessarily orthogonal to each other.

2-7. Consider a particle of mass m in a potential field $V(x)$.

- (a) On the basis of Heisenberg's equation of motion, (2.49), and the commutation relation (2.11a):

$$\frac{d}{dt} \langle \hat{x} \rangle = \frac{i}{\hbar} \langle [\frac{\hat{p}_x^2}{2m} + \hat{V}(\hat{x}), \hat{x}] \rangle = \langle \frac{\hat{p}_x}{m} \rangle .$$

- (b) On the same basis, the time variation of the expectation value of the momentum is given by :

$$\frac{d}{dt} \langle \hat{p}_x \rangle = \frac{i}{\hbar} \langle [\frac{\hat{p}_x^2}{2m} + \hat{V}(\hat{x}), \hat{p}_x] \rangle = - \langle \frac{dV(x)}{dx} \rangle = F_x \quad ,$$

which is known as Ehrenfest's theorem.

Chapter 3

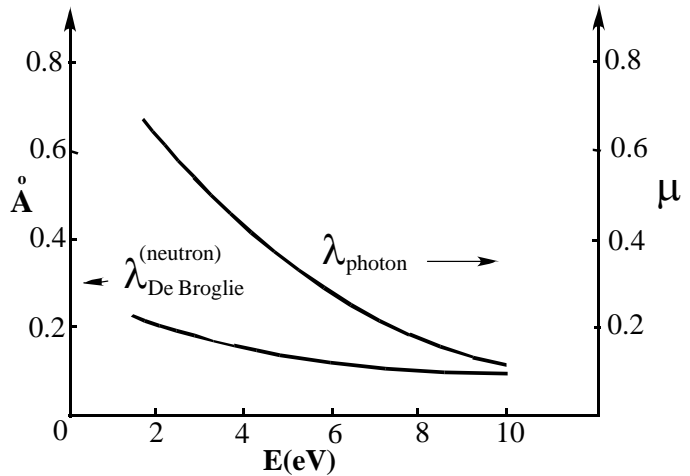
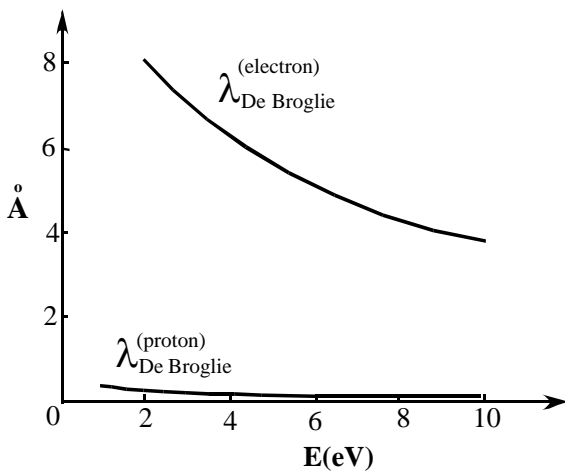
3-1.

$$(a) \quad \lambda_{deBroglie}^{(electron)} = \frac{h}{\sqrt{2mE}} = \frac{12.3}{\sqrt{E(in\ eV)}} \text{ \AA} \quad .$$

$$\lambda_{deBroglie}^{(proton)} = \frac{0.3}{\sqrt{E(in\ eV)}} \text{ \AA} \quad .$$

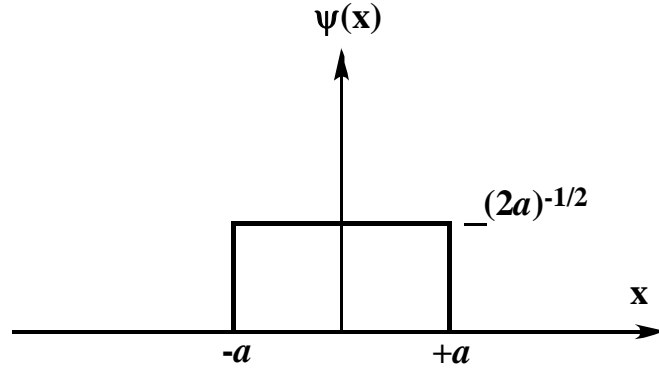
$$(b) \quad \lambda_{deBroglie}^{(neutron)} \cong \lambda_{deBroglie}^{(proton)} = \frac{0.3}{\sqrt{E(in\ eV)}} \text{ \AA}$$

$$\lambda_{deBroglie}^{(photon)} = \frac{1.24}{E(eV)} \mu$$



3-2. Suppose we know that there is a free particle initially located in the range $-a < x < a$ with a spatially uniform probability.

- (a) The normalized state function $\Psi(x, t = 0)$ of the particle in the Schrodinger-representation is, assuming the phase of the wave function is arbitrarily chosen to be zero:



(b) The corresponding momentum representation is:

$$\Psi(p) = \sqrt{\frac{\hbar}{\pi a}} \frac{1}{p_x} \sin\left(\frac{p_x}{\hbar} a\right) \quad .$$

(c) The corresponding state function at an arbitrary later time $\Psi(x, t > 0)$ in the integral form is :

$$\Psi(x, t) = \frac{1}{\pi} \sqrt{\frac{1}{2a}} \int_{-\infty}^{+\infty} \frac{\sin\left(\frac{p_x}{\hbar} a\right)}{p_x} e^{i\left(\frac{p_x x}{\hbar} - \frac{p_x^2}{2m\hbar} t\right)} dp_x \quad .$$

3-3. Consider a free particle with the initial state function in the form of:

$$\Psi(x, t = 0) = A e^{-ax^2 + ikx} \quad .$$

(a) To normalize this state function:

$$1 = |A|^2 \int_{-\infty}^{+\infty} e^{-2ax^2} dx = |A|^2 \sqrt{\frac{\pi}{2a}} \quad ; \quad \therefore A = \left(\frac{2a}{\pi}\right)^{1/4}$$

- (b) After a considerable amount of algebra by first completing the square of the exponential in Fourier-transform integral, it can be shown that the corresponding momentum representation of this state function is:

$$\Psi(p) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{+\infty} \left(\frac{2a}{\pi}\right)^{1/4} e^{-ax^2 + ikx - ip_x x/\hbar} dx = \left[\frac{1}{2\pi(\Delta p_x^2)}\right]^{1/4} e^{-\frac{(p_x - \langle p_x \rangle)^2}{4\Delta p_x^2}},$$

where

$$\Delta p_x = \frac{\hbar}{2\Delta x} = \hbar\sqrt{a}, \quad \frac{\langle p_x \rangle}{\hbar} = k, \quad \Delta x = \sqrt{\frac{1}{4a}}.$$

- (c) The corresponding state function $\Psi(x, t > 0)$ is:

$$\begin{aligned} \Psi(x, t) &= \frac{1}{\sqrt{2\pi\hbar}} \left(\frac{1}{2\pi\Delta p_x^2}\right)^{1/4} \int_{-\infty}^{+\infty} e^{-\frac{(p_x - \langle p_x \rangle)^2}{4\Delta p_x^2}} e^{-i\frac{p_x^2}{2m\hbar}t + i\frac{p_x x}{\hbar}} dp_x \\ &= \left(\frac{1}{2\pi\hbar^2}\right)^{1/4} \left[\frac{1}{4\Delta p_x^2} + \frac{i}{\hbar} \frac{t}{2m}\right]^{-1/4} e^{-\left[\frac{(x - \langle p_x \rangle t)^2}{4\hbar^2\left(\frac{1}{4\Delta p_x^2} + \frac{i}{\hbar} \frac{t}{2m}\right)} + \frac{i\langle p_x \rangle}{\hbar}(x - \frac{\langle p_x \rangle}{2m}t) + i\theta\right]}, \end{aligned}$$

where θ is a time-dependent phase-shift of no physical consequence that goes to zero at $t = 0$.

- (d) From c above, the expectation value and the corresponding uncertainty of the position for $t > 0$ are, respectively:

$$\langle x \rangle = \frac{\hbar k}{m} t \quad \text{and} \quad \Delta x = \frac{1}{2\sqrt{a}} \left[1 + \left(\frac{2\hbar a}{m} t\right)^2\right]^{1/2}.$$

Similarly, the expectation value and the corresponding uncertainty of the linear momentum for $t > 0$ are, respectively:

$$\langle p_x \rangle_t = \hbar k \quad \text{and} \quad \Delta p_x(t) = \Delta p_x(0) = \hbar\sqrt{a} \quad .$$

(e) The uncertainty product of the position and momentum for this state is:

$$(\Delta x) (\Delta p_x) = \frac{\hbar}{2} \left[1 + \left(\frac{2\hbar a}{m} t \right)^2 \right]^{\frac{1}{2}} \geq \frac{\hbar}{2} \quad ,$$

which satisfies Heisenberg's uncertainty principle for all time $t \geq 0$.

Chapter 4

4-1. From Eq. (4-19):

$$\frac{F}{A} = \frac{e^{-ik_3d}}{\left[\cos k_2d - i \frac{k_1^2 + k_2^2}{2k_1k_2} \sin k_2d \right]}$$

The corresponding transmission coefficient is :

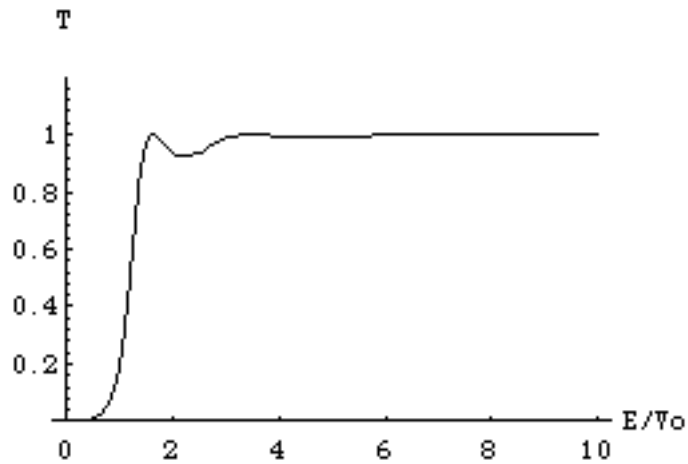
$$\begin{aligned} T &= \left| \frac{F}{A} \right|^2 = \left[\cos^2 k_2d + \left(\frac{k_1^2 + k_2^2}{2k_1k_2} \right)^2 \sin^2 k_2d \right]^{-1} \\ &= \left\{ 1 + \left[\frac{(2E - V_0)^2}{4E(E - V_0)} - 1 \right] \sin^2 k_2d \right\}^{-1} \\ &= \left[1 + \frac{V_0^2}{4E(E - V_0)} \sin^2 k_2d \right]^{-1} \\ &= \left[1 + \frac{\Delta V^2}{4(E - V_I)(E - V_{II})} \sin^2 k_2d \right]^{-1} \end{aligned}$$

which is Eq. (4.20a).

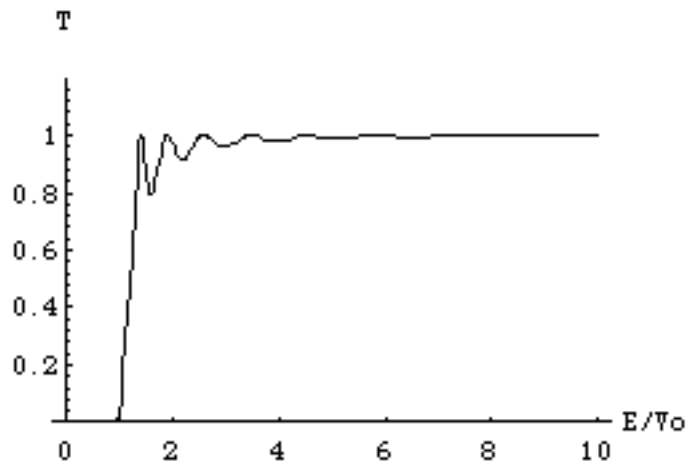
In the limit of $(E - V_0) \rightarrow 0$, $\sin^2 k_2d \rightarrow \frac{2m(E - V_0)}{\hbar^2} d^2$; therefore,

$$\lim_{E \rightarrow V_0} T = \left[1 + \frac{2mV_0d^2}{4\hbar^2} \right]^{-1} = \left[1 + \frac{\beta^2}{4} \right]^{-1}$$

Plots of T for $\beta = 4$:



and $\beta = 10$:



4 -2. A particle with energy E in a region of zero potential is incident on a potential well of depth V_0 and width " d ". From the expression for the probability of transmission T of the particle past the well given in (4.20a), the approximate values of E (in terms of $\hbar^2/2md^2$) corresponding to the maxima and minima in T :

(a) for $\beta = 10$ are:

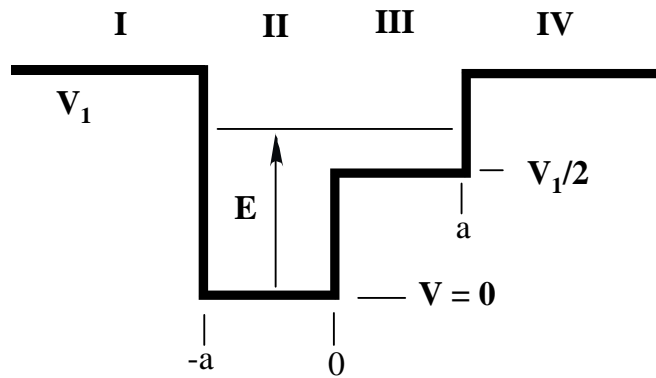
$$E_n \cong \frac{\hbar^2}{2md^2} [n^2 \pi^2 + 10^2] \quad \text{and} \quad E_n \cong \frac{\hbar^2}{2md^2} \left[\frac{(n+1)^2 \pi^2}{4} + 10^2 \right], \text{ respectively ;}$$

(b) for $\beta = 250$ are:

$$E_n \cong \frac{\hbar^2}{2md^2} [n^2 \pi^2 + 250^2] \quad \text{and} \quad E_n \cong \frac{\hbar^2}{2md^2} \left[\frac{(n+1)^2 \pi^2}{4} + 250^2 \right], \quad \text{respectively.}$$

4-3. Consider a one-dimensional rectangular potential well structure such as that shown in Figure 4.9 below.

$$\begin{aligned} V &= V_1 & \text{for} & \quad x < -a \\ V &= 0 & \text{for} & \quad -a < x < 0 \\ V &= V_1/2 & \text{for} & \quad 0 < x < a \\ V &= V_1 & \text{for} & \quad x > a \end{aligned}$$



The wave functions in regions I through IV and the equations describing the boundary conditions on these wave functions for

