

SOLUTIONS MANUAL

CHAPTER 1

1. The energy contained in a volume dV is

$$U(\nu, T)dV = U(\nu, T)r^2 dr \sin\theta d\theta d\phi$$

when the geometry is that shown in the figure. The energy from this source that emerges through a hole of area dA is

$$dE(\nu, T) = U(\nu, T)dV \frac{dA \cos\theta}{4\pi r^2}$$

The total energy emitted is

$$\begin{aligned} dE(\nu, T) &= \int_0^{c\Delta t} dr \int_0^{\pi/2} d\theta \int_0^{2\pi} d\phi U(\nu, T) \sin\theta \cos\theta \frac{dA}{4\pi} \\ &= \frac{dA}{4\pi} 2\pi c \Delta t U(\nu, T) \int_0^{\pi/2} d\theta \sin\theta \cos\theta \\ &= \frac{1}{4} c \Delta t dA U(\nu, T) \end{aligned}$$

By definition of the emissivity, this is equal to $E \Delta t dA$. Hence

$$E(\nu, T) = \frac{c}{4} U(\nu, T)$$

2. We have

$$w(\lambda, T) = U(\nu, T) |d\nu/d\lambda| = U\left(\frac{c}{\lambda}\right) \frac{c}{\lambda^2} = \frac{8\pi hc}{\lambda^5} \frac{1}{e^{hc/\lambda kT} - 1}$$

This density will be maximal when $dw(\lambda, T)/d\lambda = 0$. What we need is

$$\frac{d}{d\lambda} \left(\frac{1}{\lambda^5} \frac{1}{e^{A/\lambda} - 1} \right) = \left(-5 \frac{1}{\lambda^6} - \frac{1}{\lambda^5} \frac{e^{A/\lambda}}{e^{A/\lambda} - 1} \left(-\frac{A}{\lambda^2} \right) \right) \frac{1}{e^{A/\lambda} - 1} = 0$$

Where $A = hc/kT$. The above implies that with $x = A/\lambda$, we must have

$$5 - x = 5e^{-x}$$

A solution of this is $x = 4.965$ so that

$$\lambda_{max} T = \frac{hc}{4.965k} = 2.898 \times 10^{-3} m$$

In example 1.1 we were given an estimate of the sun's surface temperature as 6000 K. From this we get

$$\lambda_{max}^{sun} = \frac{28.98 \times 10^{-4} mK}{6 \times 10^3 K} = 4.83 \times 10^{-7} m = 483 nm$$

3. The relationship is

$$h\nu = K + W$$

where K is the electron kinetic energy and W is the work function. Here

$$h\nu = \frac{hc}{\lambda} = \frac{(6.626 \times 10^{-34} J.s)(3 \times 10^8 m/s)}{350 \times 10^{-9} m} = 5.68 \times 10^{-19} J = 3.55 eV$$

With K = 1.60 eV, we get W = 1.95 eV

4. We use

$$\frac{hc}{\lambda_1} - \frac{hc}{\lambda_2} = K_1 - K_2$$

since W cancels. From this we get

$$\begin{aligned} h &= \frac{1}{c} \frac{\lambda_1 \lambda_2}{\lambda_2 - \lambda_1} (K_1 - K_2) = \\ &= \frac{(200 \times 10^{-9} m)(258 \times 10^{-9} m)}{(3 \times 10^8 m/s)(58 \times 10^{-9} m)} \times (2.3 - 0.9) eV \times (1.60 \times 10^{-19} J/eV) \\ &= 6.64 \times 10^{-34} J.s \end{aligned}$$

5. The maximum energy loss for the photon occurs in a head-on collision, with the photon scattered backwards. Let the incident photon energy be $h\nu$, and the backward-scattered photon energy be $h\nu'$. Let the energy of the recoiling proton be E. Then its recoil momentum is obtained from $E = \sqrt{p^2 c^2 + m^2 c^4}$. The energy conservation equation reads

$$h\nu + mc^2 = h\nu' + E$$

and the momentum conservation equation reads

$$\frac{h\nu}{c} = -\frac{h\nu'}{c} + p$$

that is

$$h\nu = -h\nu' + pc$$

We get $E + pc - mc^2 = 2h\nu$ from which it follows that

$$p^2 c^2 + m^2 c^4 = (2h\nu - pc + mc^2)^2$$

so that

$$pc = \frac{4h^2\nu^2 + 4h\nu mc^2}{4h\nu + 2mc^2}$$

The energy loss for the photon is the kinetic energy of the proton $K = E - mc^2$. Now $h\nu = 100 \text{ MeV}$ and $mc^2 = 938 \text{ MeV}$, so that

$$pc = 182 \text{ MeV}$$

and

$$E - mc^2 = K = 17.6 \text{ MeV}$$

6. Let $h\nu$ be the incident photon energy, $h\nu'$ the final photon energy and p the outgoing electron momentum. Energy conservation reads

$$h\nu + mc^2 = h\nu' + \sqrt{p^2 c^2 + m^2 c^4}$$

We write the equation for momentum conservation, assuming that the initial photon moves in the x -direction and the final photon in the y -direction. When multiplied by c it read

$$\mathbf{i}(h\nu) = \mathbf{j}(h\nu') + (\mathbf{i}p_x c + \mathbf{j}p_y c)$$

Hence $p_x c = h\nu$; $p_y c = -h\nu'$. We use this to rewrite the energy conservation equation as follows:

$$(h\nu + mc^2 - h\nu')^2 = m^2 c^4 + c^2(p_x^2 + p_y^2) = m^2 c^4 + (h\nu)^2 + (h\nu')^2$$

From this we get

$$h\nu' = h\nu \left(\frac{mc^2}{h\nu + mc^2} \right)$$

We may use this to calculate the kinetic energy of the electron

$$K = h\nu - h\nu' = h\nu \left(1 - \frac{mc^2}{h\nu + mc^2} \right) = h\nu \frac{h\nu}{h\nu + mc^2}$$

$$= \frac{(100\text{keV})^2}{100\text{keV} + 510\text{keV}} = 16.4\text{keV}$$

Also

$$\mathbf{pc} = \mathbf{i}(100\text{keV}) + \mathbf{j}(-83.6\text{keV})$$

which gives the direction of the recoiling electron.

7. The photon energy is

$$h\nu = \frac{hc}{\lambda} = \frac{(6.63 \times 10^{-34} \text{ J}\cdot\text{s})(3 \times 10^8 \text{ m/s})}{3 \times 10^6 \times 10^{-9} \text{ m}} = 6.63 \times 10^{-17} \text{ J}$$

$$= \frac{6.63 \times 10^{-17} \text{ J}}{1.60 \times 10^{-19} \text{ J/eV}} = 4.14 \times 10^{-4} \text{ MeV}$$

The momentum conservation for collinear motion (the collision is head on for maximum energy loss), when squared, reads

$$\left(\frac{h\nu}{c} \right)^2 + p^2 + 2 \left(\frac{h\nu}{c} \right) p \eta_i = \left(\frac{h\nu'}{c} \right)^2 + p'^2 + 2 \left(\frac{h\nu'}{c} \right) p' \eta_f$$

Here $\eta_i = \pm 1$, with the upper sign corresponding to the photon and the electron moving in the same/opposite direction, and similarly for η_f . When this is multiplied by c^2 we get

$$(h\nu)^2 + (pc)^2 + 2(h\nu)pc\eta_i = (h\nu')^2 + (p'c)^2 + 2(h\nu')p'c\eta_f$$

The square of the energy conservation equation, with E expressed in terms of momentum and mass reads

$$(h\nu)^2 + (pc)^2 + m^2c^4 + 2Eh\nu = (h\nu')^2 + (p'c)^2 + m^2c^4 + 2E'h\nu'$$

After we cancel the mass terms and subtracting, we get

$$h\nu(E - \eta_i pc) = h\nu'(E' - \eta_f p'c)$$

From this can calculate $h\nu'$ and rewrite the energy conservation law in the form

$$E - E' = h\nu \left(\frac{E - \eta_i pc}{E' - p'c \eta_f} - 1 \right)$$

The energy loss is largest if $\eta_i = -1; \eta_f = 1$. Assuming that the final electron momentum is

not very close to zero, we can write $E + pc = 2E$ and $E' - p'c = \frac{(mc^2)^2}{2E'}$ so that

$$E - E' = h\nu \left(\frac{2E \times 2E'}{(mc^2)^2} \right)$$

It follows that $\frac{1}{E'} = \frac{1}{E} + 16h\nu$ with everything expressed in MeV. This leads to $E' = (100/1.64) = 61 \text{ MeV}$ and the energy loss is 39MeV.

8. We have $\lambda' = 0.035 \times 10^{-10} \text{ m}$, to be inserted into

$$\lambda' - \lambda = \frac{h}{m_e c} (1 - \cos 60^\circ) = \frac{h}{2m_e c} = \frac{6.63 \times 10^{-34} \text{ J.s}}{2 \times (0.9 \times 10^{-30} \text{ kg})(3 \times 10^8 \text{ m/s})} = 1.23 \times 10^{-12} \text{ m}$$

Therefore $\lambda = \lambda' = (3.50 - 1.23) \times 10^{-12} \text{ m} = 2.3 \times 10^{-12} \text{ m}$.

The energy of the X-ray photon is therefore

$$h\nu = \frac{hc}{\lambda} = \frac{(6.63 \times 10^{-34} \text{ J.s})(3 \times 10^8 \text{ m/s})}{(2.3 \times 10^{-12} \text{ m})(1.6 \times 10^{-19} \text{ J/eV})} = 5.4 \times 10^5 \text{ eV}$$

9. With the nucleus initially at rest, the recoil momentum of the nucleus must be equal and opposite to that of the emitted photon. We therefore have its magnitude given by $p = h\nu/c$, where $h\nu = 6.2 \text{ MeV}$. The recoil energy is

$$E = \frac{p^2}{2M} = h\nu \frac{h\nu}{2Mc^2} = (6.2 \text{ MeV}) \frac{6.2 \text{ MeV}}{2 \times 14 \times (940 \text{ MeV})} = 1.5 \times 10^{-3} \text{ MeV}$$

10. The formula $\lambda = 2a \sin \theta / n$ implies that $\lambda / \sin \theta \leq 2a / 3$. Since $\lambda = h/p$ this leads to $p \geq 3h / 2a \sin \theta$, which implies that the kinetic energy obeys

$$K = \frac{p^2}{2m} \geq \frac{9h^2}{8ma^2 \sin^2 \theta}$$

Thus the minimum energy for electrons is

$$K = \frac{9(6.63 \times 10^{-34} \text{ J.s})^2}{8(0.9 \times 10^{-30} \text{ kg})(0.32 \times 10^{-9} \text{ m})^2 (1.6 \times 10^{-19} \text{ J/eV})} = 3.35 \text{ eV}$$

For Helium atoms the mass is $4(1.67 \times 10^{-27} \text{ kg}) / (0.9 \times 10^{-30} \text{ kg}) = 7.42 \times 10^3$ larger, so that

$$K = \frac{33.5 \text{ eV}}{7.42 \times 10^3} = 4.5 \times 10^{-3} \text{ eV}$$

11. We use $K = \frac{p^2}{2m} = \frac{h^2}{2m\lambda^2}$ with $\lambda = 15 \times 10^{-9} \text{ m}$ to get

$$K = \frac{(6.63 \times 10^{-34} \text{ J.s})^2}{2(0.9 \times 10^{-30} \text{ kg})(15 \times 10^{-9} \text{ m})^2 (1.6 \times 10^{-19} \text{ J/eV})} = 6.78 \times 10^{-3} \text{ eV}$$

For $\lambda = 0.5 \text{ nm}$, the wavelength is 30 times smaller, so that the energy is 900 times larger. Thus $K = 6.10 \text{ eV}$.

12. For a circular orbit of radius r , the circumference is $2\pi r$. If n wavelengths λ are to fit into the orbit, we must have $2\pi r = n\lambda = nh/p$. We therefore get the condition

$$pr = nh / 2\pi = n\hbar$$

which is just the condition that the angular momentum in a circular orbit is an integer in units of \hbar .

13. We have $a = n\lambda / 2 \sin\theta$. For $n = 1$, $\lambda = 0.5 \times 10^{-10} \text{ m}$ and $\theta = 5^\circ$. we get $a = 2.87 \times 10^{-10} \text{ m}$. For $n = 2$, we require $\sin\theta_2 = 2 \sin\theta_1$. Since the angles are very small, $\theta_2 = 2\theta_1$. So that the angle is 10° .

14. The relation $F = ma$ leads to $mv^2/r = m\omega r$ that is, $v = \omega r$. The angular momentum quantization condition is $mvr = n\hbar$, which leads to $m\omega r^2 = n\hbar$. The total energy is therefore

$$E = \frac{1}{2}mv^2 + \frac{1}{2}m\omega^2 r^2 = m\omega^2 r^2 = n\hbar\omega$$

The analog of the Rydberg formula is

$$\nu(n \rightarrow n') = \frac{E_n - E_{n'}}{h} = \frac{\hbar\omega(n - n')}{h} = (n - n') \frac{\omega}{2\pi}$$

The frequency of radiation in the classical limit is just the frequency of rotation $\nu_{cl} = \omega / 2\pi$ which agrees with the quantum frequency when $n - n' = 1$. When the selection rule $\Delta n = 1$ is satisfied, then the classical and quantum frequencies are the same for all n .

15. With $V(r) = V_0 (r/a)^k$, the equation describing circular motion is

$$m \frac{v^2}{r} = \left| \frac{dV}{dr} \right| = \frac{1}{r} k V_0 \left(\frac{r}{a} \right)^k$$

so that

$$v = \sqrt{\frac{kV_0}{m}} \left(\frac{r}{a} \right)^{k/2}$$

The angular momentum quantization condition $mvr = n\hbar$ reads

$$\sqrt{ma^2 k V_0} \left(\frac{r}{a} \right)^{\frac{k+2}{2}} = n\hbar$$

We may use the result of this and the previous equation to calculate

$$E = \frac{1}{2} m v^2 + V_0 \left(\frac{r}{a} \right)^k = \left(\frac{1}{2} k + 1 \right) V_0 \left(\frac{r}{a} \right)^k = \left(\frac{1}{2} k + 1 \right) V_0 \left[\frac{n^2 \hbar^2}{ma^2 k V_0} \right]^{\frac{k}{k+2}}$$

In the limit of $k \gg 1$, we get

$$E \rightarrow \frac{1}{2} (kV_0)^{\frac{2}{k+2}} \left[\frac{\hbar^2}{ma^2} \right]^{\frac{k}{k+2}} (n^2)^{\frac{k}{k+2}} \rightarrow \frac{\hbar^2}{2ma^2} n^2$$

Note that V_0 drops out of the result. This makes sense if one looks at a picture of the potential in the limit of large k . For $r < a$ the potential is effectively zero. For $r > a$ it is effectively infinite, simulating a box with infinite walls. The presence of V_0 is there to provide something with the dimensions of an energy. In the limit of the infinite box *with the quantum condition* there is no physical meaning to V_0 and the energy scale is provided by $\hbar^2 / 2ma^2$.

16. The condition $L = n\hbar$ implies that

$$E = \frac{n^2 \hbar^2}{2I}$$

In a transition from n_1 to n_2 the Bohr rule implies that the frequency of the radiation is given

$$\nu_{12} = \frac{E_1 - E_2}{h} = \frac{\hbar^2}{2Ih} (n_1^2 - n_2^2) = \frac{\hbar}{4\pi I} (n_1^2 - n_2^2)$$

Let $n_1 = n_2 + \Delta n$. Then in the limit of large n we have $(n_1^2 - n_2^2) \rightarrow 2n_2\Delta n$, so that

$$\nu_{12} \rightarrow \frac{1}{2\pi} \frac{\hbar n_2}{I} \Delta n = \frac{1}{2\pi} \frac{L}{I} \Delta n$$

Classically the radiation frequency is the frequency of rotation which is $\omega = L/I$, i.e.

$$\nu_{cl} = \frac{\omega}{2\pi} = \frac{L}{2\pi I}$$

We see that this is equal to ν_{12} when $\Delta n = 1$.