(a) $E > V_1$ are:

$$\Psi_1 = e^{ik_1x} + A e^{-ik_1x}$$

$$\Psi_2 = B e^{ik_2x} + C e^{-ik_2x}$$

$$\Psi_3 = D e^{ik_3x} + F e^{-ik_3x}$$

$$\Psi_4 = G e^{ik_4x}$$

where

$$k_1 = \left[\frac{2m(E - V_1)}{\hbar^2} \right]^{\frac{1}{2}}, \quad k_2 = \left[\frac{2mE}{\hbar^2} \right]^{\frac{1}{2}}, \quad k_3 = \left[\frac{2m(E - \frac{V_1}{2})}{\hbar^2} \right]^{\frac{1}{2}}, \quad k_4 = k_1.$$

The boundary conditions (b. c.) at $x = -a$ are:

$$e^{-ik_1a} + Ae^{ik_1a} = Be^{-ik_2x} + Ce^{ik_2a} \quad \text{and} \quad k_1 [e^{-ik_1a} - Ae^{-ik_1a}] = k_2 [Be^{-ik_2x} - Ce^{ik_2a}].$$

The corresponding b.c. at $x = 0$ are:

$$B + C = D + F \quad \text{and} \quad k_2(B - C) = k_3(D - F).$$

The corresponding b.c. at $x = a$ are:

$$De^{ik_3a} + Fe^{-ik_3a} = Ge^{ik_4x} \quad \text{and} \quad k_3(De^{ik_3a} - Fe^{-ik_3a}) = k_4Ge^{ik_4x}.$$

(b) For $V_1 > E > V_1/2$, the wave functions in the various regions are:

$$\Psi_1 = Ae^{\alpha_1x}$$

$$\Psi_2 = Be^{ik_2x} + Ce^{-ik_2x}$$

$$\Psi_3 = De^{ik_3x} + Fe^{-ik_3x}$$

$$\Psi_4 = Ge^{-\alpha_4x},$$

where

$$\alpha_1 = \left[\frac{2m(V_1 - E)}{\hbar^2} \right]^{\frac{1}{2}}, \quad k_2 = \left[\frac{2mE}{\hbar^2} \right]^{\frac{1}{2}}, \quad k_3 = \left[\frac{2m(E - \frac{V_1}{2})}{\hbar^2} \right]^{\frac{1}{2}}, \quad \alpha_4 = \alpha_1.$$

The b. c. at at $x = -a$ are:

$$Ae^{-\alpha_1 a} = Be^{-ik_2 x} + Ce^{ik_2 a} \quad \text{and} \quad \alpha_1 Ae^{-\alpha_1 a} = ik_2 [Be^{-ik_2 x} - Ce^{ik_2 a}].$$

The corresponding b.c. at $x = 0$ are:

$$B + C = D + F \quad \text{and} \quad k_2(B - C) = k_3(D - F).$$

The corresponding b.c. at $x = a$ are:

$$De^{ik_3 a} + Fe^{-ik_3 a} = Ge^{-\alpha_4 a} \quad \text{and} \quad ik_3(De^{ik_3 a} - Fe^{-ik_3 a}) = -\alpha_4 Ge^{-\alpha_4 a}$$

(c) For $E < V_1/2$, the wave functions in the various regions are:

$$\Psi_1 = Ae^{\alpha_1 x}$$

$$\Psi_2 = Be^{ik_2 x} + Ce^{-ik_2 x}$$

$$\Psi_3 = De^{\alpha_3 x} + Fe^{-\alpha_3 x}$$

$$\Psi_4 = Ge^{-\alpha_4 x},$$

where

$$\alpha_1 = \left[\frac{2m(V_1 - E)}{\hbar^2} \right]^{\frac{1}{2}}, \quad k_2 = \left[\frac{2mE}{\hbar^2} \right]^{\frac{1}{2}}, \quad \alpha_3 = \left[\frac{2m(\frac{V_1}{2} - E)}{\hbar^2} \right]^{\frac{1}{2}}, \quad \alpha_4 = \alpha_1.$$

The b. c. at $x = -a$ are:

$$Ae^{-\alpha_1 a} = Be^{-ik_2 x} + Ce^{ik_2 a} \quad \text{and} \quad \alpha_1 Ae^{-\alpha a} = ik_2 [Be^{-ik_2 x} - Ce^{ik_2 a}].$$

The corresponding b.c. at $x = 0$ are:

$$B + C = D + F \quad \text{and} \quad ik_2(B - C) = \alpha_3(D - F) \quad .$$

The corresponding b.c. at $x = a$ are:

$$De^{\alpha_3 a} + Fe^{-\alpha_3 a} = Ge^{-\alpha_4 a} \quad \text{and} \quad \alpha_3(De^{\alpha_3 a} - Fe^{-\alpha_3 a}) = -\alpha_4 Ge^{-\alpha_4 a}$$

- 4-4.** Suppose the following wave function describe the state of an electron in an infinite square potential well, $0 < x < a$, with $V(x) = 0$ inside the well:

$$\Psi(x) = \begin{cases} A \sin\left(\frac{3\pi x}{2a}\right) \cos\left(\frac{\pi x}{2a}\right), & \text{for } 0 \leq x \leq a \\ 0 & \text{elsewhere} \end{cases} \quad .$$

- (a) One way to normalize the wave function is to expand the given wave function in terms of the normalized energy eigen functions from $x = 0$ to $x = a$:

$$\Psi(x) = A \sqrt{\frac{a}{8}} \left[\sqrt{\frac{2}{a}} \sin\left(\frac{2\pi x}{a}\right) + \sqrt{\frac{2}{a}} \sin\left(\frac{\pi x}{a}\right) \right] .$$

$$1 = |A|^2 \left[\frac{a}{8} + \frac{a}{8} \right] \quad ; \quad \therefore A = \frac{2}{\sqrt{a}} \quad .$$

- (b) Time-dependence of the normalized wave function is:

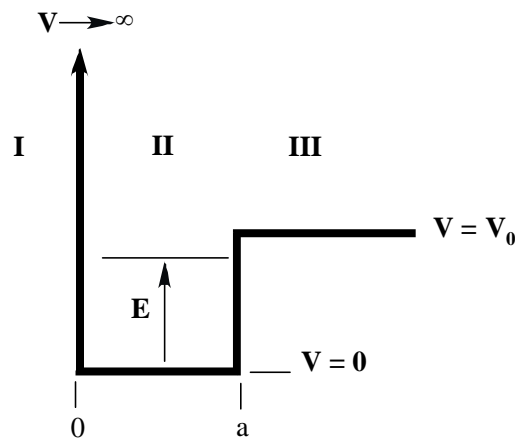
$$\Psi(x, t) = \frac{1}{\sqrt{a}} \sin\left(\frac{2\pi x}{a}\right) e^{-i \frac{2\pi^2 \hbar}{ma^2} t} + \frac{1}{\sqrt{a}} \sin\left(\frac{\pi x}{a}\right) e^{-i \frac{\pi^2 \hbar}{2ma^2} t}$$

- (c) If measurements of the energy of the electron are made, the values of the energy that will be measured and the corresponding absolute probabilities are:

<u>Energy</u>	<u>Probability</u>
$\frac{2\pi^2\hbar^2}{ma^2}$	$\frac{1}{2}$
$\frac{\pi^2\hbar^2}{2ma^2}$	$\frac{1}{2}$

4-5. Consider the one-dimensional potential of Figure 4.10:

		Region
$V = \infty$	$x < 0$	I
$V = 0$	$0 < x < a$	II
$V = V_0$	$a < x$	III



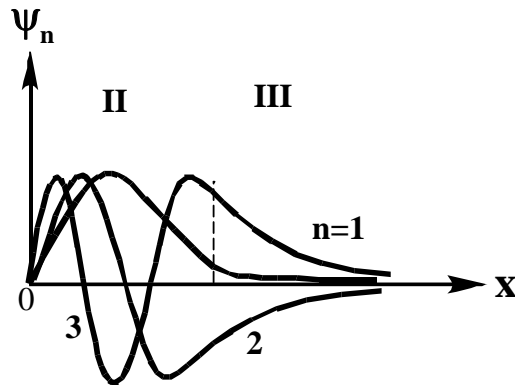
- (a) The equations whose solution give the eigen energies of the bound states ($E < V_0$) of the above potential well are the same as those for the antisymmetric solutions of a full potential well of depth V_0 from $x = -a$ to $x = a$, namely:

$$-\xi_n \cot \xi_n = \eta_n \quad , \quad \xi_n^2 + \eta_n^2 = \beta^2 \quad ,$$

where

$$\xi_n = k_n a = \frac{\sqrt{2mE_n}}{\hbar} a \quad , \quad \eta_n = \frac{\sqrt{2m(V_0 - E_n)}}{\hbar} a \quad , \quad \beta = \frac{\sqrt{2mV_0}}{\hbar} a \quad .$$

- (b) The eigenfunctions of the three lowest energies assuming V_0 is sufficiently large so that there are at least three bound states are qualitatively as shown in the following figure:



- 4 -6.** Consider the case of an electron ($m_e = 0.91 \times 10^{-27} \text{ g}$) in a finite potential well of depth 1.25 V and width 145 Å.

(a)

$$2a = d \quad 2a = d = 145 \text{ \AA} \quad , \quad V_0 = 125 \text{ eV} = 2 \times 10^{-12} \text{ erg.}$$

$$\frac{\beta}{a} = \left[\frac{2mV_0}{\hbar^2} \right]^{\frac{1}{2}} = 5.75 \times 10^7 \text{ cm}^{-1} \quad , \quad \beta = 41.7 \quad ,$$

$$(N-1)(\pi/2) < 41.7 < N(\pi/2) \quad ;$$

therefore, the estimated number of bound states $N = 27$.

- (b) To calculate the energies of the lowest two bound states, we must find the numerical solutions of the secular equations:

$$\xi \tan \xi = [\beta^2 - \xi^2]^{1/2} \quad \text{for the symmetric modes ,}$$

and

$$-\xi \cot \xi = [\beta^2 - \xi^2]^{1/2} \quad \text{for the anti-symmetric modes .}$$

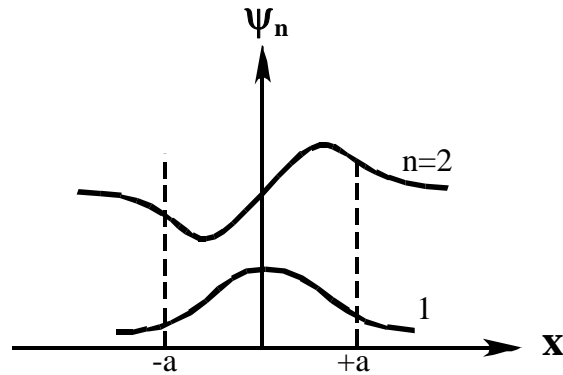
Solving these equations using, for example, Mathematica gives:

$$\xi_1 = 1.534 \quad \text{and} \quad \xi_2 = 3.07 \quad .$$

The corresponding bound-state energies are, respectively:

$$E_1 = V_0 \left(\frac{\xi_1}{\beta} \right)^2 = 1.69 \text{ meV} \quad \text{and} \quad E_2 = V_0 \left(\frac{\xi_2}{\beta} \right)^2 = 6.79 \text{ meV} \quad .$$

- (c) The wave functions for the lowest two bound states are sketched qualitatively below:

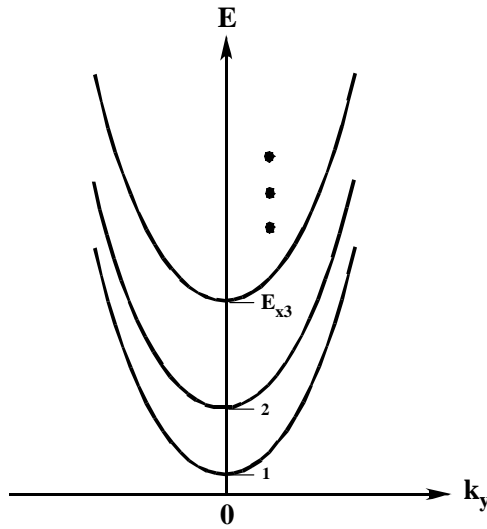


- 4-7.** A particle of mass m is confined to move in a quantum-well in the (x,y) plane which consists of a pair of impenetrable walls at $x = \pm a$ but is unbounded for motion in the y -direction.

- (a) Let the total energy of the particle be E and the energy associated with the motion in the x - and y -directions be E_x and E_y , respectively. The allowed values of E_x , E_y , and E are, respectively:

$$E_x = \frac{n^2 \pi^2 \hbar^2}{8ma^2}, \quad E_y = 0 \rightarrow \infty \text{ is unlimited, and } E = E_x + E_y.$$

- (b) E versus k_y for various allowed values of E_x are sketched below:



- (c)
$$E_y = E - E_x = E - \frac{\hbar^2 \pi^2}{2ma^2}.$$

- (d) A possible, un-normalized, space- and time-dependent wave function to describe the particle in Part c above is:

$$\Psi(x, t) = \sin(\pi x / a) e^{i \frac{\sqrt{2mE_y}}{\hbar} y - \frac{i}{\hbar} E t}$$

- (e) If the particle's total energy is $E = \pi^2 \hbar^2 / 4ma^2$, n_x can only be 1 and $E_y = \frac{\hbar^2 k^2}{2m} = \frac{\pi^2 \hbar^2}{8ma^2}$. The corresponding wave function of the particle must be of the

form:

$$\Psi(x, y, t) = \cos(\pi x / 2a) [A e^{i \frac{\pi}{2a} y} + B e^{-i \frac{\pi}{2a} y}] e^{-i \left(\frac{\pi^2 \hbar}{4ma^2} \right) t} .$$

- (f) Suppose now an infinite potential barrier at $y = \pm a$ is imposed. The particle's energy cannot be measured to be $3\pi^2 \hbar^2 / 4ma^2$, because

$$E_x + E_y = \frac{\pi^2 \hbar^2}{8ma^2} (n_x^2 + n_y^2) .$$

For the total energy to be equal to $3\pi^2 \hbar^2 / 4ma^2$, $(n_x^2 + n_y^2)$ must equal to 6, which is not possible for any integer values of n_x and n_y .