17. The energy gap between low-lying levels of rotational spectra is of the order of $\hbar^2 / I = (1/2\pi)h\hbar / MR^2$, where M is the reduced mass of the two nuclei, and R is their separation. (Equivalently we can take $2 \times m(R/2)^2 = MR^2$). Thus

$$h\nu = \frac{hc}{\lambda} = \frac{1}{2\pi} h \frac{\hbar}{MR^2}$$

This implies that

$$R = \sqrt{\frac{\hbar\lambda}{2\pi Mc}} = \sqrt{\frac{\hbar\lambda}{\pi mc}} = \sqrt{\frac{(1.05 \times 10^{-34} \text{ J}\cdot\text{s})(10^{-3} \text{ m})}{\pi(1.67 \times 10^{-27} \text{ kg})(3 \times 10^8 \text{ m/s})}} = 26 \text{ nm}$$

CHAPTER 2

1. We have

$$\psi(x) = \int_{-\infty}^{\infty} dk A(k) e^{ikx} = \int_{-\infty}^{\infty} dk \frac{N}{k^2 + \alpha^2} e^{ikx} = \int_{-\infty}^{\infty} dk \frac{N}{k^2 + \alpha^2} \cos kx$$

because only the even part of $e^{ikx} = \cos kx + i \sin kx$ contributes to the integral. The integral can be looked up. It yields

$$\psi(x) = N \frac{\pi}{\alpha} e^{-\alpha|x|}$$

so that

$$|\psi(x)|^2 = \frac{N^2 \pi^2}{\alpha^2} e^{-2\alpha|x|}$$

If we look at $|A(k)|^2$ we see that this function drops to 1/4 of its peak value at $k = \pm \alpha$. We may therefore estimate the width to be $\Delta k = 2\alpha$. The square of the wave function drops to about 1/3 of its value when

$x = \pm 1/2\alpha$. This choice then gives us $\Delta k \Delta x = 1$. Somewhat different choices will give slightly different numbers, but in all cases the product of the widths is independent of α .

2. the definition of the group velocity is

$$v_g = \frac{d\omega}{dk} = \frac{2\pi d\nu}{2\pi d(1/\lambda)} = \frac{d\nu}{d(1/\lambda)} = -\lambda^2 \frac{d\nu}{d\lambda}$$

The relation between wavelength and frequency may be rewritten in the form

$$v^2 - v_0^2 = \frac{c^2}{\lambda^2}$$

so that

$$-\lambda^2 \frac{d\nu}{d\lambda} = \frac{c^2}{v\lambda} = c \sqrt{1 - (v_0/v)^2}$$

3. We may use the formula for v_g derived above for

$$v = \sqrt{\frac{2\pi T}{\rho}} \lambda^{-3/2}$$

to calculate

$$v_g = -\lambda^2 \frac{dv}{d\lambda} = \frac{3}{2} \sqrt{\frac{2\pi T}{\rho\lambda}}$$

4. For deep gravity waves,

$$v = \sqrt{g/2\pi\lambda^{-1/2}}$$

from which we get, in exactly the same way $v_g = \frac{1}{2} \sqrt{\frac{\lambda g}{2\pi}}$.

5. With $\omega = \hbar k^2/2m$, $\beta = \hbar/m$ and with the original width of the packet $w(0) = \sqrt{2}\alpha$, we have

$$\frac{w(t)}{w(0)} = \sqrt{1 + \frac{\beta^2 t^2}{2\alpha^2}} = \sqrt{1 + \frac{\hbar^2 t^2}{2m^2 \alpha^2}} = \sqrt{1 + \frac{2\hbar^2 t^2}{m^2 w^4(0)}}$$

(a) With $t = 1$ s, $m = 0.9 \times 10^{-30}$ kg and $w(0) = 10^{-6}$ m, the calculation yields $w(1) = 1.7 \times 10^2$ m

With $w(0) = 10^{-10}$ m, the calculation yields $w(1) = 1.7 \times 10^6$ m.

These are very large numbers. We can understand them by noting that the characteristic velocity associated with a particle spread over a range Δx is $v = \hbar/m\Delta x$ and here m is very small.

(b) For an object with mass 10^{-3} kg and $w(0) = 10^{-2}$ m, we get

$$\frac{2\hbar^2 t^2}{m^2 w^4(0)} = \frac{2(1.05 \times 10^{-34} \text{ J}\cdot\text{s})^2 t^2}{(10^{-3} \text{ kg})^2 \times (10^{-2} \text{ m})^4} = 2.2 \times 10^{-54}$$

for $t = 1$. This is a totally negligible quantity so that $w(t) = w(0)$.

6. For the 13.6 eV electron $v/c = 1/137$, so we may use the nonrelativistic expression for the kinetic energy. We may therefore use the same formula as in problem 5, that is

$$\frac{w(t)}{w(0)} = \sqrt{1 + \frac{\beta^2 t^2}{2\alpha^2}} = \sqrt{1 + \frac{\hbar^2 t^2}{2m^2 \alpha^2}} = \sqrt{1 + \frac{2\hbar^2 t^2}{m^2 w^4(0)}}$$

We calculate t for a distance of 10^4 km = 10^7 m, with speed $(3 \times 10^8 \text{ m}/137)$ to be 4.6 s. We are given that $w(0) = 10^{-3}$ m. In that case

$$w(t) = (10^{-3} \text{ m}) \sqrt{1 + \frac{2(1.05 \times 10^{-34} \text{ J}\cdot\text{s})^2 (4.6 \text{ s})^2}{(0.9 \times 10^{-30} \text{ kg})^2 (10^{-3} \text{ m})^4}} = 7.5 \times 10^{-2} \text{ m}$$

For a 100 MeV electron $E = pc$ to a very good approximation. This means that $\beta = 0$ and therefore the packet does not spread.

7. For any massless particle $E = pc$ so that $\beta = 0$ and there is no spreading.

8. We have

$$\begin{aligned}\phi(p) &= \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} dx A e^{-\mu|x|} e^{-ipx/\hbar} = \frac{A}{\sqrt{2\pi\hbar}} \left\{ \int_{-\infty}^0 dx e^{(\mu-ik)x} + \int_0^{\infty} dx e^{-(\mu+ik)x} \right\} \\ &= \frac{A}{\sqrt{2\pi\hbar}} \left\{ \frac{1}{\mu-ik} + \frac{1}{\mu+ik} \right\} = \frac{A}{\sqrt{2\pi\hbar}} \frac{2\mu}{\mu^2 + k^2}\end{aligned}$$

where $k = p/\hbar$.

9. We want

$$\int_{-\infty}^{\infty} dx A^2 e^{-2\mu|x|} = A^2 \left\{ \int_{-\infty}^0 dx e^{2\mu x} + \int_0^{\infty} dx e^{-2\mu x} \right\} = A^2 \frac{1}{\mu} = 1$$

so that

$$A = \sqrt{\mu}$$

10. Done in text.

11. Consider the Schrodinger equation with $V(x)$ complex. We now have

$$\frac{\partial \psi(x,t)}{\partial t} = \frac{i\hbar}{2m} \frac{\partial^2 \psi(x,t)}{\partial x^2} - \frac{i}{\hbar} V(x) \psi(x,t)$$

and

$$\frac{\partial \psi^*(x,t)}{\partial t} = -\frac{i\hbar}{2m} \frac{\partial^2 \psi^*(x,t)}{\partial x^2} + \frac{i}{\hbar} V^*(x) \psi(x,t)$$

Now

$$\begin{aligned}\frac{\partial}{\partial t} (\psi^* \psi) &= \frac{\partial \psi^*}{\partial t} \psi + \psi^* \frac{\partial \psi}{\partial t} \\ &= \left(-\frac{i\hbar}{2m} \frac{\partial^2 \psi^*}{\partial x^2} + \frac{i}{\hbar} V^*(x) \psi^* \right) \psi + \psi^* \left(\frac{i\hbar}{2m} \frac{\partial^2 \psi}{\partial x^2} - \frac{i}{\hbar} V(x) \psi \right) \\ &= -\frac{i\hbar}{2m} \left(\frac{\partial^2 \psi^*}{\partial x^2} \psi - \psi^* \frac{\partial^2 \psi}{\partial x^2} \right) + \frac{i}{\hbar} (V^* - V) \psi^* \psi \\ &= -\frac{i\hbar}{2m} \frac{\partial}{\partial x} \left\{ \frac{\partial \psi^*}{\partial x} \psi - \psi^* \frac{\partial \psi}{\partial x} \right\} + \frac{2 \operatorname{Im} V(x)}{\hbar} \psi^* \psi\end{aligned}$$

Consequently

$$\frac{\partial}{\partial t} \int_{-\infty}^{\infty} dx |\psi(x,t)|^2 = \frac{2}{\hbar} \int_{-\infty}^{\infty} dx (\text{Im}V(x)) |\psi(x,t)|^2$$

We require that the left hand side of this equation is negative. This does not tell us much about $\text{Im}V(x)$ except that it cannot be positive everywhere. If it has a fixed sign, it must be *negative*.

12. The problem just involves simple arithmetic. The class average

$$\langle g \rangle = \sum_g g n_g = 38.5$$

$$(\Delta g)^2 = \langle g^2 \rangle - \langle g \rangle^2 = \sum_g g^2 n_g - (38.5)^2 = 1570.8 - 1482.3 = 88.6$$

The table below is a result of the numerical calculations for this system

g	n_g	$(g - \langle g \rangle)^2 / (\Delta g)^2 = \lambda$	$e^{-\lambda}$	$C e^{-\lambda}$
60	1	5.22	0.0054	0.097
55	2	3.07	0.0463	0.833
50	7	1.49	0.2247	4.04
45	9	0.48	0.621	11.16
40	16	0.025	0.975	17.53
35	13	0.138	0.871	15.66
30	3	0.816	0.442	7.96
25	6	2.058	0.128	2.30
20	2	3.864	0.021	0.38
15	0	6.235	0.002	0.036
10	1	9.70	0.0001	0.002
5	0	12.97	"0"	"0"

15. We want

$$1 = 4N^2 \int_{-\infty}^{\infty} dx \frac{\sin^2 kx}{x^2} = 4N^2 k \int_{-\infty}^{\infty} dt \frac{\sin^2 t}{t^2} = 4\pi N^2 k$$

$$\text{so that } N = \sqrt{\frac{1}{4\pi k}}$$

16. We have

$$\langle x^n \rangle = \left(\frac{\alpha}{\pi} \right)^{1/2} \int_{-\infty}^{\infty} dx x^n e^{-\alpha x^2}$$

Note that this integral vanishes for n an odd integer, because the rest of the integrand is even.

For $n = 2m$, an even integer, we have

$$\langle x^{2m} \rangle = \left(\frac{\alpha}{\pi} \right)^{1/2} = \left(\frac{\alpha}{\pi} \right)^{1/2} \left(-\frac{d}{d\alpha} \right)^m \int_{-\infty}^{\infty} dx e^{-\alpha x^2} = \left(\frac{\alpha}{\pi} \right)^{1/2} \left(-\frac{d}{d\alpha} \right)^m \left(\frac{\pi}{\alpha} \right)^{1/2}$$

For $n = 1$ as well as $n = 17$ this is zero, while for $n = 2$, that is, $m = 1$, this is $\frac{1}{2\alpha}$.

$$17. \quad \phi(p) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} dx e^{-ipx/\hbar} \left(\frac{\alpha}{\pi} \right)^{1/4} e^{-\alpha x^2/2}$$

The integral is easily evaluated by rewriting the exponent in the form

$$-\frac{\alpha}{2} x^2 - ix \frac{p}{\hbar} = -\frac{\alpha}{2} \left(x + \frac{ip}{\hbar\alpha} \right)^2 - \frac{p^2}{2\hbar^2\alpha}$$

A shift in the variable x allows us to state the value of the integral as and we end up with

$$\phi(p) = \frac{1}{\sqrt{\pi\hbar}} \left(\frac{\pi}{\alpha} \right)^{1/4} e^{-p^2/2\alpha\hbar^2}$$

We have, for n even, i.e. $n = 2m$,

$$\begin{aligned} \langle p^{2m} \rangle &= \frac{1}{\pi\hbar} \left(\frac{\pi}{\alpha} \right)^{1/2} \int_{-\infty}^{\infty} dp p^{2m} e^{-p^2/\alpha\hbar^2} = \\ &= \frac{1}{\pi\hbar} \left(\frac{\pi}{\alpha} \right)^{1/2} \left(-\frac{d}{d\beta} \right)^m \left(\frac{\pi}{\beta} \right)^{1/2} \end{aligned}$$

where at the end we set $\beta = \frac{1}{\alpha\hbar^2}$. For odd powers the integral vanishes.

18. Specifically for $m = 1$ we have We have

$$(\Delta x)^2 = \langle x^2 \rangle = \frac{1}{2\alpha}$$

$$(\Delta p)^2 = \langle p^2 \rangle = \frac{\alpha \hbar^2}{2}$$

so that $\Delta p \Delta x = \frac{\hbar}{2}$. This is, in fact, the smallest value possible for the product of the dispersions.

22. We have

$$\int_{-\infty}^{\infty} dx \psi^*(x) x \psi(x) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} dx \psi^*(x) x \int_{-\infty}^{\infty} dp \phi(p) e^{ipx/\hbar}$$

$$= \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} dx \psi^*(x) \int_{-\infty}^{\infty} dp \phi(p) \frac{\hbar}{i} \frac{\partial}{\partial p} e^{ipx/\hbar} = \int_{-\infty}^{\infty} dp \phi^*(p) i\hbar \frac{\partial \phi(p)}{\partial p}$$

In working this out we have shamelessly interchanged orders of integration. The justification of this is that the wave functions are expected to go to zero at infinity faster than any power of x , and this is also true of the momentum space wave functions, in their dependence on p .

CHAPTER 3.

1. The linear operators are (a), (b), (f)

2. We have

$$\int_{-\infty}^x dx' x' \psi(x') = \lambda \psi(x)$$

To solve this, we differentiate both sides with respect to x , and thus get

$$\lambda \frac{d\psi(x)}{dx} = x\psi(x)$$

A solution of this is obtained by writing $d\psi/\psi = (1/\lambda)x dx$ from which we can immediately state that

$$\psi(x) = C e^{\lambda x^2/2}$$

The existence of the integral that defines $O_6\psi(x)$ requires that $\lambda < 0$.

3, (a)

$$\begin{aligned} & O_2 O_6 \psi(x) - O_6 O_2 \psi(x) \\ &= x \frac{d}{dx} \int_{-\infty}^x dx' x' \psi(x') - \int_{-\infty}^x dx' x'^2 \frac{d\psi(x')}{dx'} \\ &= x^2 \psi(x) - \int_{-\infty}^x dx' \frac{d}{dx'} (x'^2 \psi(x')) + 2 \int_{-\infty}^x dx' x' \psi(x') \\ &= 2 O_6 \psi(x) \end{aligned}$$

Since this is true for every $\psi(x)$ that vanishes rapidly enough at infinity, we conclude that

$$[O_2, O_6] = 2O_6$$

(b)

$$\begin{aligned} & O_1 O_2 \psi(x) - O_2 O_1 \psi(x) \\ &= O_1 \left(x \frac{d\psi}{dx} \right) - O_2 (x^3 \psi) = x^4 \frac{d\psi}{dx} - x \frac{d}{dx} (x^3 \psi) \\ &= -3x^3 \psi(x) = -3O_1 \psi(x) \end{aligned}$$

so that

$$[O_1, O_2] = -3O_1$$

4. We need to calculate

$$\langle x^2 \rangle = \frac{2}{a} \int_0^a dx x^2 \sin^2 \frac{n\pi x}{a}$$

With $\pi x/a = u$ we have

$$\langle x^2 \rangle = \frac{2}{a} \frac{a^3}{\pi^3} \int_0^\pi du u^2 \sin^2 nu = \frac{a^2}{\pi^3} \int_0^\pi du u^2 (1 - \cos 2nu)$$

The first integral is simple. For the second integral we use the fact that

$$\int_0^\pi du u^2 \cos \alpha u = -\left(\frac{d}{d\alpha}\right)^2 \int_0^\pi du \cos \alpha u = -\left(\frac{d}{d\alpha}\right)^2 \frac{\sin \alpha \pi}{\alpha}$$

At the end we set $\alpha = n\pi$. A little algebra leads to

$$\langle x^2 \rangle = \frac{a^2}{3} - \frac{a^2}{2\pi^2 n^2}$$

For large n we therefore get $\Delta x = \frac{a}{\sqrt{3}}$. Since $\langle p^2 \rangle = \frac{\hbar^2 n^2 \pi^2}{a^2}$, it follows that

$\Delta p = \frac{\hbar \pi n}{a}$, so that

$$\Delta p \Delta x \approx \frac{n \pi \hbar}{\sqrt{3}}$$

The product of the uncertainties thus grows as n increases.

5. With $E_n = \frac{\hbar^2 \pi^2}{2ma^2} n^2$ we can calculate

$$E_2 - E_1 = 3 \frac{(1.05 \times 10^{-34} \text{ J.s})^2}{2(0.9 \times 10^{-30} \text{ kg})(10^{-9} \text{ m})^2} \frac{1}{(1.6 \times 10^{-19} \text{ J/eV})} = 0.115 \text{ eV}$$

We have $\Delta E = \frac{hc}{\lambda}$ so that $\lambda = \frac{2\pi \hbar c}{\Delta E} = \frac{2\pi(2.6 \times 10^{-7} \text{ eV.m})}{0.115 \text{ eV}} = 1.42 \times 10^{-5} \text{ m}$

where we have converted $\hbar c$ from J.m units to eV.m units.

6. (a) Here we write

$$n^2 = \frac{2ma^2 E}{\hbar^2 \pi^2} = \frac{2(0.9 \times 10^{-30} \text{ kg})(2 \times 10^{-2} \text{ m})^2 (1.5 \text{ eV})(1.6 \times 10^{-19} \text{ J/eV})}{(1.05 \times 10^{-34} \text{ J.s})^2 \pi^2} = 1.59 \times 10^{15}$$

so that $n = 4 \times 10^7$.

(b) We have

$$\begin{aligned} \Delta E &= \frac{\hbar^2 \pi^2}{2ma^2} 2n \Delta n = \frac{(1.05 \times 10^{-34} \text{ J.s})^2 \pi^2}{2(0.9 \times 10^{-30} \text{ kg})(2 \times 10^{-2} \text{ m})^2} 2(4 \times 10^7) = 1.2 \times 10^{-26} \text{ J} \\ &= 7.6 \times 10^{-8} \text{ eV} \end{aligned}$$

7. The longest wavelength corresponds to the lowest frequency. Since ΔE is proportional to $(n+1)^2 - n^2 = 2n+1$, the lowest value corresponds to $n=1$ (a state with $n=0$ does not exist). We therefore have

$$h \frac{c}{\lambda} = 3 \frac{\hbar^2 \pi^2}{2ma^2}$$

If we assume that we are dealing with electrons of mass $m = 0.9 \times 10^{-30} \text{ kg}$, then

$$a^2 = \frac{3\hbar\pi\lambda}{4mc} = \frac{3\pi(1.05 \times 10^{-34} \text{ J.s})(4.5 \times 10^{-7} \text{ m})}{4(0.9 \times 10^{-30} \text{ kg})(3 \times 10^8 \text{ m/s})} = 4.1 \times 10^{-19} \text{ m}^2$$

so that $a = 6.4 \times 10^{-10} \text{ m}$.

8. The solutions for a box of width a have energy eigenvalues $E_n = \frac{\hbar^2 \pi^2 n^2}{2ma^2}$ with $n = 1, 2, 3, \dots$. The odd integer solutions correspond to solutions even under $x \rightarrow -x$, while the even integer solutions correspond to solutions that are odd under reflection. These solutions vanish at $x=0$, and it is these solutions that will satisfy the boundary conditions for the “half-well” under consideration. Thus the energy eigenvalues are given by E_n above *with n even*.

9. The general solution is

$$\psi(x, t) = \sum_{n=1}^{\infty} C_n u_n(x) e^{-iE_n t/\hbar}$$

with the C_n defined by

$$C_n = \int_{-a/2}^{a/2} dx u_n^*(x) \psi(x, 0)$$

(a) It is clear that the wave function does not remain localized on the l.h.s. of the box at later times, since the special phase relationship that allows for a total interference for $x > 0$ no longer persists for $t \neq 0$.

(b) With our wave function we have $C_n = \sqrt{\frac{2}{a}} \int_{-a/2}^0 dx u_n(x)$. We may work this out by using the solution of the box extending from $x = 0$ to $x = a$, since the shift has no physical consequences. We therefore have

$$C_n = \sqrt{\frac{2}{a}} \int_0^{a/2} dx \sqrt{\frac{2}{a}} \sin \frac{n\pi x}{a} = \frac{2}{a} \left[-\frac{a}{n\pi} \cos \frac{n\pi x}{a} \right]_0^{a/2} = \frac{2}{n\pi} \left[1 - \cos \frac{n\pi}{2} \right]$$

Therefore $P_1 = |C_1|^2 = \frac{4}{\pi^2}$ and $P_2 = |C_2|^2 = \frac{1}{\pi^2} |1 - (-1)|^2 = \frac{4}{\pi^2}$

10. (a) We use the solution of the above problem to get

$$P_n = |C_n|^2 = \frac{4}{n^2 \pi^2} f_n$$

where $f_n = 1$ for $n = \text{odd integer}$; $f_n = 0$ for $n = 4, 8, 12, \dots$ and $f_n = 4$ for $n = 2, 6, 10, \dots$

(b) We have

$$\sum_{n=1}^{\infty} P_n = \frac{4}{\pi^2} \sum_{\text{odd}} \frac{1}{n^2} + \frac{4}{\pi^2} \sum_{n=2,6,10,\dots} \frac{4}{n^2} = \frac{8}{\pi^2} \sum_{\text{odd}} \frac{1}{n^2} = 1$$

Note. There is a typo in the statement of the problem. The sum should be restricted to *odd* integers.

11. We work this out by making use of an identity. The hint tells us that

$$\begin{aligned} (\sin x)^5 &= \left(\frac{1}{2i} \right)^5 (e^{ix} - e^{-ix})^5 = \frac{1}{16} \frac{1}{2i} (e^{5ix} - 5e^{3ix} + 10e^{ix} - 10e^{-ix} + 5e^{-3ix} - e^{-5ix}) \\ &= \frac{1}{16} (\sin 5x - 5 \sin 3x + 10 \sin x) \end{aligned}$$

Thus

$$\psi(x, 0) = A \sqrt{\frac{a}{2}} \frac{1}{16} (u_5(x) - 5u_3(x) + 10u_1(x))$$

(a) It follows that

$$\psi(x,t) = A\sqrt{\frac{a}{2}} \frac{1}{16} (u_5(x)e^{-iE_5t/\hbar} - 5u_3(x)e^{-iE_3t/\hbar} + 10u_1(x)e^{-iE_1t/\hbar})$$

(b) We can calculate A by noting that $\int_0^a dx |\psi(x,0)|^2 = 1$. This however is equivalent to the statement that the sum of the probabilities of finding *any* energy eigenvalue adds up to 1. Now we have

$$P_5 = \frac{a}{2} A^2 \frac{1}{256}; P_3 = \frac{a}{2} A^2 \frac{25}{256}; P_1 = \frac{a}{2} A^2 \frac{100}{256}$$

so that

$$A^2 = \frac{256}{63a}$$

The probability of finding the state with energy E_3 is 25/126.

12. The initial wave function vanishes for $x \leq -a$ and for $x \geq a$. In the region in between it is proportional to $\cos \frac{\pi x}{2a}$, since this is the first nodeless trigonometric function that vanishes at $x = \pm a$. The normalization constant is obtained by requiring that

$$1 = N^2 \int_{-a}^a dx \cos^2 \frac{\pi x}{2a} = N^2 \left(\frac{2a}{\pi} \right) \int_{-\pi/2}^{\pi/2} du \cos^2 u = N^2 a$$

so that $N = \sqrt{\frac{1}{a}}$. We next expand this in eigenstates of the infinite box potential with boundaries at $x = \pm b$. We write

$$\sqrt{\frac{1}{a}} \cos \frac{\pi x}{2a} = \sum_{n=1}^{\infty} C_n u_n(x;b)$$

so that

$$C_n = \int_{-b}^b dx u_n(x;b) \psi(x) = \int_{-a}^a dx u_n(x;b) \sqrt{\frac{1}{a}} \cos \frac{\pi x}{2a}$$

In particular, after a little algebra, using $\cos u \cos v = (1/2)[\cos(u-v) + \cos(u+v)]$, we get

$$C_1 = \sqrt{\frac{1}{ab}} \int_{-a}^a dx \cos \frac{\pi x}{2b} \cos \frac{\pi x}{2a} = \sqrt{\frac{1}{ab}} \int_{-a}^a dx \frac{1}{2} \left[\cos \frac{\pi x(b-a)}{2ab} + \cos \frac{\pi x(b+a)}{2ab} \right]$$

$$= \frac{4b\sqrt{ab}}{\pi(b^2 - a^2)} \cos \frac{\pi a}{2b}$$

so that

$$P_1 = |C_1|^2 = \frac{16ab^3}{\pi^2(b^2 - a^2)^2} \cos^2 \frac{\pi a}{2b}$$

The calculation of C_2 is trivial. The reason is that while $\psi(x)$ is an *even* function of x , $u_2(x)$ is an *odd* function of x , and the integral over an interval symmetric about $x = 0$ is zero. Hence P_2 will be zero.

13. We first calculate

$$\phi(p) = \int_0^a dx \sqrt{\frac{2}{a}} \sin \frac{n\pi x}{a} \frac{e^{ipx/\hbar}}{\sqrt{2\pi\hbar}} = \frac{1}{i} \sqrt{\frac{1}{4\pi\hbar a}} \left(\int_0^a dx e^{ix(n\pi/a + p/\hbar)} - (n \leftrightarrow -n) \right)$$

$$= \sqrt{\frac{1}{4\pi\hbar a}} \left(\frac{e^{iap/\hbar} (-1)^n - 1}{p/\hbar - n\pi/a} - \frac{e^{iap/\hbar} (-1)^n - 1}{p/\hbar + n\pi/a} \right)$$

$$= \sqrt{\frac{1}{4\pi\hbar a}} \frac{2n\pi/a}{(n\pi/a)^2 - (p/\hbar)^2} \{ (-1)^n \cos pa/\hbar - 1 + i(-1)^n \sin pa/\hbar \}$$

From this we get

$$P(p) = |\phi(p)|^2 = \frac{2n^2\pi}{a^3\hbar} \frac{1 - (-1)^n \cos pa/\hbar}{[(n\pi/a)^2 - (p/\hbar)^2]^2}$$

The function $P(p)$ does not go to infinity at $p = n\pi\hbar/a$, but it definitely peaks there. If we write $p/\hbar = n\pi/a + \varepsilon$, then the numerator becomes $1 - \cos a\varepsilon \approx a^2\varepsilon^2/2$ and the denominator becomes $(2n\pi\varepsilon/a)^2$, so that at the peak $P\left(\frac{n\pi\hbar}{a}\right) = a/4\pi\hbar$. The fact that the peaking occurs at

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

suggests agreement with the correspondence principle, since the kinetic energy of the particle is, as the r.h.s. of this equation shows, just the energy of a particle in the infinite box of width a . To confirm this, we need to show that the distribution is strongly peaked for large n . We do this by looking at the numerator, which vanishes when $a\varepsilon = \pi/2$, that is, when $p/\hbar = n\pi/a + \pi/2a = (n+1/2)\pi/a$. This implies that the width of the

distribution is $\Delta p = \pi\hbar/2a$. Since the x -space wave function is localized to $0 \leq x \leq a$ we only know that $\Delta x = a$. The result $\Delta p \Delta x \approx (\pi/2)\hbar$ is consistent with the uncertainty principle.

14. We calculate

$$\begin{aligned}\phi(p) &= \int_{-\infty}^{\infty} dx \left(\frac{\alpha}{\pi}\right)^{1/4} e^{-\alpha x^2/2} \frac{1}{\sqrt{2\pi\hbar}} e^{-ipx/\hbar} \\ &= \left(\frac{\alpha}{\pi}\right)^{1/4} \left(\frac{1}{2\pi\hbar}\right)^{1/2} \int_{-\infty}^{\infty} dx e^{-\alpha(x-ip/\hbar)^2} e^{-p^2/2\alpha\hbar^2} \\ &= \left(\frac{1}{\pi\alpha\hbar^2}\right)^{1/4} e^{-p^2/2\alpha\hbar^2}\end{aligned}$$

From this we find that the probability the momentum is in the range $(p, p + dp)$ is

$$|\phi(p)|^2 dp = \left(\frac{1}{\pi\alpha\hbar^2}\right)^{1/2} e^{-p^2/\alpha\hbar^2} dp$$

To get the expectation value of the energy we need to calculate

$$\begin{aligned}\left\langle \frac{p^2}{2m} \right\rangle &= \frac{1}{2m} \left(\frac{1}{\pi\alpha\hbar^2}\right)^{1/2} \int_{-\infty}^{\infty} dp p^2 e^{-p^2/\alpha\hbar^2} \\ &= \frac{1}{2m} \left(\frac{1}{\pi\alpha\hbar^2}\right)^{1/2} \frac{\sqrt{\pi}}{2} (\alpha\hbar^2)^{3/2} = \frac{\alpha\hbar^2}{2m}\end{aligned}$$

An estimate on the basis of the uncertainty principle would use the fact that the “width” of the packet is $1/\sqrt{\alpha}$. From this we estimate $\Delta p \approx \hbar/\Delta x = \hbar\sqrt{\alpha}$, so that

$$E \approx \frac{(\Delta p)^2}{2m} = \frac{\alpha\hbar^2}{2m}$$

The *exact* agreement is fortuitous, since both the definition of the width and the numerical statement of the uncertainty relation are somewhat elastic.

15. We have

$$\begin{aligned}
 j(x) &= \frac{\hbar}{2im} \left(\psi^*(x) \frac{d\psi(x)}{dx} - \frac{d\psi^*(x)}{dx} \psi(x) \right) \\
 &= \frac{\hbar}{2im} \left[(A^* e^{-ikx} + B^* e^{ikx})(ikAe^{ikx} - ikBe^{-ikx}) - c.c. \right] \\
 &= \frac{\hbar}{2im} [ik|A|^2 - ik|B|^2 + ikAB^*e^{2ikx} - ikA^*Be^{-2ikx} \\
 &\quad - (-ik)|A|^2 - (-ik)|B|^2 - (-ik)A^*Be^{-2ikx} - ikAB^*e^{2ikx}] \\
 &= \frac{\hbar k}{m} [|A|^2 - |B|^2]
 \end{aligned}$$

This is a sum of a flux to the right associated with $A e^{ikx}$ and a flux to the left associated with $B e^{-ikx}$.

16. Here

$$\begin{aligned}
 j(x) &= \frac{\hbar}{2im} \left[u(x)e^{-ikx} (iku(x)e^{ikx} + \frac{du(x)}{dx} e^{ikx}) - c.c. \right] \\
 &= \frac{\hbar}{2im} \left[(iku^2(x) + u(x) \frac{du(x)}{dx}) - c.c. \right] = \frac{\hbar k}{m} u^2(x)
 \end{aligned}$$

(c) Under the reflection $x \rightarrow -x$ both x and $p = -i\hbar \frac{\partial}{\partial x}$ change sign, and since the function consists of an odd power of x and/or p , it is an odd function of x . Now the eigenfunctions for a box symmetric about the x axis have a definite parity. So that $u_n(-x) = \pm u_n(x)$. This implies that the integrand is *antisymmetric* under $x \rightarrow -x$. Since the integral is over an interval symmetric under this exchange, it is zero.

(d) We need to prove that

$$\int_{-\infty}^{\infty} dx (P\psi(x))^* \psi(x) = \int_{-\infty}^{\infty} dx \psi(x)^* P\psi(x)$$

The left hand side is equal to

$$\int_{-\infty}^{\infty} dx \psi^*(-x)\psi(x) = \int_{-\infty}^{\infty} dy \psi^*(y)\psi(-y)$$

with a change of variables $x \rightarrow -y$, and this is equal to the right hand side.