Chapter 5

5-1. For an eigen state of a one-dimensional harmonic oscillator, the following results are true:

(a) The expectation values of the position and momentum are zero:

$$\langle n | \hat{x} | n \rangle = i \sqrt{\frac{\hbar}{2m\omega_0}} \langle n | (\hat{a}^+ - \hat{a}^-) | n \rangle = 0 \quad , \quad \text{and}$$

$$\langle n | \hat{p}_x | n \rangle = \sqrt{\frac{\hbar m \omega_0}{2}} \langle n | (\hat{a}^+ + \hat{a}^-) | n \rangle = 0 \quad .$$

(b) The expectation values of the potential energy and the kinetic energy (\hat{T}) are equal:

$$\langle n | \hat{T} | n \rangle = \langle n | \frac{p_x^2}{2m} | n \rangle = \frac{\hbar\omega_0}{4} \langle n | (\hat{a}^+ + \hat{a}^-)(\hat{a}^+ + \hat{a}^-) | n \rangle = \frac{\hbar\omega_0}{4}(2n+1) \quad ,$$

$$\langle n | \hat{V}(x) | n \rangle = -\frac{k}{2} \frac{\hbar}{2m\omega_0} \langle n | (\hat{a}^+ - \hat{a}^-)(\hat{a}^+ - \hat{a}^-) | n \rangle = \frac{\hbar\omega_0}{4}(2n+1) = \langle n | T | n \rangle \quad .$$

(c) The uncertainty product of the position and momentum $\Delta x \Delta p_x$ is equal to

$(n + \frac{1}{2})\hbar$:

$$\Delta p_x^2 = \langle p_x^2 \rangle - \langle p_x \rangle^2 = \frac{\hbar m \omega_0}{2} (2n+1) \quad ,$$

$$\Delta x^2 = \langle x^2 \rangle - \langle x \rangle^2 = \frac{\hbar}{2m\omega_0} (2n+1) \quad ;$$

$$\therefore \Delta p_x \Delta x = (n + \frac{1}{2})\hbar \quad .$$

5-2. For a one-dimensional harmonic oscillator, in the basis in which the Hamiltonian is diagonal, the matrix representations of :

(a) the position and momentum operators \hat{x} and \hat{p}_x are, respectively :

$$\hat{x} = -i\sqrt{\frac{\hbar}{2m\omega_0}} \begin{pmatrix} 0 & -\sqrt{1} & 0 & 0 & \bullet & \bullet \\ \sqrt{1} & 0 & -\sqrt{2} & 0 & \bullet & \bullet \\ 0 & \sqrt{2} & 0 & -\sqrt{3} & \bullet & \bullet \\ 0 & 0 & \sqrt{3} & 0 & \bullet & \bullet \\ \bullet & \bullet & \bullet & \bullet & \bullet & \bullet \\ \bullet & \bullet & \bullet & \bullet & \bullet & \bullet \end{pmatrix} ,$$

$$\hat{p}_x = \sqrt{\frac{\hbar m\omega_0}{2}} \begin{pmatrix} 0 & \sqrt{1} & 0 & 0 & \bullet & \bullet \\ \sqrt{1} & 0 & \sqrt{2} & 0 & \bullet & \bullet \\ 0 & \sqrt{2} & 0 & \sqrt{3} & \bullet & \bullet \\ 0 & 0 & \sqrt{3} & 0 & \bullet & \bullet \\ \bullet & \bullet & \bullet & \bullet & \bullet & \bullet \\ \bullet & \bullet & \bullet & \bullet & \bullet & \bullet \end{pmatrix} ;$$

(b) the operator products $\hat{a}^+\hat{a}^-$ and $\hat{a}^-\hat{a}^+$, respectively:

$$\hat{a}^+ \hat{a}^- = \begin{pmatrix} 0 & 0 & 0 & 0 & \bullet & \bullet \\ 0 & 1 & 0 & 0 & \bullet & \bullet \\ 0 & 0 & 2 & 0 & \bullet & \bullet \\ 0 & 0 & 0 & 3 & \bullet & \bullet \\ \bullet & \bullet & \bullet & \bullet & \bullet & \bullet \\ \bullet & \bullet & \bullet & \bullet & \bullet & \bullet \end{pmatrix}, \quad \text{and} \quad \hat{a}^- \hat{a}^+ = \begin{pmatrix} 1 & 0 & 0 & 0 & \bullet & \bullet \\ 0 & 2 & 0 & 0 & \bullet & \bullet \\ 0 & 0 & 3 & 0 & \bullet & \bullet \\ 0 & 0 & 0 & 4 & \bullet & \bullet \\ \bullet & \bullet & \bullet & \bullet & \bullet & \bullet \\ \bullet & \bullet & \bullet & \bullet & \bullet & \bullet \end{pmatrix}.$$

(c) Using the above matrices, it can be shown immediately that the commutator of \hat{a}^- and \hat{a}^+ is :

$$\hat{a}^- \hat{a}^+ - \hat{a}^+ \hat{a}^- = \begin{pmatrix} 1 & 0 & 0 & 0 & \bullet & \bullet \\ 0 & 1 & 0 & 0 & \bullet & \bullet \\ 0 & 0 & 1 & 0 & \bullet & \bullet \\ 0 & 0 & 0 & 1 & \bullet & \bullet \\ \bullet & \bullet & \bullet & \bullet & \bullet & \bullet \\ \bullet & \bullet & \bullet & \bullet & \bullet & \bullet \end{pmatrix} = 1.$$

5-3. Substituting the wave function of the form :

$$\Psi_{E_n}(x) = C_n H_n \left(\sqrt{\frac{m\omega_0}{\hbar}} x \right) e^{-\frac{m\omega_0}{2\hbar} x^2}$$

into the Schroedinger-equation gives :

$$\left[-\frac{\hbar^2}{2m} \frac{d^2 H_n(x)}{dx^2} + \hbar\omega_0 x \frac{dH_n(x)}{dx} + \frac{\hbar\omega_0}{2} H_n(x) \right] e^{-\frac{\hbar\omega_0}{2\hbar} x^2} = E_n \Psi_n(x)$$

Change the variable from x to $u \equiv \sqrt{\frac{m\omega_0}{\hbar}} x$ gives indeed Eq.(5.33), which defines the Hermit polynomials:

$$\frac{d^2 H_n(u)}{du^2} - 2u \frac{dH_n(u)}{du} + 2\left(\frac{E_n}{\hbar \omega_0} - \frac{1}{2}\right) H_n(u) = 0 \quad .$$

5-4. Suppose the harmonic oscillator is initially in a superposition state $|\Psi(t=0)\rangle = \frac{1}{\sqrt{2}}[|0\rangle + |1\rangle]$, the expectation value of the position of the oscillator $\langle x \rangle_t \equiv \langle \Psi(t) | x | \Psi(t) \rangle$ as a function of time is:

$$\begin{aligned} \langle x \rangle_t &\equiv \langle \Psi(t) | x | \Psi(t) \rangle \\ &= \frac{1}{2} [\langle 0 | + \langle 1 | e^{-i\omega_0 t}] [-i \sqrt{\frac{\hbar}{2m\omega_0}} (\hat{a}^+ - \hat{a}^-)] [|0\rangle + e^{i\omega_0 t} |1\rangle] \\ &= \sqrt{\frac{\hbar}{2m\omega_0}} \sin \omega_0 t. \end{aligned}$$

5-5. From Maxwell equations, (5.65 a-d), and the condition for transverse waves $\nabla \cdot \vec{E} = 0$ that

$$\nabla^2 \vec{E} - \frac{1}{c^2} \frac{\partial^2 \vec{E}}{\partial t^2} = 0 \quad .$$

It is clear that

$$\vec{E}(\vec{r}, t) \equiv E_x(z, t) \mathbf{e}_x = i \sqrt{\frac{2\pi\hbar\omega_k}{L}} (a_k^- e^{-i\omega_k t + ikz} - a_k^+ e^{i\omega_k t - ikz}) \mathbf{e}_x \quad (5.68a)$$

satisfies the above wave equation as long as $k^2 = \frac{\omega_k^2}{c^2}$. Under the same condition, it can be shown that (5.68a) and

$$\vec{B}(\vec{r}, t) \equiv B_y(z, t) \mathbf{e}_y = i \sqrt{\frac{2\pi\hbar\omega_k}{L}} (a_k^- e^{-i\omega_k t + ikz} - a_k^+ e^{i\omega_k t - ikz}) \mathbf{e}_y \quad (5.68b)$$

satisfy (5.65c).

Substituting (5.68a) and (5.68b) into

$$\frac{1}{8\pi} \int_0^L [E_x^2(z,t) + B_y^2(z,t)] dz$$

and making use of the commutation relationship (5.69) after changing the a^\pm 's into operators gives (5.70):

$$\hat{H} = [\hat{a}_k^+ \hat{a}_k^- + \frac{1}{2}] \hbar \omega_k$$

and

$$E_{kn} = \langle n | \hat{H} | n \rangle = (n + \frac{1}{2}) \hbar \omega_0 \quad .$$

5-6. The Rayleigh-Jeans law and Planck's law for black-body radiation as functions of wavelength and in units of energy per volume per wavelength-interval:

Since $\nu = \frac{c}{\lambda}$, Planck's radiation law as a function of the wavelength is:

$$\rho_b(\lambda) d\lambda = \rho_b(\nu = \frac{c}{\lambda}) \left| \frac{\partial \nu}{\partial \lambda} \right| d\lambda = \frac{8\pi hc}{\lambda^5} \cdot \frac{1}{e^{hc/\lambda k_B T} - 1} d\lambda \quad .$$

In the limit of $\frac{h}{\lambda} \ll k_B T$, it reduces to the classical Rayleigh-Jeans law:

$$\lim_{\lambda \rightarrow 0} \rho_b(\lambda) = \frac{8\pi k_B T}{\lambda^4}$$

with its I^{-4} dependence on wavelength and, therefore, diverges in the ultraviolet limit $I \rightarrow 0$.

Chapter 6

- 6-1.** The matrix representations of the angular momentum operators $\hat{L}_x, \hat{L}_y, \hat{L}_z, \hat{L}_+, \hat{L}_-$, and \hat{L}^2 , for $\ell = 0, 1$, and 2 , in the basis in which \hat{L}_z and \hat{L}^2 are diagonal can be found from (6.29) – (6.31) and (6.8):

For the trivial case of $\ell = 0$, all these operators are equal to zero.

For $\ell = 1$, the matrices are:

$$\hat{L}^2 = \begin{pmatrix} 2 & 0 & 0 \\ 0 & 2 & 0 \\ 0 & 0 & 2 \end{pmatrix} \hbar^2, \quad \hat{L}_z = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix} \hbar, \quad \hat{L}_x = \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix} \frac{\hbar}{\sqrt{2}},$$

$$\hat{L}_y = \begin{pmatrix} 0 & -1 & 0 \\ 1 & 0 & -1 \\ 0 & 1 & 0 \end{pmatrix} \frac{i\hbar}{\sqrt{2}}, \quad \hat{L}_+ = \begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 0 & 0 & 0 \end{pmatrix} \sqrt{2}\hbar, \quad \hat{L}_- = \begin{pmatrix} 0 & 0 & 0 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix} \sqrt{2}\hbar.$$

For $\ell = 2$, the matrices are:

$$\hat{L}^2 = \begin{pmatrix} 6 & 0 & 0 & 0 & 0 \\ 0 & 6 & 0 & 0 & 0 \\ 0 & 0 & 6 & 0 & 0 \\ 0 & 0 & 0 & 6 & 0 \\ 0 & 0 & 0 & 0 & 6 \end{pmatrix} \hbar^2, \quad \hat{L}_z = \begin{pmatrix} 2 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 0 & -2 \end{pmatrix} \hbar, \quad \hat{L}_x = \begin{pmatrix} 0 & 1 & 0 & 0 & 0 \\ 1 & 0 & \frac{\sqrt{3}}{2} & 0 & 0 \\ 0 & \frac{\sqrt{3}}{2} & 0 & \frac{\sqrt{3}}{2} & 0 \\ 0 & 0 & \frac{\sqrt{3}}{2} & 0 & 1 \\ 0 & 0 & 0 & 1 & 0 \end{pmatrix} \hbar$$

$$\hat{L}_y = \begin{pmatrix} 0 & -1 & 0 & 0 & 0 \\ 1 & 0 & -\frac{\sqrt{3}}{2} & 0 & 0 \\ 0 & \frac{\sqrt{3}}{2} & 0 & -\frac{\sqrt{3}}{2} & 0 \\ 0 & 0 & \frac{\sqrt{3}}{2} & 0 & -1 \\ 0 & 0 & 0 & 1 & 0 \end{pmatrix} i\hbar, \quad \hat{L}_+ = \begin{pmatrix} 0 & 2 & 0 & 0 & 0 \\ 0 & 0 & \sqrt{6} & 0 & 0 \\ 0 & 0 & 0 & \sqrt{6} & 0 \\ 0 & 0 & 0 & 0 & 2 \\ 0 & 0 & 0 & 0 & 0 \end{pmatrix} \hbar,$$

$$\hat{L}_- = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 \\ 2 & 0 & 0 & 0 & 0 \\ 0 & \sqrt{6} & 0 & 0 & 0 \\ 0 & 0 & \sqrt{6} & 0 & 0 \\ 0 & 0 & 0 & 2 & 0 \end{pmatrix} \hbar .$$

6-2. From the above matrix representations of the angular momentum operators, it can be shown that all the cyclic commutation relationships among all such operators are indeed satisfied. For example, for $\ell=1$:

$$\hat{L}_x \hat{L}_y = \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix} \begin{pmatrix} 0 & -1 & 0 \\ 1 & 0 & -1 \\ 0 & 1 & 0 \end{pmatrix} \frac{i\hbar^2}{2} = \begin{pmatrix} 1 & 0 & -1 \\ 0 & 0 & 0 \\ 1 & 0 & -1 \end{pmatrix} \frac{i\hbar^2}{2} , \quad \hat{L}_y \hat{L}_x = \begin{pmatrix} -1 & 0 & -1 \\ 0 & 0 & 0 \\ 1 & 0 & 1 \end{pmatrix} \frac{i\hbar^2}{2} ;$$

$$\therefore \hat{L}_x \hat{L}_y - \hat{L}_y \hat{L}_x = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix} i\hbar^2 = i\hbar \hat{L}_z .$$

Similarly, one can show all the other cyclic commutation relationships.

6-3. No. All three components of the angular momentum operators can be specified precisely at the same time if the expectation values of all the commutators of the angular momentum operators are precisely zero in a particular state. This is the case when the hydrogen atom is in the ground state, or the s-level ($\ell=0$).