The eigenfunctions of P with eigenvalue $+1$ are functions for which $u(x) = u(-x)$, while those with eigenvalue -1 satisfy $v(x) = -v(-x)$. Now the scalar product is

$$\int_{-\infty}^{\infty} dx u^*(x)v(x) = \int_{-\infty}^{\infty} dy u^*(-x)v(-x) = -\int_{-\infty}^{\infty} dx u^*(x)v(x)$$

so that

$$\int_{-\infty}^{\infty} dx u^*(x)v(x) = 0$$

(e) A simple sketch of $\psi(x)$ shows that it is a function symmetric about $x = a/2$.

This means that the integral $\int_0^a dx \psi(x)u_n(x)$ will vanish for the $u_n(x)$ which are *odd* under the reflection about this axis. This means that the integral vanishes for $n = 2, 4, 6, \dots$

CHAPTER 4.

1. The solution to the left side of the potential region is $\psi(x) = Ae^{ikx} + Be^{-ikx}$. As shown in Problem 3-15, this corresponds to a flux

$$j(x) = \frac{\hbar k}{m} (|A|^2 - |B|^2)$$

The solution on the right side of the potential is $\psi(x) = Ce^{ikx} + De^{-ikx}$, and as above, the flux is

$$j(x) = \frac{\hbar k}{m} (|C|^2 - |D|^2)$$

Both fluxes are independent of x . Flux conservation implies that the two are equal, and this leads to the relationship

$$|A|^2 + |D|^2 = |B|^2 + |C|^2$$

If we now insert

$$C = S_{11}A + S_{12}D$$

$$B = S_{21}A + S_{22}D$$

into the above relationship we get

$$|A|^2 + |D|^2 = (S_{21}A + S_{22}D)(S_{21}^*A^* + S_{22}^*D^*) + (S_{11}A + S_{12}D)(S_{11}^*A^* + S_{12}^*D^*)$$

Identifying the coefficients of $|A|^2$ and $|D|^2$, and setting the coefficient of AD^* equal to zero yields

$$|S_{21}|^2 + |S_{11}|^2 = 1$$

$$|S_{22}|^2 + |S_{12}|^2 = 1$$

$$S_{12}S_{22}^* + S_{11}S_{12}^* = 0$$

Consider now the matrix

$$S^{tr} = \begin{pmatrix} S_{11} & S_{21} \\ S_{12} & S_{22} \end{pmatrix}$$

The unitarity of this matrix implies that

$$\begin{pmatrix} S_{11} & S_{21} \\ S_{12} & S_{22} \end{pmatrix} \begin{pmatrix} S_{11}^* & S_{12}^* \\ S_{21}^* & S_{22}^* \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$

that is,

$$\begin{aligned} |S_{11}|^2 + |S_{21}|^2 &= |S_{12}|^2 + |S_{22}|^2 = 1 \\ S_{11}S_{12}^* + S_{21}S_{22}^* &= 0 \end{aligned}$$

These are just the conditions obtained above. They imply that the matrix S^{tr} is unitary, and therefore the matrix S is unitary.

2. We have solve the problem of finding R and T for this potential well in the text. We take $V_0 < 0$. We dealt with wave function of the form

$$\begin{aligned} e^{ikx} + Re^{-ikx} & \quad x < -a \\ Te^{ikx} & \quad x > a \end{aligned}$$

In the notation of Problem 4-1, we have found that if $A = 1$ and $D = 0$, then $C = S_{11} = T$ and $B = S_{21} = R$. To find the other elements of the S matrix we need to consider the same problem with $A = 0$ and $D = 1$. This can be solved explicitly by matching wave functions at the boundaries of the potential hole, but it is possible to take the solution that we have and reflect the “experiment” by the interchange $x \rightarrow -x$. We then find that $S_{12} = R$ and $S_{22} = T$. We can easily check that

$$|S_{11}|^2 + |S_{21}|^2 = |S_{12}|^2 + |S_{22}|^2 = |R|^2 + |T|^2 = 1$$

Also

$$S_{11}S_{12}^* + S_{21}S_{22}^* = TR^* + RT^* = 2\text{Re}(TR^*)$$

If we now look at the solutions for T and R in the text we see that the product of T and R^* is of the form $(-i) \times (\text{real number})$, so that its real part is zero. This confirms that the S matrix here is unitary.

3. Consider the wave functions on the left and on the right to have the forms

$$\begin{aligned} \psi_L(x) &= Ae^{ikx} + Be^{-ikx} \\ \psi_R(x) &= Ce^{ikx} + De^{-ikx} \end{aligned}$$

Now, let us make the change $k \rightarrow -k$ and complex conjugate everything. Now the two wave functions read

$$\begin{aligned}\psi_L(x)' &= A^* e^{ikx} + B^* e^{-ikx} \\ \psi_R(x)' &= C^* e^{ikx} + D^* e^{-ikx}\end{aligned}$$

Now complex conjugation and the transformation $k \rightarrow -k$ changes the original relations to

$$\begin{aligned}C^* &= S_{11}^*(-k)A^* + S_{12}^*(-k)D^* \\ B^* &= S_{21}^*(-k)A^* + S_{22}^*(-k)D^*\end{aligned}$$

On the other hand, we are now relating outgoing amplitudes C^*, B^* to ingoing amplitude A^*, D^* , so that the relations of problem 1 read

$$\begin{aligned}C^* &= S_{11}(k)A^* + S_{12}(k)D^* \\ B^* &= S_{21}(k)A^* + S_{22}(k)D^*\end{aligned}$$

This shows that $S_{11}(k) = S_{11}^*(-k)$; $S_{22}(k) = S_{22}^*(-k)$; $S_{12}(k) = S_{21}^*(-k)$. These result may be written in the *matrix* form $\mathbf{S}(k) = \mathbf{S}^+(-k)$.

4. (a) With the given flux, the wave coming in from $x = -\infty$, has the form e^{ikx} , with unit amplitude. We now write the solutions in the various regions

$$\begin{aligned}x < b & \quad e^{ikx} + R e^{-ikx} & \quad k^2 = 2mE / \hbar^2 \\ -b < x < -a & \quad A e^{\kappa x} + B e^{-\kappa x} & \quad \kappa^2 = 2m(V_0 - E) / \hbar^2 \\ -a < x < c & \quad C e^{ikx} + D e^{-ikx} \\ c < x < d & \quad M e^{iqx} + N e^{-iqx} & \quad q^2 = 2m(E + V_1) / \hbar^2 \\ d < x & \quad T e^{ikx}\end{aligned}$$

(b) We now have

$$\begin{aligned}x < 0 & \quad u(x) = 0 \\ 0 < x < a & \quad A \sin kx & \quad k^2 = 2mE / \hbar^2 \\ a < x < b & \quad B e^{\kappa x} + C e^{-\kappa x} & \quad \kappa^2 = 2m(V_0 - E) / \hbar^2 \\ b < x & \quad e^{-ikx} + R e^{ikx}\end{aligned}$$

The fact that there is total reflection at $x = 0$ implies that $|R|^2 = 1$

5. The denominator in (4-) has the form

$$D = 2kq \cos 2qa - i(q^2 + k^2) \sin 2qa$$

With $k = i\kappa$ this becomes

$$D = i(2\kappa q \cos 2qa - (q^2 - \kappa^2) \sin 2qa)$$

The denominator vanishes when

$$\tan 2qa = \frac{2 \tan qa}{1 - \tan^2 qa} = \frac{2q\kappa}{q^2 - \kappa^2}$$

This implies that

$$\tan qa = -\frac{q^2 - \kappa^2}{2\kappa q} \pm \sqrt{1 + \left(\frac{q^2 - \kappa^2}{2\kappa q}\right)^2} = -\frac{q^2 - \kappa^2}{2\kappa q} \pm \frac{q^2 + \kappa^2}{2\kappa q}$$

This condition is identical with (4-).

The argument why this is so, is the following: When $k = i\kappa$ the wave function on the left has the form $e^{-\kappa x} + R(i\kappa)e^{\kappa x}$. The function $e^{-\kappa x}$ blows up as $x \rightarrow -\infty$ and the wave function only make sense if this term is overpowered by the other term, that is when $R(i\kappa) = \infty$. We leave it to the student to check that the numerators are the same at $k = i\kappa$.

6. The solution is
$$u(x) = \begin{cases} Ae^{ikx} + Be^{-ikx} & x < b \\ Ce^{ikx} + De^{-ikx} & x > b \end{cases}$$

The continuity condition at $x = b$ leads to

$$Ae^{ikb} + Be^{-ikb} = Ce^{ikb} + De^{-ikb}$$

And the derivative condition is

$$(ikAe^{ikb} - ikBe^{-ikb}) - (ikCe^{ikb} - ikDe^{-ikb}) = (\lambda/a)(Ae^{ikb} + Be^{-ikb})$$

With the notation

$$Ae^{ikb} = \alpha ; Be^{-ikb} = \beta ; Ce^{ikb} = \gamma ; De^{-ikb} = \delta$$

These equations read

$$\alpha + \beta = \gamma + \delta$$

$$ik(\alpha - \beta + \gamma - \delta) = (\lambda/a)(\alpha + \beta)$$

We can use these equations to write (γ, β) in terms of (α, δ) as follows

$$\gamma = \frac{2ika}{2ika - \lambda} \alpha + \frac{\lambda}{2ika - \lambda} \delta$$

$$\beta = \frac{\lambda}{2ika - \lambda} \alpha + \frac{2ika}{2ika - \lambda} \delta$$

We can now rewrite these in terms of A, B, C, D and we get for the S matrix

$$S = \begin{pmatrix} \frac{2ika}{2ika - \lambda} & \frac{\lambda}{2ika - \lambda} e^{-2ikb} \\ \frac{\lambda}{2ika - \lambda} e^{2ikb} & \frac{2ika}{2ika - \lambda} \end{pmatrix}$$

Unitarity is easily established:

$$|S_{11}|^2 + |S_{12}|^2 = \frac{4k^2 a^2}{4k^2 a^2 + \lambda^2} + \frac{\lambda^2}{4k^2 a^2 + \lambda^2} = 1$$

$$S_{11} S_{12}^* + S_{12} S_{22}^* = \left(\frac{2ika}{2ika - \lambda} \right) \left(\frac{\lambda}{-2ika - \lambda} e^{-2ikb} \right) + \left(\frac{\lambda}{2ika - \lambda} e^{-2ikb} \right) \left(\frac{-2ika}{-2ika - \lambda} \right) = 0$$

The matrix elements become infinite when $2ika = \lambda$. In terms of $\kappa = -ik$, this condition becomes $\kappa = -\lambda/2a = |\lambda|/2a$.

7. The exponent in $T = e^{-S}$ is

$$S = \frac{2}{\hbar} \int_A^B dx \sqrt{2m(V(x) - E)}$$

$$= \frac{2}{\hbar} \int_A^B dx \sqrt{2m \left(\frac{m\omega^2}{2} \left(x^2 - \frac{x^3}{a} \right) \right) - \frac{\hbar\omega}{2}}$$

where A and B are turning points, that is, the points at which the quantity under the square root sign vanishes.

We first simplify the expression by changing to dimensionless variables:

$$x = \sqrt{\hbar/m\omega} y; \quad \eta = a/\sqrt{\hbar/m\omega} \ll 1$$

The integral becomes

$$2 \int_{y_1}^{y_2} dy \sqrt{y^2 - \eta y^3 - 1} \quad \text{with } \eta \ll 1$$

where now y_1 and y_2 are the turning points. A sketch of the potential shows that y_2 is very large. In that region, the -1 under the square root can be neglected, and to a good approximation $y_2 = 1/\eta$. The other turning point occurs for y not particularly large, so that we can neglect the middle term under the square root, and the value of y_1 is 1. Thus we need to estimate

$$\int_1^{1/\eta} dy \sqrt{y^2 - \eta y^3 - 1}$$

The integrand has a maximum at $2y - 3\eta y^2 = 0$, that is at $y = 2\eta/3$. We estimate the contribution from that point on by neglecting the -1 term in the integrand. We thus get

$$\int_{2/3\eta}^{1/\eta} dy y \sqrt{1 - \eta y} = \frac{2}{\eta^2} \left[\frac{(1 - \eta y)^{5/2}}{5} - \frac{(1 - \eta y)^{3/2}}{3} \right]_{2/3\eta}^{1/\eta} = \frac{8\sqrt{3}}{135} \frac{1}{\eta^2}$$

To estimate the integral in the region $1 < y < 2/3\eta$ is more difficult. In any case, we get a lower limit on S by just keeping the above, so that

$$S > 0.21/\eta^2$$

The factor e^S must be multiplied by a characteristic time for the particle to move back and forth inside the potential with energy $\hbar\omega/2$ which is necessarily of order $1/\omega$. Thus the estimated time is *longer* than $\frac{\text{const.}}{\omega} e^{0.2/\eta^2}$.

8. The barrier factor is e^S where

$$S = \frac{2}{\hbar} \int_{R_0}^b dx \sqrt{\frac{\hbar^2 l(l+1)}{x^2} - 2mE}$$

where b is given by the value of x at which the integrand vanishes, that is, with $2mE/\hbar^2 = k^2$, $b = \sqrt{l(l+1)}/k$. We have, after some algebra

$$\begin{aligned} S &= 2\sqrt{l(l+1)} \int_{R_0/b}^1 \frac{du}{u} \sqrt{1-u^2} \\ &= 2\sqrt{l(l+1)} \left[\ln \frac{1 + \sqrt{1 - (R_0/b)^2}}{R_0/b} - \sqrt{1 - (R_0/b)^2} \right] \end{aligned}$$

We now introduce the variable $f = (R_0/b) \approx kR_0/l$ for large l . Then

$$e^S e^S = \left[\frac{1 + \sqrt{1-f^2}}{f} \right]^{2l} e^{-2l\sqrt{1-f^2}} \approx \left(\frac{e}{2} \right)^{-2l} f^{-2l}$$

for $f \ll 1$. This is to be multiplied by the time of traversal inside the box. The important factor is f^{2l} . It tells us that the lifetime is proportional to $(kR_0)^{-2l}$ so that it grows as a power of l for small k . Equivalently we can say that the probability of decay falls as $(kR_0)^{2l}$.

9. The argument fails because the electron is not localized inside the potential. In fact, for weak binding, the electron wave function extends over a region $R = 1/\alpha = \hbar\sqrt{2mE_B}$, which, for weak binding is much larger than a .

10. For a bound state, the solution for $x > a$ must be of the

$$\text{form } u(x) = Ae^{-\alpha x}, \quad \text{where } \alpha = \sqrt{2mE_B} / \hbar. \text{ Matching } \frac{1}{u} \frac{du}{dx} \text{ at } x = a$$

yields $-\alpha = f(E_B)$. If $f(E)$ is a constant, then we immediately know α . Even if $f(E)$ varies only slightly over the energy range that overlaps small positive E , we can determine the binding energy in terms of the reflection coefficient. For positive energies the wave function $u(x)$ for $x > a$ has the form $e^{-ikx} + R(k)e^{ikx}$, and matching yields

$$f(E) \approx -\alpha = -ik \frac{e^{-ika} - Re^{ika}}{e^{-ika} + Re^{ika}} = -ik \frac{1 - Re^{2ika}}{1 + Re^{2ika}}$$

so that

$$R = e^{-2ika} \frac{k + i\alpha}{k - i\alpha}$$

We see that $|R|^2 = 1$.