6-4. Show that the $n=2$, $\ell=1$, and $m_\ell=1$ wave function indeed satisfies the time-independent Schrodinger's equation given in the text for the hydrogen atom:

$$\Psi_{211}(r, \theta, \phi) = R_{21}(r) Y_{11}(\theta, \phi) = [(2a_0)^{-3/2} \frac{1}{\sqrt{3}} \frac{r}{a_0} e^{-r/2a_0}] [-\sqrt{\frac{3}{8\pi}} e^{i\phi} \sin\theta] ,$$

$$\frac{\partial}{\partial r} \left(r^2 \frac{\partial}{\partial r} \right) \left[(2a_0)^{-3/2} \frac{1}{\sqrt{3}} \frac{r}{a_0} e^{-r/2a_0} \right] = (2a_0)^{-3/2} \frac{1}{\sqrt{3}} \frac{r}{a_0} \left[2 - 2 \frac{r}{a_0} + \frac{r^2}{(2a_0)^2} \right] e^{-r/2a_0} ,$$

$$\left(\frac{1}{\sin \theta} \frac{\partial}{\partial \theta} \sin \theta \frac{\partial}{\partial \theta} + \frac{1}{\sin^2 \theta} \frac{\partial^2}{\partial \phi^2} \right) e^{i\phi} \sin \theta = -2 e^{i\phi} \sin \theta .$$

Therefore,

$$\begin{aligned} & \left\{ -\frac{\hbar^2}{2m} \left[\frac{1}{r^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial}{\partial r} \right) + \frac{1}{r^2 \sin \theta} \frac{\partial}{\partial \theta} \left(\sin \theta \frac{\partial}{\partial \theta} \right) + \frac{1}{r^2 \sin^2 \theta} \frac{\partial^2}{\partial \phi^2} \right] - \frac{e^2}{r} \right\} \Psi_{211}(r, \theta, \phi) \\ &= \left\{ -\frac{\hbar^2}{2m r^2} \left[2 - 2 \frac{r}{a_0} + \frac{r^2}{(2a_0)^2} - 2 \right] - \frac{e^2}{r} \right\} \Psi_{211}(r, \theta, \phi) = \left[-\frac{\hbar^2}{2m (2a_0)^2} \right] \Psi_{211}(r, \theta, \phi) \\ &= E_{21} \Psi_{211}(r, \theta, \phi), \end{aligned}$$

and

$$E_{211} = -\frac{\hbar^2}{2m a_0^2 2^2} = -\frac{me^4}{2\hbar^2 2^2} . \quad \text{Q.E.D.}$$

Also, the wave function is indeed normalized:

$$\int_0^{\pi} \int_0^{2\pi} \int_0^{\infty} |\Psi_{211}|^2 r^2 \sin \theta dr d\theta d\phi = \left[\int_0^{\infty} (2a_0)^{-3} \frac{r^4}{3a_0^2} e^{-r/a_0} dr \right] \left[\frac{3}{4} \int_0^{\pi} \sin^3 \theta d\theta \right] = 1. \quad \text{Q.E.D.}$$

6-5. A particle is known to be in a state such that $\hat{L}^2 = 2\hbar^2$. It is also known that measurement of \hat{L}_z will yield the value $+\hbar$ with the probability $1/3$ and the value $-\hbar$ with the probability $2/3$.

(a) The normalized wave function, $\Psi(\theta, \phi)$, of this particle in terms of the spherical harmonics is:

$$\Psi(r, \theta, \phi) = \frac{1}{\sqrt{3}} Y_{11}(\theta, \phi) + \sqrt{\frac{2}{3}} Y_{1-1}(\theta, \phi) \quad .$$

- (b) The expectation value, $\langle \hat{L}_z \rangle$, of the z-component of the angular momentum of this particle is:

$$\langle \hat{L}_z \rangle = \frac{1}{3} \hbar - \frac{2}{3} \hbar = -\frac{1}{3} \hbar \quad .$$

- 6-6.** The wave function of a particle of mass m moving in a potential well is, at a particular time t :

$$\Psi(x, y, z) = (x + y + z) e^{-\alpha \sqrt{x^2 + y^2 + z^2}}$$

- (a) Ψ in the spherical coordinate system is:

$$\Psi(x, y, z) = (x + y + z) e^{-\alpha \sqrt{x^2 + y^2 + z^2}} = [r \sin \theta \cos \phi + r \sin \theta \sin \phi + r \cos \theta] e^{-\alpha r}$$

$$= \left[\left(\frac{-1+i}{2} \right) \sqrt{\frac{8\pi}{3}} Y_{11} + \left(\frac{1+i}{2} \right) \sqrt{\frac{8\pi}{3}} Y_{1-1} + \sqrt{\frac{4\pi}{3}} Y_{10} \right] r e^{-\alpha r} .$$

To normalize:

$$1 = \int |\Psi(\theta, \phi)|^2 \sin \theta d\theta d\phi = N^2 \left[\left(\frac{2}{4} + \frac{2}{4} \right) \frac{8\pi}{3} + \frac{4\pi}{3} \right] ; \quad \therefore N = \sqrt{\frac{1}{4\pi}} \quad .$$

The corresponding normalized wave function is:

$$\Psi(\theta, \phi) = \left(\frac{-1+i}{\sqrt{6}} \right) Y_{11} + \left(\frac{1+i}{\sqrt{6}} \right) Y_{1-1} + \sqrt{\frac{1}{3}} Y_{10} .$$

- (b) The probability measurement of \hat{L}^2 and \hat{L}_z gives the values $2\hbar^2$ and 0, respectively, is:

$$\text{Probability} = \frac{1/3}{1/3 + 1/3 + 1/3} = \frac{1}{3}$$

6-7. Consider a mixed state of hydrogen:

$$\Psi = R_{21}(r)Y_{11}(\theta, \phi) + 2R_{32}(r)Y_{21}(\theta, \phi)$$

(a) The normalized Ψ is:

$$\Psi = \frac{1}{\sqrt{5}}R_{21}(r)Y_{11}(\theta, \phi) + \frac{2}{\sqrt{5}}R_{32}(r)Y_{21}(\theta, \phi)$$

(b) Ψ is not an eigen function of \hat{L}^2 , but is an eigen function of \hat{L}_z corresponding to the eigen value \hbar .

(c) The expectation value $\langle \Psi | \hat{L}^2 | \Psi \rangle$ is :

$$\langle \Psi | \hat{L}^2 | \Psi \rangle = \frac{2}{5}\hbar^2 + \frac{4}{5}6\hbar^2 = \frac{26}{5}\hbar^2$$

(d) The $\langle \Psi | \hat{L}_z | \Psi \rangle$ is \hbar .

(e) $\langle \Psi | \hat{H} | \Psi \rangle = -\left(\frac{1}{5} \cdot \frac{1}{4} + \frac{4}{5} \cdot \frac{1}{9}\right) 13.6 \text{ eV}$

6-8. Consider a hydrogen atom in the following mixed state at $t=0$:

$$\Psi(r, \theta, \phi, t=0) = 3R_{32}(r)Y_{20}(\theta, \phi) + R_{21}(r)Y_{11}(\theta, \phi)$$

(a) The normalized the wave function is:

$$\Psi(r, \theta, \phi, t = 0) = \frac{3}{\sqrt{10}} R_{32}(r) Y_{20}(\theta, \phi) + \frac{1}{\sqrt{10}} R_{21}(r) Y_{11}(\theta, \phi) \quad .$$

- (b) The atom is not in a stationary state, because it is in a mixed state of $n=2$ and $n=3$.
- (c) The expectation value of the energy for $t > 0$ is:

$$\langle \Psi | \hat{H} | \Psi \rangle = -\left(\frac{9}{10} \cdot \frac{1}{9} + \frac{1}{10} \cdot \frac{1}{4} \right) 13.6 \text{ eV} \quad .$$

- (d) The expectation values are :

$$\langle \Psi | \hat{L}^2 | \Psi \rangle = \left(\frac{9}{10} \cdot 6 + \frac{1}{10} \cdot 2 \right) \hbar^2 = \frac{28}{5} \hbar^2$$

$$\langle \Psi | \hat{L}_z | \Psi \rangle = \left(\frac{9}{10} \cdot 0 + \frac{1}{10} \right) \hbar = \frac{1}{10} \hbar$$

- (e) The uncertainty of \hat{L}_z in this state is:

$$\Delta L_z = \left[\langle \Psi | \hat{L}_z^2 | \Psi \rangle - \langle \Psi | \hat{L}_z | \Psi \rangle^2 \right]^{\frac{1}{2}} = \left[\frac{1}{10} - \frac{1}{100} \right]^{1/2} \hbar = \frac{3}{10} \hbar \quad .$$

- 6-9.** This problem is somewhat like the finite square-well potential problem considered in the text, Sect. 4.4. The Hamiltonian of a particle of mass m in a finite spherical potential well:

$$V(r) = \begin{cases} 0, & \text{if } r \leq a \\ V_0, & \text{if } r \geq a \end{cases}$$

is:

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

For $\ell = 0$, it is:

$$\hat{H} = -\frac{\hbar^2}{2m} \left[\frac{1}{r^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial}{\partial r} \right) \right] + V(r) \quad .$$

The corresponding Schroedinger's equation is

$$\left\{ -\frac{\hbar^2}{2m} \left[\frac{1}{r^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial}{\partial r} \right) \right] + V(r) \right\} R_{n0}(r) = E_n R_{n0}(r) \quad , \quad \text{for } r \leq a \quad ,$$

and

$$\left\{ -\frac{\hbar^2}{2m} \left[\frac{1}{r^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial}{\partial r} \right) \right] \right\} R_{n0}(r) = E_n R_{n0}(r) \quad , \quad \text{for } r \geq a \quad .$$

The equation for $r \leq a$ can be converted to:

$$\frac{d^2}{dr^2} U(r) = -\frac{2mE}{\hbar^2} U(r) \quad ,$$

where $U(r) = r R(r)$. The general solution of this equation is:

$$U(r) = A \cos kr + B \sin kr$$

where $k = \frac{\sqrt{2mE}}{\hbar}$. To satisfy the boundary condition that $R_{n0}(r)$ must be finite at $r=0$,

A must be equal to 0, or

$$U(r) = B \sin kr \quad , \quad \text{for } r \leq a .$$

Similarly, for $r \geq a$,

$$U(r) = C e^{\alpha r} + D e^{-\alpha r} \quad ,$$

where $\alpha = \frac{\sqrt{2m(V_0 - E)}}{\hbar}$. For $U(r)$ or $R_{n0}(r)$ to be finite at $r \rightarrow \infty$, C must be equal

to zero and:

$$U(r) = D e^{-\alpha r} \quad , \quad \text{for } r \geq a .$$

Continuity of the wave function $R_{n0}(r)$ and its derivative at $r = a$ leads to the secular equation:

$$-k \cot ka = \alpha \quad .$$

Defining $\xi = ka$, the above equation is of exactly the same form as that corresponding to the antisymmetric solution of the finite square potential-well problem:

$$-\xi \cot \xi = \sqrt{\beta^2 - \xi^2} \quad , \quad \text{where } \beta^2 = \frac{2mV_0 a^2}{\hbar^2} .$$

Just like in that problem, there is no solution, if $\beta < \frac{\pi}{2}$ or

$$V_0 a^2 < \frac{\pi^2 \hbar^2}{8m} \quad . \quad \text{Q.E.D.}$$

Chapter 7

7-1. The Slater-determinant for a 2-electron atom in the form given in (7.11) is:

$$\Psi_{a_1 a_2} = \frac{1}{\sqrt{2}} \begin{vmatrix} \Psi_{a_1}(\vec{r}_1) & \Psi_{a_1}(\vec{r}_2) \\ \Psi_{a_2}(\vec{r}_1) & \Psi_{a_2}(\vec{r}_2) \end{vmatrix} .$$

It is indeed normalized:

$$\begin{aligned} \int \int |\Psi_{a_1 a_2}|^2 d\vec{r}_1 d\vec{r}_2 &= \frac{1}{2} \left[\int |\Psi_{a_1}(\vec{r}_1)|^2 d\vec{r}_1 \cdot \int |\Psi_{a_2}(\vec{r}_2)|^2 d\vec{r}_2 + \int |\Psi_{a_1}(\vec{r}_2)|^2 d\vec{r}_2 \cdot \int |\Psi_{a_2}(\vec{r}_1)|^2 d\vec{r}_1 \right. \\ &\quad \left. - \int \Psi_{a_1}(\vec{r}_1)^* \Psi_{a_2}(\vec{r}_1) d\vec{r}_1 \cdot \int \Psi_{a_2}(\vec{r}_2)^* \Psi_{a_1}(\vec{r}_2) d\vec{r}_2 - \int \Psi_{a_1}(\vec{r}_2)^* \Psi_{a_2}(\vec{r}_2) d\vec{r}_2 \cdot \int \Psi_{a_2}(\vec{r}_1)^* \Psi_{a_1}(\vec{r}_1) d\vec{r}_1 \right] \\ &= \frac{1}{2} [1 \cdot 1 + 1 \cdot 1 - 0 \cdot 0 - 0 \cdot 0] = 1 \quad . \quad \text{Q.E.D.} \end{aligned}$$

7-1. The Slater-determinant for a 2-electron atom in terms of the radial wave functions and the spherical harmonics in the Schrodinger-representation and the spin state functions (α and β) in the Heisenberg-representation of a hydrogenic atom is:

$$\Psi_{a_1 a_2} = \frac{1}{\sqrt{2}} \begin{vmatrix} R_{n_1 \ell_1}(r_1) Y_{\ell_1 m_1}(\theta_1, \phi_1) \alpha_1 & R_{n_1 \ell_1}(r_2) Y_{\ell_1 m_1}(\theta_2, \phi_2) \alpha_2 \\ R_{n_2 \ell_2}(r_1) Y_{\ell_2 m_2}(\theta_1, \phi_1) \beta_1 & R_{n_2 \ell_2}(r_2) Y_{\ell_2 m_2}(\theta_2, \phi_2) \beta_2 \end{vmatrix}$$

7-3. The total orbital and spin angular momentum quantum numbers of the ground-state of helium atom:

$$2 \text{ Electrons} : \ell = 0 \quad , \quad m_\ell = 0 \quad , \quad s = \frac{1}{2} \quad , \quad m_s = \frac{1}{2} \text{ and } -\frac{1}{2} \quad .$$

$$\text{Atom:} \quad L = 0 \quad , \quad M_L = 0 \quad , \quad S = 0 \quad , \quad M_S = 0 \quad .$$

For lithium atom:

$$3 \text{ Electrons : } \ell = 0 \text{ , } m_\ell = 0 \text{ , } s = \frac{1}{2} \text{ , } m_s = \frac{1}{2} \text{ and } -\frac{1}{2} \text{ .}$$

$$\ell = 1 \text{ , } m_\ell = 0 \text{ or } \pm 1 \text{ , } s = \frac{1}{2} \text{ , } m_s = \frac{1}{2} \text{ or } -\frac{1}{2}$$

$$\text{Atom: } L = 1 \text{ , } M_L = 0 \text{ or } \pm 1 \text{ , } S = \frac{1}{2} \text{ , } M_S = \frac{1}{2} \text{ or } -\frac{1}{2} \text{ .}$$

7-4.	Ground state configuration	Degeneracy
Carbon:	$(1s)^2 (2s)^2 (2p)^2$	$(6 \cdot 5 \div 2 = 15) \text{ .}$
Silicon:	$(1s)^2 (2s)^2 (2p)^6 (3s)^2 (3p)^2$	$(6 \cdot 5 \div 2 = 15) \text{ .}$

7-5. The ground state configuration of -

$$\text{Ga : } (1s)^2 (2s)^2 (2p)^6 (3s)^2 (3p)^6 (3d)^{10} (4s)^2 (4p)^1$$

$$\text{As : } (1s)^2 (2s)^2 (2p)^6 (3s)^2 (3p)^6 (3d)^{10} (4s)^2 (4p)^3 \text{ .}$$

Chapter 8

8-1. Substituting (8.17) into the left side of (8.5) gives:

$$i\hbar \frac{\partial}{\partial t} \Psi(\vec{r}, t) \cong E_i \Psi_{E_i}(\vec{r}) e^{-\frac{i}{\hbar} E_i t} + \sum_{j \neq i} e z_{ij} \tilde{E}_z \left[E_j \frac{(1 - e^{i(\omega_{ji} - \omega)t})}{\hbar(\omega_{ji} - \omega)} + e^{i(\omega_{ji} - \omega)t} \right] \Psi_{E_j}(\vec{r}) e^{-\frac{i}{\hbar} E_j t} + 0(\epsilon^2) .$$

Substituting (8.17) into the right side of (8.5) gives in the limit of $\epsilon \rightarrow 1$:

$$[\hat{H}_0 + \epsilon \hat{V}_1] \Psi = E_i \Psi_{E_i}(\vec{r}) e^{-\frac{i}{\hbar} E_i t} + \sum_{j \neq i} e z_{ij} \tilde{E}_z \left[E_j \frac{(1 - e^{i(\omega_{ji} - \omega)t})}{\hbar(\omega_{ji} - \omega)} + e^{i(\omega_{ji} - \omega)t} \right] \Psi_{E_j}(\vec{r}) e^{-\frac{i}{\hbar} E_j t} ,$$

which is the same as the left side.