11. Since the well is symmetric about $x = 0$, we need only match wave functions at $x = b$ and a . We look at $E < 0$, so that we introduce $\alpha^2 = 2m|E|/\hbar^2$ and

$$q^2 = 2m(V_0 - |E|)/\hbar^2. \text{ We now write down}$$

Even solutions:

$$\begin{aligned} u(x) &= \cosh\alpha x & 0 < x < b \\ &= A \sin qx + B \cos qx & b < x < a \\ &= C e^{-\alpha x} & a < x \end{aligned}$$

Matching $\frac{1}{u(x)} \frac{du(x)}{dx}$ at $x = b$ and at $x = a$ leads to the equations

$$\alpha \tanh \alpha b = q \frac{A \cos qb - B \sin qb}{A \sin qb + B \cos qb}$$

$$-\alpha = q \frac{A \cos qa - B \sin qa}{A \sin qa + B \cos qa}$$

From the first equation we get

$$\frac{B}{A} = \frac{q \cos qb - \alpha \tanh \alpha b \sin qb}{q \sin qb + \alpha \tanh \alpha b \cos qb}$$

and from the second

$$\frac{B}{A} = \frac{q \cos qa + \alpha \sin qa}{q \sin qa - \alpha \cos qa}$$

Equating these, cross-multiplying, we get after a little algebra

$$q^2 \sin q(a-b) - \alpha \cos q(a-b) = \alpha \tanh \alpha b [\alpha \sin q(a-b) + q \cos q(a-b)]$$

from which it immediately follows that

$$\frac{\sin q(a-b)}{\cos q(a-b)} = \frac{\alpha q (\tanh \alpha b + 1)}{q^2 - \alpha^2 \tanh \alpha b}$$

Odd Solution

Here the only difference is that the form for $u(x)$ for $0 < x < b$ is $\sinh \alpha x$. The result of this is that we get the same expression as above, with $\tanh \alpha b$ replaced by $\coth \alpha b$.

11. (a) The condition that there are at most two bound states is equivalent to stating that there is at most one *odd* bound state. The relevant figure is Fig. 4-8, and we ask for the condition that there be no intersection point with the tangent curve that starts up at $3\pi/2$. This means that

$$\frac{\sqrt{\lambda - y^2}}{y} = 0$$

for $y \leq 3\pi/2$. This translates into $\lambda = y^2$ with $y < 3\pi/2$, i.e. $\lambda < 9\pi^2/4$.

(b) The condition that there be at most three bound states implies that there be at most two *even* bound states, and the relevant figure is 4-7. Here the condition is that $y < 2\pi$ so that $\lambda < 4\pi^2$.

(c) We have $y = \pi$ so that the second *even* bound state have zero binding energy. This means that $\lambda = \pi^2$. What does this tell us about the first bound state? All we know is that y is a solution of Eq. (4-54) with $\lambda = \pi^2$. Eq.(4-54) can be rewritten as follows:

$$\tan^2 y = \frac{1 - \cos^2 y}{\cos^2 y} = \frac{\lambda - y^2}{y^2} = \frac{1 - (y^2 / \lambda)}{(y^2 / \lambda)}$$

so that the *even* condition is $\cos y = y / \sqrt{\lambda}$, and in the same way, the *odd* condition is $\sin y = y / \sqrt{\lambda}$. Setting $\sqrt{\lambda} = \pi$ still leaves us with a transcendental equation. All we can say is that the binding energy of the even state will be larger than that of the odd one.

13.(a) As $b \rightarrow 0$, $\tan q(a-b) \rightarrow \tan qa$ and the r.h.s. reduces to α/q . Thus we get, for the even solution

$$\tan qa = \alpha/q$$

and, for the odd solution,

$$\tan qa = -q/\alpha.$$

These are just the single well conditions.

(b) This part is more complicated. We introduce notation $c = (a-b)$, which will be held fixed. We will also use the notation $z = \alpha b$. We will also use the subscript "1" for the even solutions, and "2" for the odd solutions. For b large,

$$\begin{aligned} \tanh z &= \frac{e^z - e^{-z}}{e^z + e^{-z}} = \frac{1 - e^{-2z}}{1 + e^{-2z}} \approx 1 - 2e^{-2z} \\ \coth z &\approx 1 + 2e^{-2z} \end{aligned}$$

The eigenvalue condition for the even solution now reads

$$\tan q_1 c = \frac{q_1 \alpha_1 (1 + 1 - 2e^{-2z_1})}{q_1^2 - \alpha_1^2 (1 - 2e^{-2z_1})} \approx \frac{2q_1 \alpha_1}{q_1^2 - \alpha_1^2} \left(1 - \frac{q_1^2 + \alpha_1^2}{q_1^2 - \alpha_1^2} e^{-2z_1}\right)$$

The condition for the odd solution is obtained by just changing the sign of the e^{-2z} term, so that

$$\tan q_2 c = \frac{q_2 \alpha_2 (1 + 1 + 2e^{-2z_2})}{q_2^2 - \alpha_2^2 (1 + 2e^{-2z_2})} \approx \frac{2q_2 \alpha_2}{q_2^2 - \alpha_2^2} \left(1 + \frac{q_2^2 + \alpha_2^2}{q_2^2 - \alpha_2^2} e^{-2z_2}\right)$$

In both cases $q^2 + \alpha^2 = 2mV_0/\hbar^2$ is fixed. The two eigenvalue conditions only differ in the e^{-2z} terms, and the difference in the eigenvalues is therefore proportional to e^{-2z} , where z here is some mean value between $\alpha_1 b$ and $\alpha_2 b$.

This can be worked out in more detail, but this becomes an exercise in Taylor expansions with no new physical insights.

14. We write

$$\begin{aligned} \left\langle x \frac{dV(x)}{dx} \right\rangle &= \int_{-\infty}^{\infty} dx \psi(x) x \frac{dV(x)}{dx} \psi(x) \\ &= \int_{-\infty}^{\infty} dx \left[\frac{d}{dx} (\psi^2 x V) - 2\psi \frac{d\psi}{dx} x V - \psi^2 V \right] \end{aligned}$$

The first term vanishes because ψ goes to zero rapidly. We next rewrite

$$\begin{aligned} -2 \int_{-\infty}^{\infty} dx \frac{d\psi}{dx} x V \psi &= -2 \int_{-\infty}^{\infty} dx \frac{d\psi}{dx} x \left(E + \frac{\hbar^2}{2m} \frac{d^2}{dx^2} \right) \psi \\ &= -E \int_{-\infty}^{\infty} dx x \frac{d\psi^2}{dx} - \frac{\hbar^2}{2m} \int_{-\infty}^{\infty} dx x \frac{d}{dx} \left(\frac{d\psi}{dx} \right)^2 \end{aligned}$$

Now

$$\int_{-\infty}^{\infty} dx x \frac{d\psi^2}{dx} = \int_{-\infty}^{\infty} dx \frac{d}{dx} (x \psi^2) - \int_{-\infty}^{\infty} dx \psi^2$$

The first term vanishes, and the second term is unity. We do the same with the second term, in which only the second integral

$$\int_{-\infty}^{\infty} dx \left(\frac{d\psi}{dx} \right)^2$$

remains. Putting all this together we get

$$\left\langle x \frac{dV}{dx} \right\rangle + \langle V \rangle = \frac{\hbar^2}{2m} \int_{-\infty}^{\infty} dx \left(\frac{d\psi}{dx} \right)^2 + E \int_{-\infty}^{\infty} dx \psi^2 = \left\langle \frac{p^2}{2m} \right\rangle + E$$

so that

$$\frac{1}{2} \left\langle x \frac{dV}{dx} \right\rangle = \left\langle \frac{p^2}{2m} \right\rangle$$

CHAPTER 5.

1. We are given

$$\int_{-\infty}^{\infty} dx (A\Psi(x))^* \Psi(x) = \int_{-\infty}^{\infty} dx \Psi(x)^* A\Psi(x)$$

Now let $\Psi(x) = \phi(x) + \lambda\psi(x)$, where λ is an arbitrary complex number. Substitution into the above equation yields, on the l.h.s.

$$\begin{aligned} & \int_{-\infty}^{\infty} dx (A\phi(x) + \lambda A\psi(x))^* (\phi(x) + \lambda\psi(x)) \\ &= \int_{-\infty}^{\infty} dx \left[(A\phi)^* \phi + \lambda (A\phi)^* \psi + \lambda^* (A\psi)^* \phi + |\lambda|^2 (A\psi)^* \psi \right] \end{aligned}$$

On the r.h.s. we get

$$\begin{aligned} & \int_{-\infty}^{\infty} dx (\phi(x) + \lambda\psi(x))^* (A\phi(x) + \lambda A\psi(x)) \\ &= \int_{-\infty}^{\infty} dx \left[\phi^* A\phi + \lambda^* \psi^* A\phi + \lambda\phi^* A\psi + |\lambda|^2 \psi^* A\psi \right] \end{aligned}$$

Because of the hermiticity of A , the first and fourth terms on each side are equal. For the rest, since λ is an arbitrary complex number, the coefficients of λ and λ^* are independent, and we may therefore identify these on the two sides of the equation. If we consider λ , for example, we get

$$\int_{-\infty}^{\infty} dx (A\phi(x))^* \psi(x) = \int_{-\infty}^{\infty} dx \phi(x)^* A\psi(x)$$

the desired result.

2. We have $A^+ = A$ and $B^+ = B$, therefore $(A + B)^+ = (A + B)$. Let us call $(A + B) = X$. We have shown that X is hermitian. Consider now

$$(X^+)^n = X^+ X^+ X^+ \dots X^+ = X X X \dots X = (X)^n$$

which was to be proved.

3. We have

$$\langle A^2 \rangle = \int_{-\infty}^{\infty} dx \psi^*(x) A^2 \psi(x)$$

Now define $A\psi(x) = \phi(x)$. Then the above relation can be rewritten as

$$\begin{aligned}\langle A^2 \rangle &= \int_{-\infty}^{\infty} dx \psi(x) A \phi(x) = \int_{-\infty}^{\infty} dx (A \psi(x))^* \phi(x) \\ &= \int_{-\infty}^{\infty} dx (A \psi(x))^* A \psi(x) \geq 0\end{aligned}$$

4. Let $U = e^{iH} = \sum_{n=0}^{\infty} \frac{i^n H^n}{n!}$. Then $U^\dagger = \sum_{n=0}^{\infty} \frac{(-i)^n (H^n)^\dagger}{n!} = \sum_{n=0}^{\infty} \frac{(-i)^n (H^n)}{n!} = e^{-iH}$, and thus

the hermitian conjugate of e^{iH} is e^{-iH} provided $H = H^\dagger$.

5. We need to show that

$$e^{iH} e^{-iH} = \sum_{n=0}^{\infty} \frac{i^n}{n!} H^n \sum_{m=0}^{\infty} \frac{(-i)^m}{m!} H^m = 1$$

Let us pick a particular coefficient in the series, say $k = m + n$ and calculate its coefficient. We get, with $m = k - n$, the coefficient of H^k is

$$\begin{aligned}\sum_{n=0}^k \frac{i^n}{n!} \frac{(-i)^{k-n}}{(k-n)!} &= \frac{1}{k!} \sum_{n=0}^k \frac{k!}{n!(k-n)!} i^n (-i)^{k-n} \\ &= \frac{1}{k!} (i - i)^k = 0\end{aligned}$$

Thus in the product only the $m = n = 0$ term remains, and this is equal to unity.

6. We write $I(\lambda, \lambda^*) = \int_{-\infty}^{\infty} dx (\phi(x) + \lambda \psi(x))^* (\phi(x) + \lambda \psi(x)) \geq 0$. The left hand side, in abbreviated notation can be written as

$$I(\lambda, \lambda^*) = \int |\phi|^2 + \lambda^* \int \psi^* \phi + \lambda \int \phi^* \psi + \lambda \lambda^* \int |\psi|^2$$

Since λ and λ^* are independent, the minimum value of this occurs when

$$\begin{aligned}\frac{\partial I}{\partial \lambda^*} &= \int \psi^* \phi + \lambda \int |\psi|^2 = 0 \\ \frac{\partial I}{\partial \lambda} &= \int \phi^* \psi + \lambda^* \int |\psi|^2 = 0\end{aligned}$$

When these values of λ and λ^* are inserted in the expression for $I(\lambda, \lambda^*)$ we get

$$I(\lambda_{min}, \lambda_{min}^*) = \int |\phi|^2 - \frac{\int \phi^* \psi \int \psi^* \phi}{\int |\psi|^2} \geq 0$$

from which we get the Schwartz inequality.

7. We have $UU^+ = 1$ and $VV^+ = 1$. Now $(UV)^+ = V^+U^+$ so that

$$(UV)(UV)^+ = UVV^+U^+ = UU^+ = 1$$

8. Let $U\psi(x) = \lambda\psi(x)$, so that λ is an eigenvalue of U . Since U is unitary, $U^+U = 1$. Now

$$\begin{aligned} \int_{-\infty}^{\infty} dx (U\psi(x))^* U\psi(x) &= \int_{-\infty}^{\infty} dx \psi^*(x) U^+ U\psi(x) = \\ &= \int_{-\infty}^{\infty} dx \psi^*(x) \psi(x) = 1 \end{aligned}$$

On the other hand, using the eigenvalue equation, the integral may be written in the form

$$\int_{-\infty}^{\infty} dx (U\psi(x))^* U\psi(x) = \lambda^* \lambda \int_{-\infty}^{\infty} dx \psi^*(x) \psi(x) = |\lambda|^2$$

It follows that $|\lambda|^2 = 1$, or equivalently $\lambda = e^{ia}$, with a real.

9. We write

$$\begin{aligned} \int_{-\infty}^{\infty} dx \phi(x)^* \phi(x) &= \int_{-\infty}^{\infty} dx (U\psi(x))^* U\psi(x) = \int_{-\infty}^{\infty} dx \psi^*(x) U^+ U\psi(x) = \\ &= \int_{-\infty}^{\infty} dx \psi^*(x) \psi(x) = 1 \end{aligned}$$

10. We write, in abbreviated notation

$$\int v_a^* v_b = \int (Uu_a)^* Uu_b = \int u_a^* U^+ Uu_b = \int u_a^* u_b = \delta_{ab}$$

11. (a) We are given $A^+ = A$ and $B^+ = B$. We now calculate

$$\begin{aligned} (i[A, B])^+ &= (iAB - iBA)^+ = -i(AB)^+ - (-i)(BA)^+ = -i(B^+A^+) + i(A^+B^+) \\ &= -iBA + iAB = i[A, B] \end{aligned}$$

$$\begin{aligned} (b) [AB, C] &= ABC - CAB = ABC - ACB + ACB - CAB = A(BC - CB) - (AC - CA)B \\ &= A[B, C] - [A, C]B \end{aligned}$$

(c) The Jacobi identity written out in detail is

$$[A, [B, C]] + [B, [C, A]] + [C, [A, B]] =$$

$$\begin{aligned}
& A(BC - CB) - (BC - CB)A + B(CA - AC) - (CA - AC)B + C(AB - BA) - (AB - BA)C \\
& = ABC - ACB - BCA + CBA + BCA - BAC - CAB + ACB + CAB - CBA - ABC + BAC
\end{aligned}$$

It is easy to see that the sum is zero.

12. We have

$$e^A B e^{-A} = (1 + A + A^2/2! + A^3/3! + A^4/4! + \dots)B (1 - A + A^2/2! - A^3/3! + A^4/4! - \dots)$$

Let us now take the term independent of A : it is B .

The terms of first order in A are $AB - BA = [A, B]$.

The terms of second order in A are

$$\begin{aligned}
A^2 B / 2! - ABA + BA^2 / 2! &= (1/2!)(A^2 B - 2ABA + BA^2) \\
&= (1/2!)(A(AB - BA) - (AB - BA)A) = (1/2!)\{A[A, B] - [A, B]A\} \\
&= (1/2!)[A, [A, B]]
\end{aligned}$$

The terms of third order in A are $A^3 B / 3! - A^2 BA / 2! + ABA^2 / 2! - BA^3$. One can again rearrange these and show that this term is $(1/3!)[A, [A, [A, B]]]$.

There is actually a neater way to do this. Consider

$$F(\lambda) = e^{\lambda A} B e^{-\lambda A}$$

Then

$$\frac{dF(\lambda)}{d\lambda} = e^{\lambda A} A B e^{-\lambda A} - e^{\lambda A} B A e^{-\lambda A} = e^{\lambda A} [A, B] e^{-\lambda A}$$

Differentiating again we get

$$\frac{d^2 F(\lambda)}{d\lambda^2} = e^{\lambda A} [A, [A, B]] e^{-\lambda A}$$

and so on. We now use the Taylor expansion to calculate $F(1) = e^A B e^{-A}$.

$$\begin{aligned}
F(1) &= F(0) + F'(0) + \frac{1}{2!} F''(0) + \frac{1}{3!} F'''(0) + \dots \\
&= B + [A, B] + \frac{1}{2!} [A, [A, B]] + \frac{1}{3!} [A, [A, [A, B]]] + \dots
\end{aligned}$$

13. Consider the eigenvalue equation $Hu = \lambda u$. Applying H to this equation we get

$H^2 u = \lambda^2 u$; $H^3 u = \lambda^3 u$ and $H^4 u = \lambda^4 u$. We are given that $H^4 = 1$, which means that H^4 applied to any function yields 1. In particular this means that $\lambda^4 = 1$. The solutions of this are $\lambda = 1, -1, i, \text{ and } -i$. However, H is hermitian, so that the eigenvalues are real. Thus only $\lambda = \pm 1$ are possible eigenvalues. If H is not hermitian, then all four eigenvalues are acceptable.