[Note: To derive the right side equation above, use is made of the fact that \hat{V}_1 in the representation in which \hat{H}_0 is diagonal is:

$$\hat{V}_1 = \hat{1} \cdot \hat{V}_1 \cdot \hat{1} = \sum_{j \neq i} |E_j\rangle \langle E_j| e z \tilde{E}_z |E_j\rangle \langle E_j| e^{-i\omega t} \quad \text{and} \quad \langle E_j | E_i \rangle = \mathbf{d}_{ji} .]$$

8-2. For circularly polarized waves:

$$\vec{E}(\vec{r}, t) = \frac{\tilde{E}_{\pm}}{\sqrt{2}} (\hat{\mathbf{e}}_x \mp i \hat{\mathbf{e}}_y) e^{i\omega t} \quad \text{and} \quad \hat{V}_{\pm} = \frac{e \tilde{E}_{\pm}}{\sqrt{2}} (x \mp i y) e^{i\omega t} .$$

Therefore,

$$W_{ij} = \frac{\pi e^2}{\hbar^2} [|x_{ij}|^2 + |y_{ij}|^2] |E_{\pm}|^2 \delta(\omega_{ij} - \omega) .$$

For spherically symmetric systems, such as atoms:

$$W_{ij} = \frac{2\pi e^2}{3\hbar^2} |r|^2 |E_{\pm}|^2 \delta(\omega_{ij} - \omega) \quad ,$$

where $|r|^2 = |x|^2 + |y|^2 + |z|^2 = 3|x|^2 = 3|y|^2 = 3|z|^2$.

8-3. For the selection rules on the orbital angular momentum,

$$\langle \ell m_{\ell} | Y_{10} | \ell' m_{\ell'} \rangle = \int_0^{2\pi} \int_0^{\pi} Y_{\ell m_{\ell}}^* Y_{10} Y_{\ell' m_{\ell'}} \sin \theta d\theta d\phi \propto \delta_{m_{\ell} m_{\ell'}} \quad ,$$

$$\langle \ell m_{\ell} | Y_{1\pm 1} | \ell' m_{\ell'} \rangle = \int_0^{2\pi} \int_0^{\pi} Y_{\ell m_{\ell}}^* Y_{10} Y_{\ell' m_{\ell'}} \sin \theta d\theta d\phi \propto \delta_{m_{\ell}, (m_{\ell'} \pm 1)} \quad ,$$

and from the known properties of the integrals of three spherical harmonics, $|\Delta \ell| \equiv |\ell - \ell'| \leq 1$. On the basis of parity considerations, ℓ and ℓ' must be of opposite parity; therefore, $\Delta \ell \equiv \ell - \ell' = \pm 1$.

8-4. According to the Rydberg formula (8.24):

$$\frac{1}{\lambda_{1s,2p}} = R_H \left(1 - \frac{1}{n^2} \right) \quad ,$$

$$\lambda_{1s,2p} = 91.127 \times \frac{n^2}{n^2 - 1} \text{ nm} \quad .$$

For Lyman series:

n	2	3	4	5	6	
Experiment	121.6	102.6	97.3	95.0	93.8	nm
Rydberg Formula	121.5	102.5	97.2	94.9	93.7	nm

8-5. Give the expectation value of the z-component of the electric dipole moment of the hydrogen atom in the mixed state:

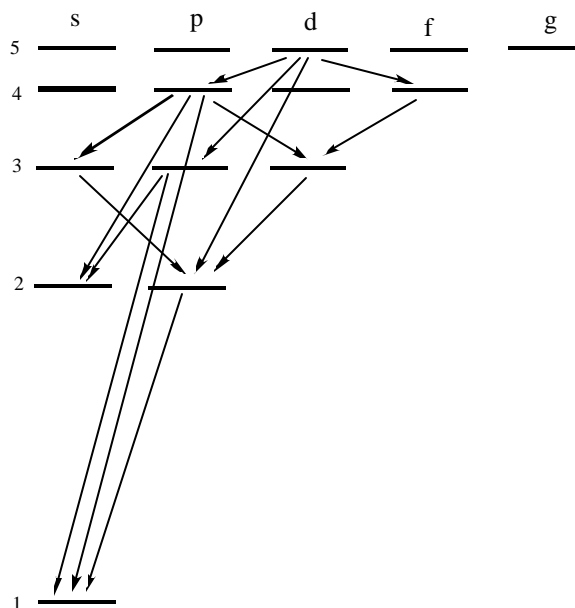
$$\begin{aligned} \langle \Psi | (-ez) | \Psi \rangle &= \frac{-e}{1 + |C_{12}|^2} \langle 100 | z | 210 \rangle C_{12} + \text{complex conjugate} \\ &= \frac{-C_{21}e}{1 + |C_{12}|^2} \int_0^\infty R_{10} r R_{21} r^2 dr \int_0^\pi Y_{00} \cos \theta Y_{10} \sin \theta d\theta + C.C. \\ &\cong \frac{-C_{21}e}{1 + |C_{12}|^2} 1.5 a_0 + C.C. \end{aligned}$$

8.6 An electron in the $n = 3, \ell = 0, m = 0$ state of hydrogen decays by a sequence of (electric dipole) transitions to the ground state.

(a) The decay routes open to it are:

$$\begin{aligned} |300\rangle &\rightarrow |210\rangle \rightarrow |100\rangle \\ &\rightarrow |21\pm 1\rangle \rightarrow |100\rangle \end{aligned}$$

(b) The allowed transitions from the 5d states of hydrogen to the lower states are:



- 8.7.** Assume a Lorentzian fluorescence linewidth of 10 Ghz. The stimulated emission cross-section (in cm^2) defined in connection with (8.31) for a hypothetical hydrogen laser with linearly polarized emission at 121.56 nm (Lyman- α line) is:

$$\sigma_{st} = \frac{4\pi^2 e^2 \nu}{\hbar c} |x_{12}| g_f(\nu) \cong 7.1 \times 10^4 |x_{12}|^2 \quad .$$

Using the value of the dipole moment found in Problem 8-5, $|x_{12}|^2 \approx 0.62 \times 10^{-16} \text{ cm}^2$,

$$\therefore \sigma_{st} \approx 4.4 \times 10^{-12} \text{ cm}^2 \quad .$$

Assuming all the degenerate states in the 2p level are equally populated, the corresponding spatial gain coefficient (in cm^{-1}) is:

$$g = (N_2 - N_1) \sigma_{st} \approx 4.4 \times 10^{-2} \text{ cm}^{-1} \quad ,$$

if the total population inversion between the 1s and 2p levels of hydrogen in the gaseous medium is 10^{10} cm^{-3} .

Chapter 9

9-1. The spin-orbit interaction in hydrogen is of the form, (6.62) :

$$\hat{H}_{s-o} = \left(\frac{Ze^2}{2m^2 c^2 r^3} \right) \hat{L} \cdot \hat{S} \equiv \zeta(r) \hat{L} \cdot \hat{S}$$

The corresponding matrix for $\ell = 1$ in the representation in which \hat{L}^2 , \hat{L}_z , \hat{S}^2 , \hat{S}_z are diagonal is a 6x6 matrix. To diagonalize this matrix within the manifold of degenerate states $|n, \ell = 1, m_\ell, s = 1/2, m_s \rangle$, the columns and rows corresponding to the pairs of (m_ℓ, m_s) values are arranged in a particular order:

$$\begin{matrix} (m_\ell, m_s) & (-1, -\frac{1}{2}) & (-1, +\frac{1}{2}) & (0, -\frac{1}{2}) & (0, +\frac{1}{2}) & (+1, -\frac{1}{2}) & (+1, +\frac{1}{2}) \\ \begin{pmatrix} (-1, -1/2) \\ (-1, +1/2) \\ (0, -1/2) \\ (0, +1/2) \\ (+1, -1/2) \\ (+1, +1/2) \end{pmatrix} & \begin{pmatrix} 1/2 & 0 & 0 & 0 & 0 & 0 \\ 0 & -1/2 & 1/\sqrt{2} & 0 & 0 & 0 \\ 0 & 1/\sqrt{2} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1/\sqrt{2} & 0 \\ 0 & 0 & 0 & 1/\sqrt{2} & -1/2 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1/2 \end{pmatrix} & \cdot \mathbf{z}_{n\ell} \hbar^2 \end{matrix} .$$

This matrix breaks down into two 2x2 and two 1x1 matrices which can be easily diagonalized. Doing so according to the degenerate perturbation theory yields two new eigen values: $\mathbf{z}_{n\ell} \hbar^2 / 2$ and $-\mathbf{z}_{n\ell} \hbar^2$. These correspond to the two new sets of 4-fold $(j = \frac{3}{2}, m_j = \pm \frac{1}{2}, \pm \frac{3}{2})$ and 2-fold $(j = \frac{1}{2}, m_j = \pm \frac{1}{2})$ degenerate levels split from the original 6-fold degenerate level in the absence of spin-orbit interaction as given in Sect. 6.5. The two sets of new eigen states correspond to the spin-orbit coupled $j = 3/2, m_j = \pm 3/2, \pm 1/2$ and $j = 1/2, m_j = \pm 1/2$ hydrogenic states. The diagonalization procedure gives also the relevant vector-coupling coefficients

$\langle \ell m_\ell s m_s / j m_j \ell s \rangle$ defined in (6.59) for the eigen functions for this particular case. For example, the vector-coupling coefficients:

$$\langle j m_j \ell s | \ell m_\ell s m_s \rangle = \langle 3/2, \pm 3/2, 1, 1/2 | 1, \pm 1, 1/2, \pm 1/2 \rangle = 1 \quad ,$$

$$\langle j m_j \ell s | \ell m_\ell s m_s \rangle = \langle 3/2, -1/2, 1, 1/2 | 1, -1, 1/2, 1/2 \rangle = \sqrt{\frac{1}{3}} \quad ,$$

$$\langle j m_j \ell s | \ell m_\ell s m_s \rangle = \langle 3/2, -1/2, 1, 1/2 | 1, 0, 1/2, -1/2 \rangle = \sqrt{\frac{2}{3}} \quad ,$$

etc.

This is the procedure for calculating vector-coupling coefficients in general.

9-2. The perturbation theory for the covalent bonded homo-nuclear diatomic molecule can be extended to the case of hetero-nuclear diatomic molecules:

$$\begin{pmatrix} E_A & \hat{H}_{AB} \\ \hat{H}_{BA} & E_B \end{pmatrix} \begin{pmatrix} C_{Ag} \\ C_{Bg} \end{pmatrix} = E_g \begin{pmatrix} C_{Ag} \\ C_{Bg} \end{pmatrix}$$

where

$$E_A \equiv \langle A | \hat{H} | A \rangle \neq E_B \equiv \langle B | \hat{H} | B \rangle, \quad H_{AB} \equiv \langle A | \hat{H} | B \rangle = H_{BA}^* \equiv \langle B | \hat{H} | A \rangle^* \quad .$$

Setting the corresponding secular determinant to zero gives:

$$E_g^2 - (E_A + E_B) E_g - |H_{AB}|^2 + E_A E_B = 0 \quad ,$$

which gives the bonding and anti-bonding levels of the heteronuclear molecule:

$$E_{a,b} = \frac{(E_A + E_B)}{2} \pm \frac{1}{2} \left[(E_A - E_B)^2 + 4|H_{AB}|^2 \right]^{1/2}$$

$$\approx E_B \pm \frac{|H_{AB}|^2}{(E_A - E_B)},$$

for $(E_A - E_B) \gg |H_{AB}|^2$ and $E_A > E_B$. The corresponding wave functions of the bonding and antibonding orbitals of the molecule are:

$$|b\rangle = C_A^{(b)}|A\rangle + C_B^{(b)}|B\rangle \quad \text{and} \quad |a\rangle = C_A^{(a)}|A\rangle + C_B^{(a)}|B\rangle,$$

where $(E_A - E_{a,b})C_A^{(a,b)} + H_{AB}C_B^{(a,b)} = 0$.

More specifically, they are:

$$C_A^{(a,b)} = \frac{|H_{AB}|}{\left[|H_{AB}|^2 + (E_A - E_{a,b})^2 \right]} \quad \text{and} \quad C_B^{(a,b)} = \frac{E_A - E_{a,b}}{\left[|H_{AB}|^2 + (E_A - E_{a,b})^2 \right]}.$$

[Note: $H_{AB} = -|H_{AB}|$.]

9-3. Suppose the un-normalized molecular orbital of a diatomic homo-nuclear diatomic molecule is:

$$\Psi_{mo} = C_A |A\rangle + C_B |B\rangle$$

where $|A\rangle$ and $|B\rangle$ are the normalized atomic orbitals.

(a) The normalized molecular orbital is:

$$\Psi_{m.o.} = \frac{1}{\sqrt{|C_A|^2 + |C_B|^2 + 2SC_A C_B}} [C_A |A\rangle + C_B |B\rangle],$$

where $S \equiv \langle A | B \rangle$ is the overlap integral between the atomic orbitals and C_A and C_B are assumed to be real.

(b) The corresponding molecular energy is:

$$E_m \equiv \langle \Psi_m | \hat{H} | \Psi_m \rangle = \frac{|C_A|^2 E_A + |C_B|^2 E_B + 2C_A C_B H_{AB}}{|C_A|^2 + |C_B|^2 + 2SC_A C_B},$$

and

$$E_m [|C_A|^2 + |C_B|^2 + 2SC_A C_B] = |C_A|^2 E_A + |C_B|^2 E_B + 2C_A C_B H_{AB}.$$

Following the basic concept of Coulson's molecular-orbital theory, differentiate the above equation against variations in C_A gives:

$$\frac{\partial E_m}{\partial C_A} [|C_A|^2 + |C_B|^2 + 2SC_A C_B] + 2E_m [C_A + S C_B] = 2 [C_A E_A + C_B H_{AB}]$$

Minimizing the molecular energy against variations in C_A , or setting $\partial E_m / \partial C_A = 0$, yields one condition that E_m , C_A , and C_B must satisfy:

$$(E_A - E_m) C_A + (H_{AB} - E_m S) C_B = 0.$$

Similarly, by minimizing the molecular energy against variations in C_B , or setting $\partial E_m / \partial C_B = 0$, yields another condition E_m , C_A , and C_B must satisfy:

$$(H_{BA} - E_m S) C_A + (E_B - E_m) C_B = 0.$$

The secular determinant of these two homogeneous equations must be zero:

$$\begin{vmatrix} E_A - E_m & H_{AB} \\ H_{BA} & E_B - E_m \end{vmatrix} \cong 0 \quad ,$$

assuming the overlap integral is negligible or $S \approx 0$. This result is the same as that obtained in Problem 9-2 above according to degenerate perturbation theory.

9-4. The number of atoms per cubic cell of volume a^3 in such a lattice:

$$\frac{N}{a^3} = 2 \cdot \left[\left(8 \cdot \frac{1}{8} \right) + 6 \cdot \frac{1}{2} \right] = \frac{8}{a^3} \quad .$$

The number of valence electrons per conventional unit cell of diamond lattice = $4 \cdot \frac{8}{a^3}$.

9-5. The primitive translational vectors for;

$$\text{SCC:} \quad \vec{a} = a \mathbf{e}_x \quad , \quad \vec{b} = a \mathbf{e}_y \quad , \quad \vec{c} = a \mathbf{e}_z \quad ;$$

$$\text{FCC:} \quad \vec{a} = \frac{a}{2} (\mathbf{e}_x + \mathbf{e}_y) \quad , \quad \vec{b} = \frac{a}{2} (\mathbf{e}_y + \mathbf{e}_z) \quad , \quad \vec{c} = \frac{a}{2} (\mathbf{e}_x + \mathbf{e}_z)$$

9-6. Diamond lattice = FCC with 2 atoms per basis at $(0, 0, 0)$ and $\left(\frac{1}{4}, \frac{1}{4}, \frac{1}{4} \right)$. It is, therefore, equivalent to two inter-laced FCC lattice displaced one quarter the distance along the body diagonal of the FCC.

9-7. The C-C bond length in the diamond structure = $\frac{\sqrt{3}}{4} a$.

Chapter 10

10-1. For a two-dimensional electron gas, the density-of-state is independent of the energy; therefore, the Fermi energy is directly proportional to the electron density:

$$N_e = \int_0^{E_F} D^{(2)}(E) dE = \frac{m}{\pi \hbar^2} E_F \quad .$$

10-2.

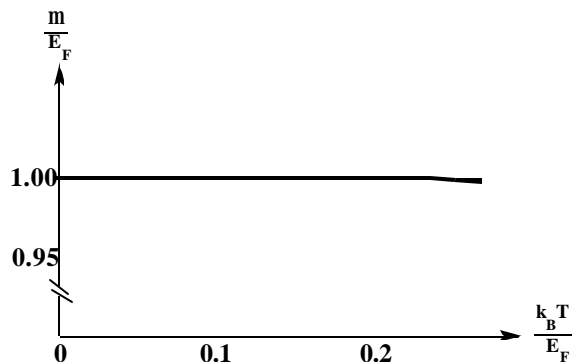
(a) The chemical potential of a free-electron gas in two dimensions is given can be found from Eq.(10.29):

$$N_e = \int_0^{\infty} \frac{m k_B T}{\pi \hbar^2} \frac{1}{e^{(E-\mu)/k_B T} + 1} \frac{dE}{k_B T} = \frac{m k_B T}{\pi \hbar^2} \ln [e^{\mu/k_B T} + 1] \quad ;$$

$$\therefore \quad \mu(T) = k_B T \ln [e^{\frac{\pi \hbar^2 N_e}{m k_B T}} - 1] \quad ,$$

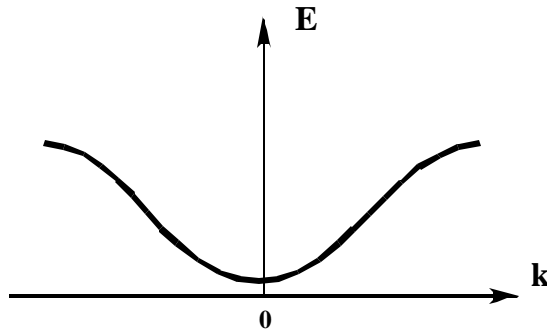
for N_e electrons per unit area.

(b) Plot $\mu(T)/E_F$ as a function of kT/E_F as in Figure 10.6(b):

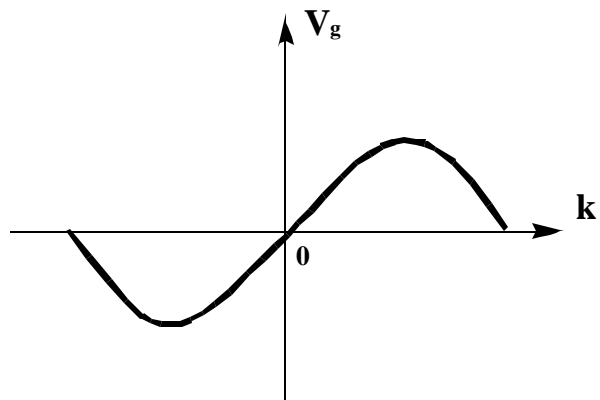


10-3. For a typical 1-D energy band, sketch graphs of the relationships between the wave vector, k , of an electron and its:

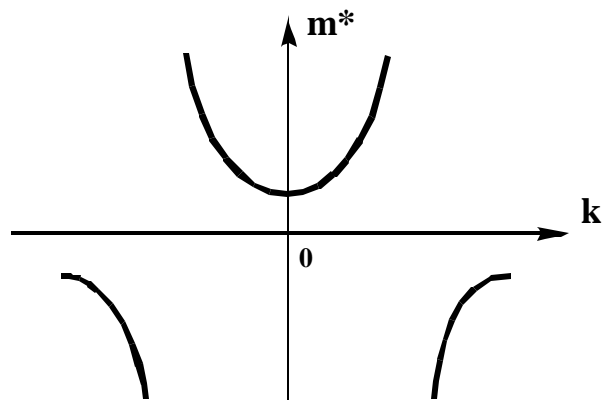
(a) energy,



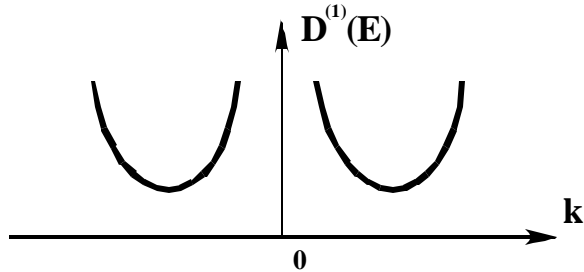
(b) group velocity,



(c) and effective mass.



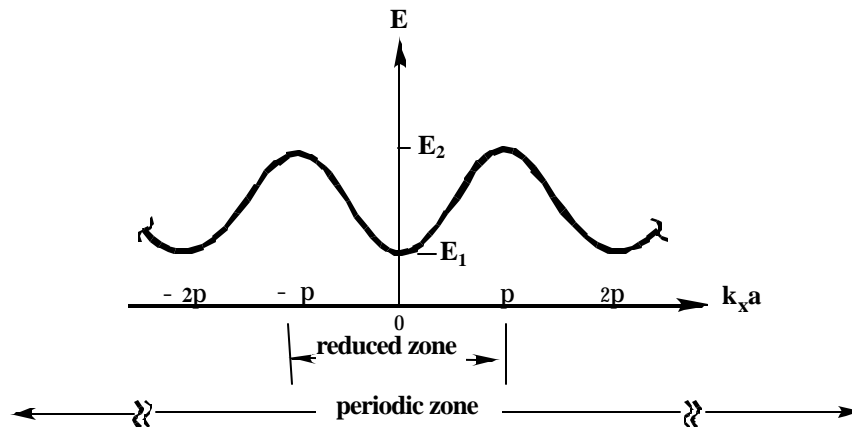
- d. The approximate density-of-states $D^{(1)}(E)$ for the energy band of part a above is



- 10-4.** The $E(k_x)$ vs. k_x dependence for an electron in the conduction band of a one-dimensional semiconductor crystal with lattice constant $a = 4 \text{ \AA}$ is given by:

$$E(k_x) = E_2 - (E_2 - E_1) \cos^2[k_x a / 2]; \quad E_2 > E_1$$

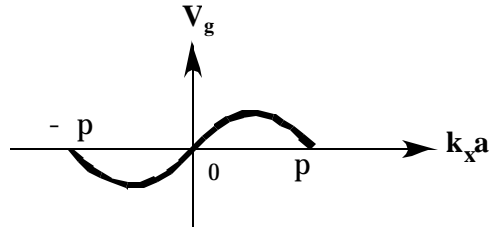
- (a) The $E(k_x)$ for this band in the reduced and periodic zone schemes.



- (b) The group velocity of an electron in this band is:

$$v_g = \left[\frac{1}{\hbar} \frac{\partial E}{\partial k} \right] = \frac{(E_2 - E_1) a}{2\hbar} \sin k_x a$$

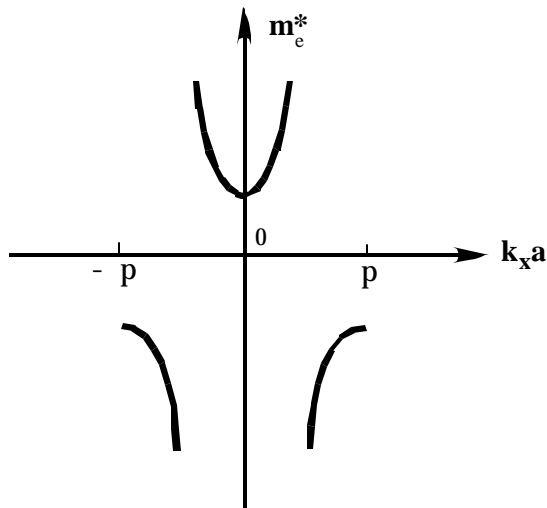
and is sketched below as a function of k_x :



- (c) The effective mass of an electron in this band as a function of k_x is:

$$m^* = \hbar^2 \left[\frac{\partial^2 E}{\partial^2 k} \right]^{-1} = \hbar^2 \left[\frac{(E_2 - E_1) a^2}{2} \cos k_x a \right]^{-1}$$

and is sketched below it in the reduced-zone scheme:



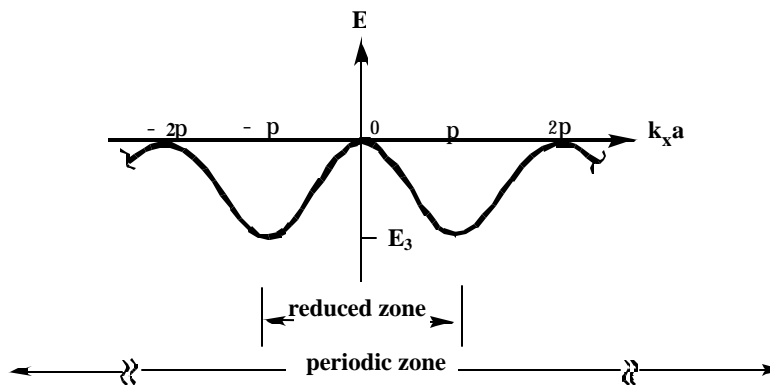
A uniform electric field E_x is applied in the x -direction, the motion of the electron is as follows:

$\underline{k_x a}$	$\underline{v_g}$	$\underline{m_e^*}$	<u>Acceleration</u>
0.2π	> 0	> 0	-x direction
0.5π	> 0	$\rightarrow \infty$	$= 0$
0.9π	> 0	< 0	+x direction

10-5. Suppose now the corresponding electron energy $E(k_x)$ vs. k_x curve in the valence band is:

$$E(k_x) = -E_3 + E_3 \cos^2[k_x a / 2]$$

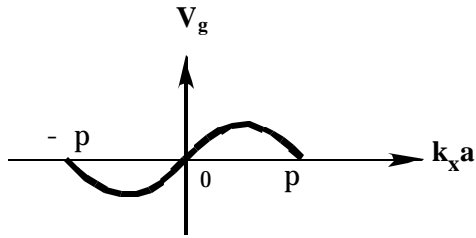
(a) The $E(k_x)$ sketch for this band in the reduced- and periodic-zone schemes:



(b) The group velocity of a hole in this band is:

$$v_g = \left[-\frac{1}{\hbar} \frac{\nabla E_h}{\nabla k} \right] = \frac{E_3 a}{2\hbar} \sin k_x a$$

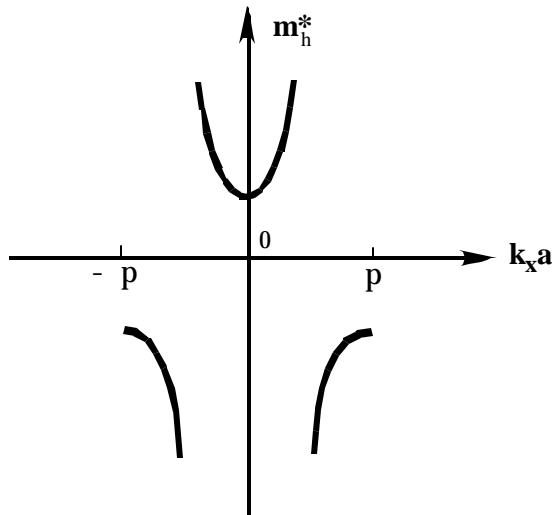
and is sketched below as a function k_x :



- (c) The effective mass of the hole in this band as a function of k_x in the reduced zone scheme is:

$$m^* = \hbar^2 \left[-\frac{\partial^2 E_e}{\partial^2 k} \right]^{-1} = \hbar^2 \left[\frac{E_3 a^2}{2} \cos k_x a \right]^{-1} .$$

The corresponding effective mass of an electron in the valence band is



- (d) A uniform electric field E_x is applied in the x -direction, the motion of the holes is as follows:

<u>$\mathbf{k_x a}$</u>	<u>$\mathbf{v_g}$</u>	<u>$\mathbf{m_h^*}$</u>	<u>Acceleration</u>
0.2 π	> 0	> 0	+x direction
0.5 π	> 0	$\rightarrow \infty$	= 0
0.9 π	> 0	< 0	-x direction .