14. We have the equations

$$\begin{aligned} B u_a^{(1)} &= b_{11} u_a^{(1)} + b_{12} u_a^{(2)} \\ B u_a^{(2)} &= b_{21} u_a^{(1)} + b_{22} u_a^{(2)} \end{aligned}$$

Let us now introduce functions $(v_a^{(1)}, v_a^{(2)})$ that satisfy the equations $B v_a^{(1)} = b_1 v_a^{(1)}$; $B v_a^{(2)} = b_2 v_a^{(2)}$. We write, with simplified notation,

$$\begin{aligned} v_1 &= \alpha u_1 + \beta u_2 \\ v_2 &= \gamma u_1 + \delta u_2 \end{aligned}$$

The b_1 - eigenvalue equation reads

$$b_1 v_1 = B (\alpha u_1 + \beta u_2) = \alpha (b_{11} u_1 + b_{12} u_2) + \beta (b_{21} u_1 + b_{22} u_2)$$

We write the l.h.s. as $b_1(\alpha u_1 + \beta u_2)$. We can now take the coefficients of u_1 and u_2 separately, and get the following equations

$$\begin{aligned} \alpha (b_1 - b_{11}) &= \beta b_{21} \\ \beta (b_1 - b_{22}) &= \alpha b_{12} \end{aligned}$$

The product of the two equations yields a quadratic equation for b_1 , whose solution is

$$b_1 = \frac{b_{11} + b_{22}}{2} \pm \sqrt{\frac{(b_{11} - b_{22})^2}{4} + b_{12} b_{21}}$$

We may choose the + sign for the b_1 eigenvalue. An examination of the equation involving v_2 leads to an identical equation, and we associate the - sign with the b_2 eigenvalue. Once we know the eigenvalues, we can find the ratios α/β and γ/δ . These suffice, since the normalization condition implies that

$$\alpha^2 + \beta^2 = 1 \quad \text{and} \quad \gamma^2 + \delta^2 = 1$$

15. The equations of motion for the expectation values are

$$\frac{d}{dt}\langle x \rangle = \frac{i}{\hbar} \langle [H, x] \rangle = \frac{i}{\hbar} \langle [\frac{p^2}{2m}, x] \rangle = \frac{i}{m\hbar} \langle p[p, x] \rangle = \langle \frac{p}{m} \rangle$$

$$\frac{d}{dt}\langle p \rangle = \frac{i}{\hbar} \langle [H, p] \rangle = -\frac{i}{\hbar} \langle [p, \frac{1}{2}m\omega_1^2 x^2 + \omega_2 x] \rangle = -m\omega_1^2 \langle x \rangle - \omega_2$$

16. We may combine the above equations to get

$$\frac{d^2}{dt^2}\langle x \rangle = -\omega_1^2 \langle x \rangle - \frac{\omega_2}{m}$$

The solution of this equation is obtained by introducing the variable

$$X = \langle x \rangle + \frac{\omega_2}{m\omega_1^2}$$

The equation for X reads $d^2X/dt^2 = -\omega_1^2 X$, whose solution is

$$X = A\cos\omega_1 t + B\sin\omega_1 t$$

This gives us

$$\langle x \rangle_t = -\frac{\omega_2}{m\omega_1^2} + A\cos\omega_1 t + B\sin\omega_1 t$$

At $t = 0$

$$\langle x \rangle_0 = -\frac{\omega_2}{m\omega_1^2} + A$$

$$\langle p \rangle_0 = m \frac{d}{dt} \langle x \rangle_{t=0} = mB\omega_1$$

We can therefore write A and B in terms of the initial values of $\langle x \rangle$ and $\langle p \rangle$,

$$\langle x \rangle_t = -\frac{\omega_2}{m\omega_1^2} + \left(\langle x \rangle_0 + \frac{\omega_2}{m\omega_1^2} \right) \cos\omega_1 t + \frac{\langle p \rangle_0}{m\omega_1} \sin\omega_1 t$$

17. We calculate as above, but we can equally well use Eq. (5-53) and (5-57), to get

$$\frac{d}{dt}\langle x \rangle = \frac{1}{m}\langle p \rangle$$

$$\frac{d}{dt}\langle p \rangle = -\left\langle \frac{\partial V(x,t)}{\partial x} \right\rangle = eE_0 \cos\omega t$$

Finally

$$\frac{d}{dt}\langle H \rangle = \left\langle \frac{\partial H}{\partial t} \right\rangle = eE_0\omega \sin \omega t \langle x \rangle$$

18. We can solve the second of the above equations to get

$$\langle p \rangle_t = \frac{eE_0}{\omega} \sin \omega t + \langle p \rangle_{t=0}$$

This may be inserted into the first equation, and the result is

$$\langle x \rangle_t = -\frac{eE_0}{m\omega^2} (\cos \omega t - 1) + \frac{\langle p \rangle_{t=0} t}{m} + \langle x \rangle_{t=0}$$

CHAPTER 6

19. (a) We have

$$A|a\rangle = a|a\rangle$$

It follows that

$$\langle a|A|a\rangle = a\langle a|a\rangle = a$$

if the eigenstate of A corresponding to the eigenvalue a is normalized to unity. The complex conjugate of this equation is

$$\langle a|A|a\rangle^* = \langle a|A^+|a\rangle = a^*$$

If $A^+ = A$, then it follows that $a = a^*$, so that a is real.

13. We have

$$\langle \psi |(AB)^+ | \psi \rangle = \langle (AB)\psi | \psi \rangle = \langle B\psi | A^+ | \psi \rangle = \langle \psi | B^+ A^+ | \psi \rangle$$

This is true for every ψ , so that $(AB)^+ = B^+ A^+$

2.

$$\begin{aligned} \text{Tr}AB &= \sum_n \langle n | AB | n \rangle = \sum_n \langle n | A \mathbf{1} B | n \rangle \\ &= \sum_n \sum_m \langle n | A | m \rangle \langle m | B | n \rangle = \sum_n \sum_m \langle m | B | n \rangle \langle n | A | m \rangle \\ &= \sum_m \langle m | B \mathbf{1} A | m \rangle = \sum_m \langle m | BA | m \rangle = \text{Tr}BA \end{aligned}$$

3. We start with the definition of $|n\rangle$ as

$$|n\rangle = \frac{1}{\sqrt{n!}} (A^+)^n |0\rangle$$

We now take Eq. (6-47) from the text to see that

$$A|n\rangle = \frac{1}{\sqrt{n!}} A(A^+)^n |0\rangle = \frac{n}{\sqrt{n!}} (A^+)^{n-1} |0\rangle = \frac{\sqrt{n}}{\sqrt{(n-1)!}} (A^+)^{n-1} |0\rangle = \sqrt{n} |n-1\rangle$$

4. Let $f(A^+) = \sum_{n=1}^N C_n (A^+)^n$. We then use Eq. (6-47) to obtain

$$\begin{aligned}
Af(A^+) |0\rangle &= A \sum_{n=1}^N C_n(A^+)^n |0\rangle = \sum_{n=1}^N n C_n(A^+)^{n-1} |0\rangle \\
&= \frac{d}{dA^+} \sum_{n=1}^N C_n(A^+)^n |0\rangle = \frac{df(A^+)}{dA^+} |0\rangle
\end{aligned}$$

5. We use the fact that Eq. (6-36) leads to

$$\begin{aligned}
x &= \sqrt{\frac{\hbar}{2m\omega}} (A + A^+) \\
p &= i\sqrt{\frac{m\omega\hbar}{2}} (A^+ - A)
\end{aligned}$$

We can now calculate

$$\begin{aligned}
\langle k | x | n \rangle &= \sqrt{\frac{\hbar}{2m\omega}} \langle k | A + A^+ | n \rangle = \sqrt{\frac{\hbar}{2m\omega}} (\sqrt{n} \langle k | n-1 \rangle + \sqrt{k} \langle k-1 | n \rangle) \\
&= \sqrt{\frac{\hbar}{2m\omega}} (\sqrt{n} \delta_{k,n-1} + \sqrt{n+1} \delta_{k,n+1})
\end{aligned}$$

which shows that $k = n \pm 1$.

6. In exactly the same way we show that

$$\langle k | p | n \rangle = i\sqrt{\frac{m\omega\hbar}{2}} \langle k | A^+ - A | n \rangle = i\sqrt{\frac{m\omega\hbar}{2}} (\sqrt{n+1} \delta_{k,n+1} - \sqrt{n} \delta_{k,n-1})$$

7. Let us now calculate

$$\langle k | px | n \rangle = \langle k | p \mathbf{1} x | n \rangle = \sum_q \langle k | p | q \rangle \langle q | x | n \rangle$$

We may now use the results of problems 5 and 6. We get for the above

$$\begin{aligned}
&\frac{i\hbar}{2} \sum_q (\sqrt{k} \delta_{k-1,q} - \sqrt{k+1} \delta_{k+1,q}) (\sqrt{n} \delta_{q,n-1} + \sqrt{n+1} \delta_{q,n+1}) \\
&= \frac{i\hbar}{2} (\sqrt{kn} \delta_{kn} - \sqrt{(k+1)n} \delta_{k+1,n-1} + \sqrt{k(n+1)} \delta_{k-1,n+1} - \sqrt{(k+1)(n+1)} \delta_{k+1,n+1}) \\
&= \frac{i\hbar}{2} (-\delta_{kn} - \sqrt{(k+1)(k+2)} \delta_{k+2,n} + \sqrt{n(n+2)} \delta_{k,n+2})
\end{aligned}$$

To calculate $\langle k | xp | n \rangle$ we may proceed in exactly the same way. It is also possible to abbreviate the calculation by noting that since x and p are hermitian operators, it follows that

$$\langle k | xp | n \rangle = \langle n | px | k \rangle^*$$

so that the desired quantity is obtained from what we obtained before by interchanging k and n and complex-conjugating. The latter only changes the overall sign, so that we get

$$\langle k | xp | n \rangle = -\frac{i\hbar}{2}(-\delta_{kn} - \sqrt{(n+1)(n+2)}\delta_{k,n+2} + \sqrt{(k+1)(k+2)}\delta_{k+2,n})$$

8. The results of problem 7 immediately lead to

$$\langle k | xp - px | n \rangle = i\hbar\delta_{kn}$$

9. This follows immediately from problems 5 and 6.

10. We again use

$$x = \sqrt{\frac{\hbar}{2m\omega}}(A + A^+)$$

$$p = i\sqrt{\frac{m\omega\hbar}{2}}(A^+ - A)$$

to obtain the operator expression for

$$x^2 = \frac{\hbar}{2m\omega}(A + A^+)(A + A^+) = \frac{\hbar}{2m\omega}(A^2 + 2A^+A + (A^+)^2 + 1)$$

$$p^2 = -\frac{m\omega\hbar}{2}(A^+ - A)(A^+ - A) = -\frac{m\omega\hbar}{2}(A^2 - 2A^+A + (A^+)^2 - 1)$$

where we have used $[A, A^+] = 1$.

The quadratic terms change the values of the eigenvalue integer by 2, so that they do not appear in the desired expressions. We get, very simply

$$\langle n | x^2 | n \rangle = \frac{\hbar}{2m\omega}(2n + 1)$$

$$\langle n | p^2 | n \rangle = \frac{m\omega\hbar}{2}(2n + 1)$$

14. Given the results of problem 9, and of 10, we have

$$(\Delta x)^2 = \frac{\hbar}{2m\omega} (2n + 1)$$

$$(\Delta p)^2 = \frac{\hbar m\omega}{2} (2n + 1)$$

and therefore

$$\Delta x \Delta p = \hbar \left(n + \frac{1}{2}\right)$$

15. The eigenstate in $A|\alpha\rangle = \alpha|\alpha\rangle$ may be written in the form

$$|\alpha\rangle = f(A^+) |0\rangle$$

It follows from the result of problem 4 that the eigenvalue equation reads

$$Af(A^+) |0\rangle = \frac{df(A^+)}{dA^+} |0\rangle = \alpha f(A^+) |0\rangle$$

The solution of $df(x) = \alpha f(x)$ is $f(x) = C e^{\alpha x}$ so that

$$|\alpha\rangle = C e^{\alpha A^+} |0\rangle$$

The constant C is determined by the normalization condition $\langle\alpha|\alpha\rangle = 1$

This means that

$$\begin{aligned} \frac{1}{C^2} &= \langle 0 | e^{\alpha^* A} e^{\alpha A^+} | 0 \rangle = \sum_{n=0}^{\infty} \frac{(\alpha^*)^n}{n!} \langle 0 | \left(\frac{d}{dA^+} \right)^n e^{\alpha A^+} | 0 \rangle \\ &= \sum_{n=0}^{\infty} \frac{|\alpha|^{2n}}{n!} \langle 0 | e^{\alpha A^+} | 0 \rangle = \sum_{n=0}^{\infty} \frac{|\alpha|^{2n}}{n!} = e^{|\alpha|^2} \end{aligned}$$

Consequently

$$C = e^{-|\alpha|^2/2}$$

We may now expand the state as follows

$$\begin{aligned} |\alpha\rangle &= \sum_n |n\rangle \langle n|\alpha\rangle = \sum_n |n\rangle \langle 0 | \frac{A^n}{\sqrt{n!}} C e^{\alpha A^+} | 0 \rangle \\ &= C \sum_n |n\rangle \frac{1}{\sqrt{n!}} \langle 0 | \left(\frac{d}{dA^+} \right)^n e^{\alpha A^+} | 0 \rangle = C \frac{\alpha^n}{\sqrt{n!}} |n\rangle \end{aligned}$$

The probability that the state $|\alpha\rangle$ contains n quanta is

$$P_n = |\langle n | \alpha \rangle|^2 = C^2 \frac{|\alpha|^{2n}}{n!} = \frac{(|\alpha|^2)^n}{n!} e^{-|\alpha|^2}$$

This is known as the *Poisson distribution*.