10-6. From (10.46) and (10.47), $N \propto (m^*)^{3/2}$; therefore,

$$E_F \cong \frac{E_C + E_V}{2} + \frac{kT}{2} \ln\left(\frac{N_V}{N_C}\right) = \frac{E_C + E_V}{2} + \frac{3kT}{4} \ln\left(\frac{m_h^*}{m_e^*}\right) .$$

10-7. A semiconductor has $N_c = 4 \times 10^{17} \text{ cm}^{-3}$ and $N_v = 6 \times 10^{18} \text{ cm}^{-3}$ at room temperature and has a band gap of 1.4 eV. A p-n junction is made in this material with $N_a = 10^{17} \text{ cm}^{-3}$ on one side, and $N_d = 2 \times 10^{15} \text{ cm}^{-3}$ and $N_a = 10^{15} \text{ cm}^{-3}$ on the other side. Assume complete ionization of donors and acceptors.

- (a) If the semiconductor is not doped and choosing $E = 0$ to be at the top of the valence band or $E_v = 0$:

$$E_F \cong \frac{E_C + E_V}{2} + \frac{kT}{2} \ln\left(\frac{N_V}{N_C}\right) = 0.7 + \frac{1}{80} \ln\left(\frac{60}{4}\right) \cong 0.73 \text{ eV} ,$$

$$n_i = \left(N_c N_v e^{-\frac{E_g}{kT}} \right)^{1/2} \cong (12 \times 10^{-13})^{1/2} \ll \ll N_d^+ \approx N_d \quad \text{or} \quad N_a^- \approx N_a .$$

One, therefore, assume that on the p-side:

$$p = N_v e^{-(E_F - E_V)/kT} \approx N_a^- \approx N_a \quad \text{and} \quad E_F - E_V \approx kT \ln\left(\frac{N_v}{N_a}\right) \approx 0.102 \text{ eV} .$$

- (b) Similarly, on the n-side, $N_D^+ \approx N_D = N_d - N_a = 10^{15} \text{ cm}^{-3}$:

$$E_C - E_F \approx kT \ln\left(\frac{N_C}{N_D}\right) \approx 0.15 \text{ eV}$$

- (c) The built-in voltage across the junction at room temperature is then:

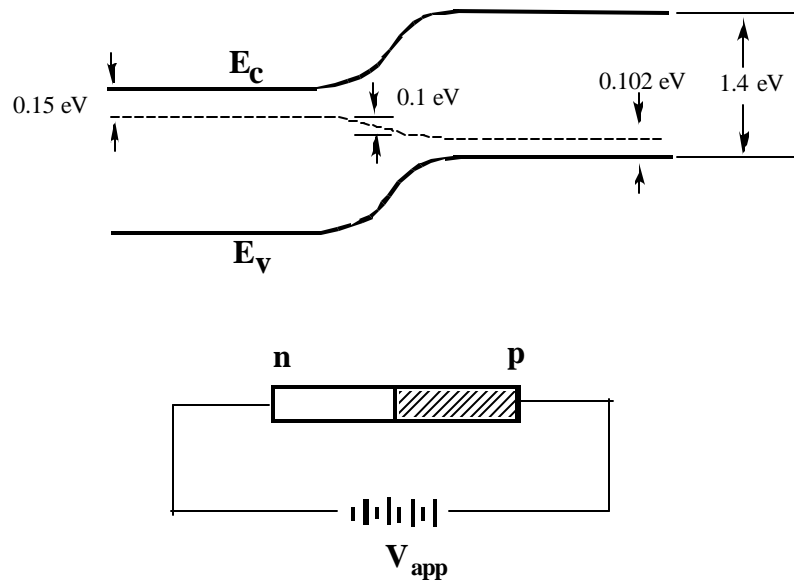
$$V_B \cong 1.4 - 0.15 - 0.102 = 1.148 \text{ Volt}$$

- (d) The equilibrium minority carrier (electron) density on the p-side of the junction at room temperature is then:

$$n_p = n_n e^{-V_B/kT} \approx N_D e^{-V_B/kT} \approx 47 \text{ m}^{-3}$$

which is extremely small!

- (e) When a forward bias of 0.1 eV is applied across the junction, the minority carrier density on the p-side increased by the factor: $e^{0.1/kT} \cong 54.6$.



Chapter 11

11-1. For a statistical ensemble of N spin-1/2 particles per volume, the matrices representing the Cartesian components of the spin angular momentum of such particles in the representation in which \hat{S}_z and \hat{S}^2 are diagonal are given in (6.50). The averaged expectation values per volume of the three components of the spin angular momentum in terms of the appropriate density matrix elements for the statistical ensemble of particles are:

$$\langle \bar{S}_z \rangle = N \text{Trace} \left[\begin{pmatrix} \mathbf{r}_{11} & \mathbf{r}_{12} \\ \mathbf{r}_{21} & \mathbf{r}_{22} \end{pmatrix} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \frac{\hbar}{2} \right] = \frac{N\hbar}{2} (\mathbf{r}_{11} - \mathbf{r}_{22}) \quad ,$$

$$\langle \bar{S}_y \rangle = N \text{Trace} \left[\begin{pmatrix} \mathbf{r}_{11} & \mathbf{r}_{12} \\ \mathbf{r}_{21} & \mathbf{r}_{22} \end{pmatrix} \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \frac{\hbar}{2} \right] = \frac{iN\hbar}{2} (\mathbf{r}_{12} - \mathbf{r}_{21}) \quad ,$$

$$\langle \bar{S}_x \rangle = N \text{Trace} \left[\begin{pmatrix} \mathbf{r}_{11} & \mathbf{r}_{12} \\ \mathbf{r}_{21} & \mathbf{r}_{22} \end{pmatrix} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \frac{\hbar}{2} \right] = \frac{N\hbar}{2} (\mathbf{r}_{12} + \mathbf{r}_{21}) \quad ,$$

11-2. An electrical charged particle with a spin angular momentum will have a magnetization proportional to the spin angular momentum. Suppose the averaged expectation value of the magnetization of the medium considered in Problem 11-1 above is $\vec{M} = N \text{Trace} [\hat{\rho} (\gamma \vec{S})]$.

(a) The three Cartesian components of the magnetization in terms of the appropriate density-matrix elements as in Problem 11-1 above are:

$$\bar{M}_z = \frac{N\gamma\hbar}{2} (\rho_{11} - \rho_{22}) \quad ,$$

$$\bar{M}_y = \frac{iN\gamma\hbar}{2} (\rho_{12} - \rho_{21}) \quad ,$$

$$\bar{M}_x = \frac{N\gamma\hbar}{2} (\rho_{12} + \rho_{21}) \quad .$$

- (b) The Hamiltonian of the spin-1/2 particles in the presence of a static magnetic field $\vec{H} = H_x \vec{x} + H_y \vec{y} + H_z \vec{z}$, but in the absence of any relaxation processes is:

$$\hat{H} = -\frac{\gamma\hbar}{2} \begin{pmatrix} H_z & H_x - i\mathbf{g}H_y \\ H_x + i\mathbf{g}H_y & -H_z \end{pmatrix}$$

From the results of Part a above, on the basis of the density-matrix equation (11.16), the dynamic equations describing the precession of the magnetization \vec{M} around such a magnetic field are:

$$\frac{d}{dt}(\rho_{11} - \rho_{22}) = -\frac{i}{\hbar} 2 [H_{12}\rho_{21} - \rho_{12}H_{21}] = \gamma [iH_x(-\rho_{12} + \rho_{21}) + H_y(\rho_{12} + \rho_{21})] \quad ,$$

which can be shown to be

$$\frac{d}{dt} \bar{M}_z = \gamma [-H_x M_y + H_y M_x] = \gamma [\vec{M} \times \vec{H}] \quad ,$$

making use of the results in (a) above. Similarly for the x- and y-components of

$$\vec{M} \quad , \quad \therefore \quad \frac{d\vec{M}}{dt} = \gamma \vec{M} \times \vec{H} \quad , \quad \text{just like in classical mechanics.}$$

- (c) Suppose a magnetic field consisting of a static component in the \vec{z} -direction and a weak oscillating component in the plane perpendicular to the \vec{z} -axis is applied to the medium: $\vec{H} = H_0 \vec{z} + H_x \vec{x} \equiv H_0 \vec{z} + H_1 \cos \omega_0 t \vec{x}$. The corresponding Hamiltonian is:

$$\hat{H} = -\frac{\gamma \hbar}{2} \begin{pmatrix} H_0 & H_1 \cos \omega_0 t \\ H_1 \cos \omega_0 t & H_0 \end{pmatrix} .$$

From (11.19),

$$\frac{d}{dt}(\rho_{11} - \rho_{22}) = -\frac{(\rho_{11} - \rho_{22}) - (\rho_{11}^{(th)} - \rho_{22}^{(th)})}{T_1} + i\gamma H_x (-\rho_{12} + \rho_{21}) .$$

Also, $\bar{M}_\pm = \bar{M}_x \pm i\bar{M}_y$. Therefore,

$$\frac{d}{dt} \bar{M}_z = -\frac{\bar{M}_z - \bar{M}_z^{(th)}}{T_1} + i\frac{\gamma H_1}{2} (\bar{M}_+ - \bar{M}_-) \cos \omega_0 t .$$

Similarly, for the other components:

$$\frac{d}{dt} \bar{M}_\pm = -\frac{\bar{M}_\pm}{T_2} \pm i\gamma H_0 \bar{M}_\mp \mp i\gamma H_1 \bar{M}_z \cos \omega_0 t .$$

These are the well-known Bloch equations in the literature on magnetic resonance phenomena.

11-3.

- (a) From the dispersion relation for light waves, $k^2 = \epsilon \omega^2 / c^2$, and the definitions $k \equiv \beta + i\alpha$ and $\epsilon \equiv \epsilon' + i\epsilon'' = \epsilon_0 + i\epsilon''$,

$$\beta \equiv \sqrt{\epsilon_0} \omega_0 / c \quad \text{and} \quad \alpha \equiv \epsilon'' \omega_0^2 / \beta c^2 .$$

Therefore, on the basis of (11.44) and near the resonance, $\mathbf{w}_0 \approx \mathbf{w}_{21}$ and :

$$\mathbf{a} \cong \frac{\mathbf{e}'' \mathbf{w}_0^2}{\mathbf{b} c^2} = \frac{\mathbf{e}'' \mathbf{w}_0}{\sqrt{\mathbf{e}_0} c} = \frac{4 \mathbf{p}^2 (N_1 - N_2) \mathbf{n}_0 e^2 |z_{12}|^2}{\sqrt{\mathbf{e}_0} \hbar c} g_f(\mathbf{n}_0) = \frac{\mathbf{w}_p^2 f}{4 \sqrt{\mathbf{e}_0} c} g_f(\mathbf{n}_0) \quad ,$$

where $\omega_p \equiv \sqrt{\frac{4\pi N e^2}{m}} \approx \sqrt{\frac{4\pi(N_1 - N_2)e^2}{m}}$, if most of atoms are in the ground state, is known as the “plasma frequency” and $f_z \equiv \frac{2m\mathbf{w}_{21}}{\hbar} |z_{21}|^2$ is known as the “oscillator strength”.

- (b) To compare the result obtained in Part a above with the classical result based on a damped harmonic oscillator model instead of the two-level atom model: Suppose the equation of motion of the harmonic oscillator is of the form:

$$\frac{d^2}{dt^2} z(t) + \Gamma \frac{d}{dt} z(t) + \mathbf{w}_{21}^2 z(t) = -\frac{f^{1/2} e}{m} (\tilde{E}_z e^{-i\mathbf{w}_0 t} + \tilde{E}_z^* e^{i\mathbf{w}_0 t})$$

which describes the oscillating motion of a particle of mass m and negative charge of the magnitude $f^{1/2}e$ bound to a fixed point in space similar to the oscillator shown in Figure 5.1. The spring constant of the harmonic oscillator is equal to $m\mathbf{w}_{21}^2$; the damping constant is Γ ; and the deviation of the particle from its equilibrium position in the absence of any electric field E_z is $z(t)$.

For the classical result, assume $\mathbf{w}_0 \approx \mathbf{w}_{21} \gg \Gamma^{-1}$ so that $\mathbf{w}_0^2 - \mathbf{w}_{21}^2 \cong 2\mathbf{w}_0(\mathbf{w}_0 - \mathbf{w}_{21})$. Solving the above equation for a damped harmonic oscillator:

$$z = -\frac{\sqrt{f} e \tilde{E}}{m} \frac{1}{4\omega_0} g_f(\mathbf{v}) \quad ;$$

and

$$\therefore \mathbf{e} = \mathbf{e}' + i \mathbf{e}'' = 4 \mathbf{p} [\mathbf{c}' + i \mathbf{c}''] = 4 \mathbf{p} \mathbf{c}' - i 4 \mathbf{p} \left(\frac{N \sqrt{f} e z}{\tilde{E}} \right) ,$$

therefore, the classical model gives also :

$$\frac{\mathbf{e}'' \mathbf{w}_0}{\sqrt{\mathbf{e}_0} c} = \frac{\mathbf{w}_p^2 f}{4\sqrt{\mathbf{e}_0} c} g_f(\mathbf{n}_0) = \mathbf{a} \quad ,$$

which is the same as the result obtained in (a) above on the basis of the quantum mechanic density-matrix equation.

- (c) Since the complex dielectric constant based on the oscillator strength f using either the quantum mechanical model or the classical harmonic oscillator model gives the same result for ϵ'' , it is obvious that the same should be true for ϵ' . The classical harmonic oscillator model, therefore, can be used to characterize the dispersion and absorption characteristics of linear optical media with only three phenomenological parameters: the oscillator strength f , that characterizes the strength of the charge e^2 , the resonance frequency ω_{21} , and the damping constant Γ associated with the bound particle in the harmonic oscillator model.

11-4. Differentiating (11.51)

$$\rho_{mn}(t) = \int_{-\infty}^t \left\{ \frac{\rho_{mn}^{(th)}}{T_{mn}} + \frac{i}{\hbar} \sum_{m'} [\rho_{mm'}(t') V(t')_{m'n} - V(t')_{mm'} \rho_{m'n}(t')] \right\} e^{(i\omega_{mn} + 1/T_{mn})(t'-t)} dt'$$

gives:

$$\frac{d}{dt} \rho_{mn} = \frac{\rho_{mn}^{(th)}}{T_{mn}} + \frac{i}{\hbar} \sum_{m'} [\rho_{mm'} V(t)_{m'n} - V(t)_{mm'} \rho_{m'n}] - (i\omega_{mn} + \frac{1}{T_{mn}}) \rho_{mn} \quad ,$$

which is Eq.(11.27). (11.51), therefore, satisfies and is a solution of (11.27).

11.5 The second-order nonlinear optical susceptibility $\tilde{\mathbf{c}}^{(2)}(\mathbf{w}_1 + \mathbf{w}_2 = \mathbf{w}_3)$ relates the induced macroscopic polarization component $P_i(\omega_3)$ to the applied electric field components $E_j(\omega_1)$ and $E_k(\omega_2)$ in the medium:

$$P_i(\omega_3) = \sum_{j,k} \tilde{\chi}_{ijk}^{(2)}(\omega_1 + \omega_2 = \omega_3) E_j(\omega_1) E_k(\omega_2) \quad .$$

For any such medium with inversion symmetry, inverting the coordinate axes leaves $\tilde{\chi}_{ijk}^{(2)}(\omega_1 + \omega_2 = \omega_3)$ invariant but changes the signs of all the vector components:

$$-P_i(\omega_3) = \sum_{j,k} \tilde{\chi}_{ijk}^{(2)}(\omega_1 + \omega_2 = \omega_3) [-E_j(\omega_1)] [-E_k(\omega_2)] = P_i(\omega_3) \quad .$$

Therefore, $\tilde{\mathbf{c}}^{(2)}(\mathbf{w}_1 + \mathbf{w}_2 = \mathbf{w}_3)$ must vanish.

11.6. Consider a laser with the following parameters: $T_l \sim 10^{-9}$ sec, $T_2 \sim 10^{-12}$ sec, $T_{ph} \sim 5 \times 10^{-12}$ sec, $R_{pump} \sim 10^{27}$ /cm³ - sec, $Bh\mathbf{n}_0 g_f(v_0) \sim 6 \times 10^{-7}$ cm³/sec. The corresponding laser rate equations are:

$$\left\{ \begin{array}{l} \frac{d}{dt} (N_2 - N_1) = -10^9 (N_2 - N_1) - 1.2 \cdot 10^{-6} (N_2 - N_1) N_{ph} + 10^{27} \\ \frac{d}{dt} N_{ph} = -2 \cdot 10^{11} N_{ph} + 6 \cdot 10^{-7} (N_2 - N_1) N_{ph} + 0(N_{ph}^{(spont)}) \end{array} \right.$$

Changing the scales: $t \rightarrow 10\tau$, $(N_2 - N_1) \rightarrow 10^{15}n$, $N_{ph} \rightarrow 10^{14}N$ so that the numbers are more manageable in the numerical computation:

$$\begin{cases} \frac{d}{d\tau} n = -10n - 1.2nN + 10^4 \\ \frac{d}{d\tau} N = -2 \cdot 10^3 N + 6nN + 0(N^{(spont)}) \end{cases} \cdot$$

The steady-state solutions of these equations are: $n_{ss} = 333.3$ and $N_{ss} \approx 16.6$.

Changing to normalized parameters: $\frac{n}{333.3} \equiv y$ and $\frac{N}{16.6} \equiv z$, the above rate equations become:

$$\begin{cases} \frac{d}{dt} y = -10y(1+2z) + 30 \\ \frac{d}{dt} z = 2 \cdot 10^3 z(y-1) + 0(z^{(spont)}) \end{cases} \cdot$$

The turn-on dynamics of such a laser can be calculated numerically on the basis of these normalized laser rate equations using, for example, the Mathematica program:

```
NDSolve[{y'[x] == -20 y[x] Abs[z[x]] - 10 y[x] + 30,
z'[x] == -2000 z[x] + 2000 y[x] z[x] + 0.001, y[0] == 0,
z[0] == 0}, {y, z}, {x, 0, 2}]
g = 0/0
Plot[Evaluate[ y[x] /. g], {x, 0, 0.5}, PlotRange-> {0, 2},
AxesOrigin->{0, 0},
AxesLabel->{"t", "n(t)/n(s.s)"}]
Plot[Evaluate[ z[x] /. g], {x, 0, 0.5}, PlotRange->{0, 10},
AxesLabel->{"t", "N(t)/N(s.s.)"}]
```

The resulting calculated dynamics for the normalized population inversion and intracavity intensity are shown in the figures (t in 10^{-7} sec) below. These results show a pattern of laser relaxation oscillations with the frequency in the range of a few tenths of a Ghz and a damping time on the order of tens of nsec, numbers characteristic of a semiconductor laser.

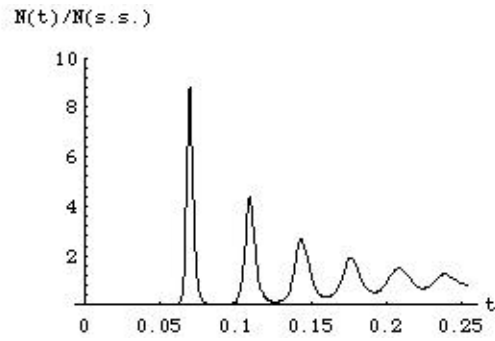
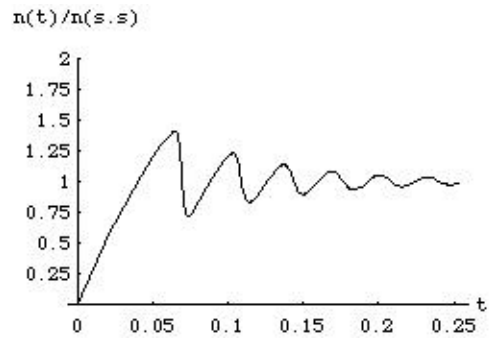


Figure 11.1 - Examples of the transient dynamics of a semiconductor laser.

Errata

Chapter 4 -

- Page 48, Eq.(419) should read :

$$\frac{F}{A} = \frac{e^{-ik_3d}}{\left[\cos k_2d - i \frac{k_1^2 + k_2^2}{2k_1k_2} \sin k_2d \right]}$$

not :

$$\frac{F}{A} = \frac{e^{-ik_3d}}{\left[\cos k_2d - i \frac{k_1^2 + k^2}{2k_1k_2} \sin k_2d \right]}$$

- Page 55, line 7 should read:

$$\hat{H} \hat{\mathcal{P}} \sum_n C_n \Psi_{E_n}(x) = \sum_n (-1)^{n+1} C_n E_n \Psi_{E_n}(x) = \hat{\mathcal{P}} \hat{H} \sum_n C_n \Psi_{E_n}(x)$$

not :

$$\hat{H} \hat{\mathcal{P}} \sum_n C_n \Psi_{E_n}(x) = \pm \sum_n C_n E_n \Psi_{E_n}(x) = \hat{\mathcal{P}} \hat{H} \sum_n C_n \Psi_{E_n}(x)$$

- Page 60, Problem 4.1, line 4 should read:

for $\beta = 4$ and $10, \dots$,

not :

for $\beta = 2$ and 6

- Page 61, Problem 4.4, equation should read:

$$\Psi(x) = \dots\dots\dots ,$$

not :

$$V(x) = \dots\dots\dots .$$

- Page 62, Problem 4.6 (c), should read:

$$\dots \text{ for the lowest two bound states} \dots\dots\dots ,$$

not :

$$\text{for the lowest three bound states } \dots\dots\dots .$$

Chapter 5 -

- Page 84, line 12 should read:

$$\Delta n = \sqrt{\langle \alpha | (\hat{a}^+ \hat{a}^-)^2 | \alpha \rangle - (\langle \alpha | \hat{a}^+ \hat{a}^- | \alpha \rangle)^2} = |\alpha| = (\bar{n})^{\frac{1}{2}} ,$$

not
$$\Delta n = \sqrt{\langle \alpha | (\hat{a}^+ \hat{a}^-)^2 | \alpha \rangle - (\langle \alpha | \hat{a}^+ \hat{a}^- | \alpha \rangle)^2} = |\alpha| = (\bar{n})^{\frac{1}{2}} .$$

- Page 82, third line from the bottom should read:

$$= |\langle 0 | \alpha \rangle|^2 \sum_n \frac{|\alpha|^{2n}}{n!} = |\langle 0 | \alpha \rangle|^2 e^{|\alpha|^2},$$

not :

$$= |\langle 0 | \alpha \rangle|^2 \sum_n \frac{\alpha^{2n}}{n!} = |\langle 0 | \alpha \rangle|^2 e^{|\alpha|^2}.$$

Chapter 6 –

- Equation (6.3) should read :

$$\left\{ -\frac{\hbar^2}{2m} \left[\frac{1}{r^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial}{\partial r} \right) + \frac{1}{r^2 \sin \theta} \frac{\partial}{\partial \theta} \left(\sin \theta \frac{\partial}{\partial \theta} \right) + \frac{1}{r^2 \sin^2 \theta} \frac{\partial^2}{\partial \phi^2} \right] - \frac{e^2}{r} \right\} \Psi_E(r, \theta, \phi)$$

$$= E \Psi_E(r, \theta, \phi),$$

not :

$$\left\{ -\frac{\hbar^2}{2m} \left[\frac{1}{r^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial}{\partial r} \right) + \frac{1}{r^2 \sin^2 \theta} \frac{\partial}{\partial \theta} \left(\sin \theta \frac{\partial}{\partial \theta} \right) + \frac{1}{r^2 \sin^2 \theta} \frac{\partial^2}{\partial \phi^2} \right] - \frac{e^2}{r} \right\} \Psi_E(r, \theta, \phi)$$

$$= E \Psi_E(r, \theta, \phi).$$

- Equation (6.36) should read:

$$\left\{ -\frac{\hbar^2}{2m} \left[\frac{1}{r^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial}{\partial r} \right) - \frac{\ell(\ell+1)}{r^2} \right] - \frac{e^2}{r} \right\} R_{E_\ell}(r) = E_\ell R_{E_\ell}(r),$$

not :

$$\left\{ -\frac{\hbar^2}{2m} \left[\frac{1}{r^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial}{\partial r} \right) \frac{\partial}{\partial r} - \frac{\ell(\ell+1)}{r^2} \right] - \frac{e^2}{r} \right\} R_{E\ell}(r) = E_\ell R_{E\ell}(r) .$$

- Page 91, Eq.(6.31) should read :

$$\langle \ell m_\ell | \hat{L}_\pm | \ell' m'_\ell \rangle = [(\ell \mp m'_\ell)(\ell \pm m'_\ell + 1)]^{\frac{1}{2}} \hbar \delta_{\ell\ell'} \delta_{m_\ell, (m'_\ell \pm 1)} ,$$

- not :

$$\langle \ell m_\ell | \hat{L}_\pm | \ell' m'_\ell \rangle = [(\ell \mp m_\ell)(\ell \pm m_\ell + 1)]^{\frac{1}{2}} \hbar \delta_{\ell\ell'} \delta_{m_\ell, (m'_\ell \pm 1)} .$$

- Page 99, equation in should read :

$$\int_0^{2\pi} \int_0^\pi |R_{10}(r) Y_{00}|^2 r^2 dr \sin \theta d\theta d\phi = |R_{10}(r)|^2 r^2 dr ,$$

not :

$$\int_0^{2\pi} \int_0^\pi |R_{10}(r)|^2 r^2 dr \sin \theta d\theta d\phi = 4\pi |R_{10}(r)|^2 r^2 dr ,$$

- Page 99, Equation (6.38) should read :

$$\dots\dots\dots \text{and } |p_y \rangle = \frac{i}{\sqrt{2}} (|p_{+1} \rangle + |p_{-1} \rangle) . \quad (6.38) ,$$

not :

..... and $|p_y\rangle = i(|p_{+1}\rangle + |p_{-1}\rangle)$. (6.38) .

- Page 103, Eq.(6.49) should read :

$$\langle jm_j | \hat{J}_\pm | j' m'_j \rangle = [(j \mp m'_j)(j \pm m'_j + 1)]^{\frac{1}{2}} \hbar \delta_{jj'} \delta_{m_j, (m'_j \pm 1)} ,$$

- not :

$$\langle jm_j | \hat{J}_\pm | j' m'_j \rangle = [(j \mp m_j)(j \pm m_j + 1)]^{\frac{1}{2}} \hbar \delta_{jj'} \delta_{m_j, (m'_j \pm 1)} .$$

- Page 109, Problem 6.8(e) should read :

$$\Delta L_z = [\langle \Psi | \hat{L}_z^2 | \Psi \rangle - \langle \Psi | \hat{L}_z | \Psi \rangle^2]^{\frac{1}{2}} ,$$

not :

$$\Delta L_z = [\langle \Psi | \hat{L}_z | \Psi \rangle - \langle \Psi | \hat{L}_z | \Psi \rangle^2]^{\frac{1}{2}} .$$

- Page 108, Problem 6.8(b) should read :

.....measurement of L^2 and L_z that gives,

not :

.....measurement of L^2 and L_z gives, .

Chapter 7 –

- line 18 should read :

$$\Psi_{a_1 a_2 \dots a_{N-1} a_N}(\vec{r}_1, \vec{r}_2, \dots, \vec{r}_{N-1}, \vec{r}_N) = \Psi_{a_2}(\vec{r}_1) \Psi_{a_1}(\vec{r}_2) \dots \Psi_{a_{N-1}}(\vec{r}_{N-1}) \Psi_{a_N}(\vec{r}_N) ,$$

not:

$$\Psi_{a_1 a_2 \dots a_{N-1} a_N}(\vec{r}_1, \vec{r}_2, \dots, \vec{r}_{N-1}, \vec{r}_N) = \Psi_{a_2}(\vec{r}_1) \Psi_{a_1}(\vec{r}_2) \dots \Psi_{n_{N-1} \ell_{N-1} m_{\ell_{N-1}} s_{N-1} m_{s_{N-1}}}(\vec{r}_{N-1}) \Psi_{n_N \ell_N m_{\ell_N} s_N m_{s_N}}(\vec{r}_N)$$

Chapter 8 –

- Equation (8.25) should read:

$$|E_f\rangle = |100\rangle e^{-\frac{i}{\hbar} E_1 t} + C_{12}^{(1)} |210\rangle e^{-\frac{i}{\hbar} E_2 t} ,$$

not :

$$|E_f\rangle = |100\rangle e^{-\frac{i}{\hbar} E_1 t} + C_{12}^{(1)} |210\rangle e^{-\frac{i}{\hbar} E_2 t} .$$

Chapter 10 –

- Eq.(10.46) should read:

$$\boxed{N_C = \frac{\pi}{\sqrt{2}} \left(\frac{m_e^* k_B T}{\pi^2 \hbar^2} \right)^{3/2}}, \quad \text{not : } N_C = \frac{1}{\sqrt{2}} \left(\frac{m_e^* k_B T}{\pi^2 \hbar^2} \right)^{3/2} .$$

- Eq.(10.47) should read :

$$\boxed{N_V = \frac{\pi}{\sqrt{2}} \left(\frac{m_h^* k_B T}{\pi^2 \hbar^2} \right)^{3/2}}, \quad \text{not : } N_V = \frac{1}{\sqrt{2}} \left(\frac{m_h^* k_B T}{\pi^2 \hbar^2} \right)^{3/2} .$$