Finally

$$\langle \alpha | N | \alpha \rangle = \langle \alpha | A^+ A | \alpha \rangle = \alpha^* \alpha = |\alpha|^2$$

13. The equations of motion read

$$\begin{aligned} \frac{dx(t)}{dt} &= \frac{i}{\hbar} [H, x(t)] = \frac{i}{\hbar} \left[\frac{p^2(t)}{2m}, x(t) \right] = \frac{p(t)}{m} \\ \frac{dp(t)}{dt} &= \frac{i}{\hbar} [mgx(t), p(t)] = -mg \end{aligned}$$

This leads to the equation

$$\frac{d^2x(t)}{dt^2} = -g$$

The general solution is

$$x(t) = \frac{1}{2}gt^2 + \frac{p(0)}{m}t + x(0)$$

14. We have, as always

$$\frac{dx}{dt} = \frac{p}{m}$$

Also

$$\begin{aligned} \frac{dp}{dt} &= \frac{i}{\hbar} \left[\frac{1}{2}m\omega^2x^2 + e\xi x, p \right] \\ &= \frac{i}{\hbar} \left(\frac{1}{2}m\omega^2x[x, p] + \frac{1}{2}m\omega^2[x, p]x + e\xi[x, p] \right) \\ &= -m\omega^2x - e\xi \end{aligned}$$

Differentiating the first equation with respect to t and rearranging leads to

$$\frac{d^2x}{dt^2} = -\omega^2x - \frac{e\xi}{m} = -\omega^2 \left(x + \frac{e\xi}{m\omega^2} \right)$$

The solution of this equation is

$$\begin{aligned} x + \frac{e\xi}{m\omega^2} &= A\cos\omega t + B\sin\omega t \\ &= \left(x(0) + \frac{e\xi}{m\omega^2} \right) \cos\omega t + \frac{p(0)}{m\omega} \sin\omega t \end{aligned}$$

We can now calculate the commutator $[x(t_1), x(t_2)]$, which should vanish when $t_1 = t_2$. In this calculation it is only the commutator $[p(0), x(0)]$ that plays a role. We have

$$\begin{aligned} [x(t_1), x(t_2)] &= [x(0)\cos\omega t_1 + \frac{p(0)}{m\omega} \sin\omega t_1, x(0)\cos\omega t_2 + \frac{p(0)}{m\omega} \sin\omega t_2] \\ &= i\hbar \left(\frac{1}{m\omega} (\cos\omega t_1 \sin\omega t_2 - \sin\omega t_1 \cos\omega t_2) \right) = \frac{i\hbar}{m\omega} \sin\omega(t_2 - t_1) \end{aligned}$$

16. We simplify the algebra by writing

$$\sqrt{\frac{m\omega}{2\hbar}} = a, \quad \sqrt{\frac{\hbar}{2m\omega}} = \frac{1}{2a}$$

Then

$$\sqrt{n!} \left(\frac{\hbar\pi}{m\omega} \right)^{1/4} u_n(x) = v_n(x) = \left(ax - \frac{1}{2a} \frac{d}{dx} \right)^n e^{-a^2 x^2}$$

Now with the notation $y = ax$ we get

$$\begin{aligned} v_1(y) &= \left(y - \frac{1}{2} \frac{d}{dy} \right) e^{-y^2} = (y + y) e^{-y^2} = 2y e^{-y^2} \\ v_2(y) &= \left(y - \frac{1}{2} \frac{d}{dy} \right) (2y e^{-y^2}) = (2y^2 - 1 + 2y^2) e^{-y^2} \\ &= (4y^2 - 1) e^{-y^2} \end{aligned}$$

Next

$$\begin{aligned}
v_3(y) &= \left(y - \frac{1}{2} \frac{d}{dy}\right) \left[(4y^2 - 1)e^{-y^2} \right] \\
&= (4y^3 - y - 4y + y(4y^2 - 1))e^{-y^2} \\
&= (8y^3 - 6y)e^{-y^2}
\end{aligned}$$

The rest is substitution $y = \sqrt{\frac{m\omega}{2\hbar}}x$

17. We learned in problem 4 that

$$Af(A^+) |0\rangle = \frac{df(A^+)}{dA^+} |0\rangle$$

Iteration of this leads to

$$A^n f(A^+) |0\rangle = \frac{d^n f(A^+)}{dA^{+n}} |0\rangle$$

We use this to get

$$e^{\lambda A} f(A^+) |0\rangle = \sum_{n=0}^{\infty} \frac{\lambda^n}{n!} A^n f(A^+) |0\rangle = \sum_{n=0}^{\infty} \frac{\lambda^n}{n!} \left(\frac{d}{dA^+}\right)^n f(A^+) |0\rangle = f(A^+ + \lambda) |0\rangle$$

18. We use the result of problem **16** to write

$$e^{\lambda A} f(A^+) e^{-\lambda A} g(A^+) |0\rangle = e^{\lambda A} f(A^+) g(A^+ - \lambda) |0\rangle = f(A^+ + \lambda) g(A^+) |0\rangle$$

Since this is true for *any* state of the form $g(A^+) |0\rangle$ we have

$$e^{\lambda A} f(A^+) e^{-\lambda A} = f(A^+ + \lambda)$$

In the above we used the first formula in the solution to **16**, which depended on the fact that $[A, A^+] = 1$. More generally we have the Baker-Hausdorff form, which we derive as follows:

Define

$$F(\lambda) = e^{\lambda A} A^+ e^{-\lambda A}$$

Differentiation w.r.t. λ yields

$$\frac{dF(\lambda)}{d\lambda} = e^{\lambda A} A A^+ e^{-\lambda A} - e^{\lambda A} A^+ A e^{-\lambda A} = e^{\lambda A} [A, A^+] e^{-\lambda A} \equiv e^{\lambda A} C_1 e^{-\lambda A}$$

Iteration leads to

$$\frac{d^2 F(\lambda)}{d\lambda^2} = e^{\lambda A} [A, [A, A^+]] e^{-\lambda A} \equiv e^{\lambda A} C_2 e^{-\lambda A}$$

.....

$$\frac{d^n F(\lambda)}{d\lambda^n} = e^{\lambda A} [A, [A, [A, [A, \dots]]] \dots] e^{-\lambda A} \equiv e^{\lambda A} C_n e^{-\lambda A}$$

with A appearing n times in C_n . We may now use a Taylor expansion for

$$F(\lambda + \sigma) = \sum_{n=0}^{\infty} \frac{\sigma^n}{n!} \frac{d^n F(\lambda)}{d\lambda^n} = \sum_{n=0}^{\infty} \frac{\sigma^n}{n!} e^{\lambda A} C_n e^{-\lambda A}$$

If we now set $\lambda = 0$ we get

$$F(\sigma) = \sum_{n=0}^{\infty} \frac{\sigma^n}{n!} C_n$$

which translates into

$$e^{\sigma A} A^+ e^{-\sigma A} = A^+ + \sigma [A, A^+] + \frac{\sigma^2}{2!} [A, [A, A^+]] + \frac{\sigma^3}{3!} [A, [A, [A, A^+]]] + \dots$$

Note that if $[A, A^+] = 1$ only the first two terms appear, so that

$$e^{\sigma A} f(A^+) e^{-\sigma A} = f(A^+ + \sigma [A, A^+]) = f(A^+ + \sigma)$$

19. We follow the procedure outlined in the hint. We define $F(\lambda)$ by

$$e^{\lambda(aA + bA^+)} = e^{\lambda a A} F(\lambda)$$

Differentiation w.r.t λ yields

$$(aA + bA^+) e^{\lambda a A} F(\lambda) = aA e^{\lambda a A} F(\lambda) + e^{\lambda a A} \frac{dF(\lambda)}{d\lambda}$$

The first terms on each side cancel, and multiplication by $e^{-\lambda a A}$ on the left yields

$$\frac{dF(\lambda)}{d\lambda} = e^{-\lambda a A} bA^+ e^{\lambda a A} F(\lambda) = bA^+ - \lambda ab [A, A^+] F(\lambda)$$

When $[A, A^+]$ commutes with A . We can now integrate w.r.t. λ and after integration

Set $\lambda = 1$. We then get

$$F(1) = e^{bA^+ - ab[A, A^+]/2} = e^{bA^+} e^{-ab/2}$$

so that

$$e^{aA+bA^+} = e^{aA} e^{bA^+} e^{-ab/2}$$

20. We can use the procedure of problem **17**, but a simpler way is to take the hermitian conjugate of the result. For a *real* function f and λ real, this reads

$$e^{-\lambda A^+} f(A) e^{\lambda A^+} = f(A + \lambda)$$

Changing λ to $-\lambda$ yields

$$e^{\lambda A^+} f(A) e^{-\lambda A^+} = f(A - \lambda)$$

The remaining steps that lead to

$$e^{aA+bA^+} = e^{bA^+} e^{aA} e^{ab/2}$$

are identical to the ones used in problem **18**.

20. For the harmonic oscillator problem we have

$$x = \sqrt{\frac{\hbar}{2m\omega}} (A + A^+)$$

This means that e^{ikx} is of the form given in problem **19** with $a = b = ik\sqrt{\hbar/2m\omega}$

This leads to

$$e^{ikx} = e^{ik\sqrt{\hbar/2m\omega}A^+} e^{ik\sqrt{\hbar/2m\omega}A} e^{-\hbar k^2/4m\omega}$$

Since $A|0\rangle = 0$ and $\langle 0|A^+ = 0$, we get

$$\langle 0|e^{ikx}|0\rangle = e^{-\hbar k^2/4m\omega}$$

21. An alternative calculation, given that $u_0(x) = (m\omega/\pi\hbar)^{1/4} e^{-m\omega x^2/2\hbar}$, is

$$\left(\frac{m\omega}{\pi\hbar}\right)^{1/2} \int_{-\infty}^{\infty} dx e^{ikx} e^{-m\omega x^2/\hbar} = \left(\frac{m\omega}{\pi\hbar}\right)^{1/2} \int_{-\infty}^{\infty} dx e^{-\frac{m\omega}{\hbar}\left(x - \frac{ikh}{2m\omega}\right)^2} e^{-\frac{\hbar k^2}{4m\omega}}$$

The integral is a simple gaussian integral and $\int_{-\infty}^{\infty} dy e^{-m\omega y^2/\hbar} = \sqrt{\frac{\hbar\pi}{m\omega}}$ which just cancels the factor in front. Thus the two results agree.

CHAPTER 7

1. (a) The system under consideration has rotational degrees of freedom, allowing it to rotate about two orthogonal axes perpendicular to the rigid rod connecting the two masses. If we define the z axis as represented by the rod, then the Hamiltonian has the form

$$H = \frac{L_x^2 + L_y^2}{2I} = \frac{\mathbf{L}^2 - L_z^2}{2I}$$

where I is the moment of inertia of the dumbbell.

- (b) Since there are no rotations about the z axis, the eigenvalue of L_z is zero, so that the eigenvalues of the Hamiltonian are

$$E = \frac{\hbar^2 \ell(\ell + 1)}{2I}$$

with $\ell = 0, 1, 2, 3, \dots$

- (c) To get the energy spectrum we need an expression for the moment of inertia. We use the fact that

$$I = M_{red} a^2$$

where the reduced mass is given by

$$M_{red} = \frac{M_C M_N}{M_C + M_N} = \frac{12 \times 14}{26} M_{nucleon} = 6.46 M_{nucleon}$$

If we express the separation a in Angstroms, we get

$$I = 6.46 \times (1.67 \times 10^{-27} \text{ kg})(10^{-10} \text{ m} / \text{A})^2 a_A^2 = 1.08 \times 10^{-46} a_A^2$$

The energy difference between the ground state and the first excited state is $2\hbar^2 / 2I$ which leads to the numerical result

$$\Delta E = \frac{(1.05 \times 10^{-34} \text{ J}\cdot\text{s})^2}{1.08 \times 10^{-46} a_A^2 \text{ kg}\cdot\text{m}^2} \times \frac{1}{(1.6 \times 10^{-19} \text{ J} / \text{eV})} = \frac{6.4 \times 10^{-4}}{a_A^2} \text{ eV}$$

2. We use the connection $\frac{x}{r} = \sin \theta \cos \phi$, $\frac{y}{r} = \sin \theta \sin \phi$; $\frac{z}{r} = \cos \theta$ to write

$$Y_{11} = -\sqrt{\frac{3}{8\pi}} e^{i\phi} \sin \theta = -\sqrt{\frac{3}{8\pi}} \left(\frac{x+iy}{r} \right)$$

$$Y_{10} = \sqrt{\frac{3}{4\pi}} \cos \theta = \sqrt{\frac{3}{4\pi}} \left(\frac{z}{r} \right)$$

$$Y_{1,-1} = (-1)Y_{11}^* = \sqrt{\frac{3}{8\pi}} e^{-i\phi} \sin \theta = \sqrt{\frac{3}{8\pi}} \left(\frac{x-iy}{r} \right)$$

Next we have

$$\begin{aligned} Y_{22} &= \sqrt{\frac{15}{32\pi}} e^{2i\phi} \sin^2 \theta = \sqrt{\frac{15}{32\pi}} (\cos 2\phi + i \sin 2\phi) \sin^2 \theta \\ &= \sqrt{\frac{15}{32\pi}} (\cos^2 \phi - \sin^2 \phi + 2i \sin \phi \cos \phi) \sin^2 \theta \\ &= \sqrt{\frac{15}{32\pi}} \left(\frac{x^2 - y^2 + 2ixy}{r^2} \right) \end{aligned}$$

$$Y_{21} = -\sqrt{\frac{15}{8\pi}} e^{i\phi} \sin \theta \cos \theta = -\sqrt{\frac{15}{8\pi}} \frac{(x+iy)z}{r^2}$$

and

$$Y_{20} = \sqrt{\frac{5}{16\pi}} (3 \cos^2 \theta - 1) = \sqrt{\frac{5}{16\pi}} \left(\frac{2z^2 - x^2 - y^2}{r^2} \right)$$

We may use Eq. (7-46) to obtain the form for $Y_{2,-1}$ and $Y_{2,-2}$.

3. We use $L_{\pm} = L_x \pm iL_y$ to calculate $L_x = \frac{1}{2}(L_+ + L_-)$; $L_y = \frac{i}{2}(L_- - L_+)$. We may now proceed

$$\langle l, m_1 | L_x | l, m_2 \rangle = \frac{1}{2} \langle l, m_1 | L_+ | l, m_2 \rangle + \frac{1}{2} \langle l, m_1 | L_- | l, m_2 \rangle$$

$$\langle l, m_1 | L_y | l, m_2 \rangle = \frac{i}{2} \langle l, m_1 | L_- | l, m_2 \rangle - \frac{i}{2} \langle l, m_1 | L_+ | l, m_2 \rangle$$

and on the r.h.s. we insert

$$\langle l, m_1 | L_+ | l, m_2 \rangle = \hbar \sqrt{(l-m_2)(l+m_2+1)} \delta_{m_1, m_2+1}$$

$$\langle l, m_1 | L_- | l, m_2 \rangle = \hbar \sqrt{(l+m_2)(l-m_2+1)} \delta_{m_1, m_2-1}$$

4. Again we use $L_x = \frac{1}{2}(L_+ + L_-)$; $L_y = \frac{i}{2}(L_- - L_+)$ to work out

$$\begin{aligned}
L_x^2 &= \frac{1}{4} (L_+ + L_-)(L_+ + L_-) = \\
&= \frac{1}{4} (L_+^2 + L_-^2 + \mathbf{L}^2 - L_z^2 + \hbar L_z + \mathbf{L}^2 - L_z^2 - \hbar L_z) \\
&= \frac{1}{4} L_+^2 + \frac{1}{4} L_-^2 + \frac{1}{2} \mathbf{L}^2 - \frac{1}{2} L_z^2
\end{aligned}$$

We calculate

$$\begin{aligned}
\langle l, m_1 | L_+^2 | l, m_2 \rangle &= \hbar \sqrt{(l - m_2)(l + m_2 + 1)} \langle l, m_1 | L_+ | l, m_2 + 1 \rangle \\
&= \hbar^2 ((l - m_2)(l + m_2 + 1)(l - m_2 - 1)(l + m_2 + 2))^{1/2} \delta_{m_1, m_2 + 2}
\end{aligned}$$

and

$$\langle l, m_1 | L_-^2 | l, m_2 \rangle = \langle l, m_2 | L_+^2 | l, m_1 \rangle^*$$

which is easily obtained from the preceding result by interchanging m_1 and m_2 .

The remaining two terms yield

$$\frac{1}{2} \langle l, m_1 | (\mathbf{L}^2 - L_z^2) | l, m_2 \rangle = \frac{\hbar^2}{2} (l(l+1) - m_2^2) \delta_{m_1, m_2}$$

The remaining calculation is simple, since

$$\langle l, m_1 | L_y^2 | l, m_2 \rangle = \langle l, m_1 | \mathbf{L}^2 - L_z^2 - L_x^2 | l, m_2 \rangle$$

5. The Hamiltonian may be written as

$$H = \frac{\mathbf{L}^2 - L_z^2}{2I_1} + \frac{L_z^2}{2I_3}$$

whose eigenvalues are

$$\hbar^2 \left[\frac{l(l+1)}{2I_1} + m^2 \left(\frac{1}{2I_3} - \frac{1}{2I_1} \right) \right]$$

where $-l \leq m \leq l$.

(b) The plot is given on the right.

(c) The spectrum in the limit that $I_1 \gg I_3$ is just $E = \frac{\hbar^2}{2I_3} m^2$,

with $m = 0, 1, 2, \dots, l$. The $m = 0$ eigenvalue is nondegenerate, while the other ones are doubly degenerate (corresponding to the negative values of m).

6. We will use the lowering operator $L_- = \hbar e^{-i\phi} \left(-\frac{\partial}{\partial \theta} + i \cot \theta \frac{\partial}{\partial \phi} \right)$ acting on Y_{44} . Since

we are not interested in the normalization, we will not carry the \hbar factor.

$$\begin{aligned} Y_{43} &\propto e^{-i\phi} \left(-\frac{\partial}{\partial \theta} + i \cot \theta \frac{\partial}{\partial \phi} \right) [e^{4i\phi} \sin^4 \theta] \\ &= e^{3i\phi} \{ -4 \sin^3 \theta \cos \theta - 4 \cot \theta \sin^4 \theta \} = -8e^{3i\phi} \sin^3 \theta \cos \theta \end{aligned}$$

$$\begin{aligned} Y_{42} &\propto e^{-i\phi} \left(-\frac{\partial}{\partial \theta} + i \cot \theta \frac{\partial}{\partial \phi} \right) [e^{3i\phi} \sin^3 \theta \cos \theta] \\ &= e^{2i\phi} \{ -3 \sin^2 \theta \cos^2 \theta + \sin^4 \theta - 3 \sin^2 \theta \cos^2 \theta \} = \\ &= e^{2i\phi} \{ -6 \sin^2 \theta + 7 \sin^4 \theta \} \end{aligned}$$

$$\begin{aligned} Y_{41} &\propto e^{-i\phi} \left(-\frac{\partial}{\partial \theta} + i \cot \theta \frac{\partial}{\partial \phi} \right) [e^{2i\phi} (-6 \sin^2 \theta + 7 \sin^4 \theta)] \\ &= e^{i\phi} \{ 12 \sin \theta \cos \theta - 28 \sin^3 \theta \cos \theta - 2(-6 \sin \theta \cos \theta + 7 \sin^3 \theta \cos \theta) \} \\ &= e^{i\phi} \{ 24 \sin \theta \cos \theta - 42 \sin^3 \theta \cos \theta \} \end{aligned}$$

$$\begin{aligned}
Y_{40} &\propto e^{-i\phi} \left(-\frac{\partial}{\partial \theta} + i \cot \theta \frac{\partial}{\partial \phi} \right) \left[e^{i\phi} (4 \sin \theta - 7 \sin^3 \theta) \cos \theta \right] \\
&= \{ -4 \cos \theta + 21 \sin^2 \theta \cos \theta \} \cos \theta + (4 \sin^2 \theta - 7 \sin^4 \theta) - (4 \cos^2 \theta - 7 \sin^2 \theta \cos^2 \theta) \\
&= \{ -8 + 40 \sin^2 \theta - 35 \sin^4 \theta \}
\end{aligned}$$

7. Consider the H given. The angular momentum eigenstates $|\ell, m\rangle$ are eigenstates of the Hamiltonian, and the eigenvalues are

$$E = \frac{\hbar^2 \ell(\ell+1)}{2I} + \alpha \hbar m$$

with $-\ell \leq m \leq \ell$. Thus for every value of ℓ there will be $(2\ell+1)$ states, no longer degenerate.

8. We calculate

$$\begin{aligned}
[x, L_x] &= [x, yp_z - zp_y] = 0 \\
[y, L_x] &= [y, yp_z - zp_y] = z[p_y, y] = -i\hbar z \\
[z, L_x] &= [z, yp_z - zp_y] = -y[p_z, z] = i\hbar y \\
[x, L_y] &= [x, zp_x - xp_z] = -z[p_x, x] = i\hbar z \\
[y, L_y] &= [y, zp_x - xp_z] = 0 \\
[z, L_y] &= [z, zp_x - xp_z] = x[p_z, z] = -i\hbar x
\end{aligned}$$

The pattern is cyclical $(x, y) \rightarrow i\hbar z$ and so on, so that we expect (and can check) that

$$\begin{aligned}
[x, L_z] &= -i\hbar y \\
[y, L_z] &= i\hbar x \\
[z, L_z] &= 0
\end{aligned}$$

9. We again expect a cyclical pattern. Let us start with

$$[p_x, L_y] = [p_x, zp_x - xp_z] = -[p_x, x]p_z = i\hbar p_z$$

and the rest follows automatically.

10. (a) The eigenvalues of L_z are known to be 2, 1, 0, -1, -2 in units of \hbar .

(b) We may write

$$(3/5)L_x - (4/5)L_y = \mathbf{n} \cdot \mathbf{L}$$

where \mathbf{n} is a *unit vector*, since $n_x^2 + n_y^2 = (3/5)^2 + (-4/5)^2 = 1$. However, we may well have chosen the \mathbf{n} direction as our selected z direction, and the eigenvalues for this are again 2,1,0,-1,-2.

(c) We may write

$$\begin{aligned} 2L_x - 6L_y + 3L_z &= \sqrt{2^2 + 6^2 + 3^2} \left(\frac{2}{7}L_x - \frac{6}{7}L_y + 3L_z \right) \\ &= 7\mathbf{n} \cdot \mathbf{L} \end{aligned}$$

Where \mathbf{n} is yet another unit vector. By the same argument we can immediately state that the eigenvalues are $7m$ i.e. 14,7,0,-7,-14.

11. For our purposes, the only part that is relevant is

$$\begin{aligned} \frac{xy + yz + zx}{r^2} &= \sin^2 \theta \sin \phi \cos \phi + (\sin \phi + \cos \phi) \sin \theta \cos \theta \\ &= \frac{1}{2} \sin^2 \theta \frac{e^{2i\phi} - e^{-2i\phi}}{2i} + \sin \theta \cos \theta \left(\frac{e^{i\phi} - e^{-i\phi}}{2i} + \frac{e^{i\phi} + e^{-i\phi}}{2} \right) \end{aligned}$$

Comparison with the table of Spherical Harmonics shows that all of these involve combinations of $\ell = 2$ functions. We can therefore immediately conclude that the probability of finding $\ell = 0$ is *zero*, and the probability of finding $6\hbar^2$ is one, since this value corresponds to $\ell = 2$. A look at the table shows that

$$\begin{aligned} e^{2i\phi} \sin^2 \theta &= \sqrt{\frac{32\pi}{15}} Y_{2,2}; & e^{-2i\phi} \sin^2 \theta &= \sqrt{\frac{32\pi}{15}} Y_{2,-2} \\ e^{i\phi} \sin \theta \cos \theta &= -\sqrt{\frac{8\pi}{15}} Y_{2,1}; & e^{-i\phi} \sin \theta \cos \theta &= \sqrt{\frac{8\pi}{15}} Y_{2,-1} \end{aligned}$$

Thus

$$\begin{aligned} \frac{xy + yz + zx}{r^2} &= \frac{1}{2} \sin^2 \theta \frac{e^{2i\phi} - e^{-2i\phi}}{2i} + \sin \theta \cos \theta \left(\frac{e^{i\phi} - e^{-i\phi}}{2i} + \frac{e^{i\phi} + e^{-i\phi}}{2} \right) \\ &= \frac{1}{4i} \sqrt{\frac{32\pi}{15}} Y_{2,2} - \frac{1}{4i} \sqrt{\frac{32\pi}{15}} Y_{2,-2} - \frac{-i+1}{2} \sqrt{\frac{8\pi}{15}} Y_{2,1} + \frac{i+1}{2} \sqrt{\frac{8\pi}{15}} Y_{2,-1} \end{aligned}$$

This is not normalized. The sum of the squares of the coefficients is

$\frac{2\pi}{15} + \frac{2\pi}{15} + \frac{4\pi}{15} + \frac{4\pi}{15} = \frac{12\pi}{15} = \frac{4\pi}{5}$, so that for normalization purposes we must multiply by $\sqrt{\frac{5}{4\pi}}$. Thus the probability of finding $m = 2$ is the same as getting $m = -2$, and it is

$$P_{\pm 2} = \frac{5}{4\pi} \frac{2\pi}{15} = \frac{1}{6}$$

Similarly $P_1 = P_{-1}$, and since all the probabilities have add up to 1,

$$P_{\pm 1} = \frac{1}{3}$$

12. Since the particles are identical, the wave function $e^{im\phi}$ must be unchanged under the rotation $\phi \rightarrow \phi + 2\pi/N$. This means that $m(2\pi/N) = 2n\pi$, so that $m = nN$, with $n = 0, \pm 1, \pm 2, \pm 3, \dots$

The energy is

$$E = \frac{\hbar^2 m^2}{2MR^2} = \frac{\hbar^2 N^2}{2MR^2} n^2$$

The gap between the ground state ($n = 0$) and the first excited state ($n = 1$) is

$$\Delta E = \frac{\hbar^2 N^2}{2MR^2} \rightarrow \infty \text{ as } N \rightarrow \infty$$

If the cylinder is nicked, then there is no such symmetry and $m = 0, \pm 1, \pm 2, \dots$ and

$$\Delta E = \frac{\hbar^2}{2MR^2}$$

CHAPTER 8

1. The solutions are of the form $\psi_{n_1 n_2 n_3}(x, y, z) = u_{n_1}(x)u_{n_2}(y)u_{n_3}(z)$

where $u_n(x) = \sqrt{\frac{2}{a}} \sin \frac{n\pi x}{a}$, and so on. The eigenvalues are

$$E = E_{n_1} + E_{n_2} + E_{n_3} = \frac{\hbar^2 \pi^2}{2ma^2} (n_1^2 + n_2^2 + n_3^2)$$

2. (a) The lowest energy state corresponds to the lowest values of the integers $\{n_1, n_2, n_3\}$, that is, $\{1, 1, 1\}$ Thus

$$E_{\text{ground}} = \frac{\hbar^2 \pi^2}{2ma^2} \times 3$$

In units of $\frac{\hbar^2 \pi^2}{2ma^2}$ the energies are

- $\{1, 1, 1\} \rightarrow 3$ nondegenerate
- $\{1, 1, 2\}, \{1, 2, 1\}, \{2, 1, 1\} \rightarrow 6$ (triple degeneracy)
- $\{1, 2, 2\}, \{2, 1, 2\}, \{2, 2, 1\} \rightarrow 9$ (triple degeneracy)
- $\{3, 1, 1\}, \{1, 3, 1\}, \{1, 1, 3\} \rightarrow 11$ (triple degeneracy)
- $\{2, 2, 2\} \rightarrow 12$ (nondegenerate)
- $\{1, 2, 3\}, \{1, 3, 2\}, \{2, 1, 3\}, \{2, 3, 1\}, \{3, 1, 2\}, \{3, 2, 1\} \rightarrow 14$ (6-fold degenerate)
- $\{2, 2, 3\}, \{2, 3, 2\}, \{3, 2, 2\} \rightarrow 17$ (triple degenerate)
- $\{1, 1, 4\}, \{1, 4, 1\}, \{4, 1, 1\} \rightarrow 18$ (triple degenerate)
- $\{1, 3, 3\}, \{3, 1, 3\}, \{3, 3, 1\} \rightarrow 19$ (triple degenerate)
- $\{1, 2, 4\}, \{1, 4, 2\}, \{2, 1, 4\}, \{2, 4, 1\}, \{4, 1, 2\}, \{4, 2, 1\} \rightarrow 21$ (6-fold degenerate)

3. The problem breaks up into three separate, here identical systems. We know that the energy for a one-dimensional oscillator takes the values $\hbar\omega(n + 1/2)$, so that here the energy eigenvalues are

$$E = \hbar\omega(n_1 + n_2 + n_3 + 3/2)$$

The ground state energy corresponds to the n values all zero. It is $\frac{3}{2} \hbar\omega$.

4. The energy eigenvalues in terms of $\hbar\omega$ with the corresponding integers are

$(0, 0, 0)$	3/2	degeneracy 1
$(0, 0, 1)$ etc	5/2	3
$(0, 1, 1)$ $(0, 0, 2)$ etc	7/2	6
$(1, 1, 1), (0, 0, 3), (0, 1, 2)$ etc	9/2	10
$(1, 1, 2), (0, 0, 4), (0, 2, 2), (0, 1, 3)$	11/2	15
$(0, 0, 5), (0, 1, 4), (0, 2, 3), (1, 2, 2)$		
$(1, 1, 3)$	13/2	21

(0,0,6),(0,1,5),(0,2,4),(0,3,3)		
(1,1,4),(1,2,3),(2,2,2),	15/2	28
(0,0,7),(0,1,6),(0,2,5),(0,3,4)		
(1,1,5),(1,2,4),(1,3,3),(2,2,3)	17/2	36
(0,0,8),(0,1,7),(0,2,6),(0,3,5)		
(0,4,4),(1,1,6),(1,2,5),(1,3,4)		
(2,2,4),(2,3,3)	19/2	45
(0,0,9),(0,1,8),(0,2,7),(0,3,6)		
(0,4,5)(1,1,7),(1,2,6),(1,3,5)		
(1,4,4),(2,2,5) (2,3,4),(3,3,3)	21/2	55

5. It follows from the relations $x = \rho \cos \phi, y = \rho \sin \phi$ that

$$dx = d\rho \cos \phi - \rho \sin \phi d\phi; \quad dy = d\rho \sin \phi + \rho \cos \phi d\phi$$

Solving this we get

$$d\rho = \cos \phi dx + \sin \phi dy; \quad \rho d\phi = -\sin \phi dx + \cos \phi dy$$

so that

$$\frac{\partial}{\partial x} = \frac{\partial \rho}{\partial x} \frac{\partial}{\partial \rho} + \frac{\partial \phi}{\partial x} \frac{\partial}{\partial \phi} = \cos \phi \frac{\partial}{\partial \rho} - \frac{\sin \phi}{\rho} \frac{\partial}{\partial \phi}$$

and

$$\frac{\partial}{\partial y} = \frac{\partial \rho}{\partial y} \frac{\partial}{\partial \rho} + \frac{\partial \phi}{\partial y} \frac{\partial}{\partial \phi} = \sin \phi \frac{\partial}{\partial \rho} + \frac{\cos \phi}{\rho} \frac{\partial}{\partial \phi}$$

We now need to work out

$$\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} =$$

$$\left(\cos \phi \frac{\partial}{\partial \rho} - \frac{\sin \phi}{\rho} \frac{\partial}{\partial \phi} \right) \left(\cos \phi \frac{\partial}{\partial \rho} - \frac{\sin \phi}{\rho} \frac{\partial}{\partial \phi} \right) + \left(\sin \phi \frac{\partial}{\partial \rho} + \frac{\cos \phi}{\rho} \frac{\partial}{\partial \phi} \right) \left(\sin \phi \frac{\partial}{\partial \rho} + \frac{\cos \phi}{\rho} \frac{\partial}{\partial \phi} \right)$$

A little algebra leads to the r.h.s. equal to

$$\frac{\partial^2}{\partial \rho^2} + \frac{1}{\rho^2} \frac{\partial^2}{\partial \phi^2}$$

The time-independent Schrodinger equation now reads

$$-\frac{\hbar^2}{2m} \left(\frac{\partial^2 \Psi(\rho, \phi)}{\partial \rho^2} + \frac{1}{\rho^2} \frac{\partial^2 \Psi(\rho, \phi)}{\partial \phi^2} \right) + V(\rho) \Psi(\rho, \phi) = E \Psi(\rho, \phi)$$

The substitution of $\Psi(\rho, \phi) = R(\rho)\Phi(\phi)$ leads to two separate ordinary differential equations. The equation for $\Phi(\phi)$, when supplemented by the condition that the solution is unchanged when $\phi \rightarrow \phi + 2\pi$ leads to

$$\Phi(\phi) = \frac{1}{\sqrt{2\pi}} e^{im\phi} \quad m = 0, \pm 1, \pm 2, \dots$$

and the radial equation is then

$$\frac{d^2 R(\rho)}{d\rho^2} - \frac{m^2}{\rho^2} R(\rho) + \frac{2mE}{\hbar^2} R(\rho) = \frac{2mV(\rho)}{\hbar^2} R(\rho)$$

6. The relation between energy difference and wavelength is

$$2\pi\hbar \frac{c}{\lambda} = \frac{1}{2} m_{red} c^2 \alpha^2 \left(1 - \frac{1}{4}\right)$$

so that

$$\lambda = \frac{16\pi}{3} \frac{\hbar}{m_e c \alpha^2} \left(1 + \frac{m_e}{M}\right)$$

where M is the mass of the second particle, bound to the electron. We need to evaluate this for the three cases: $M = m_p$; $M = 2m_p$ and $M = m_e$. The numbers are

$$\lambda(in \ m) = 1215.0226 \times 10^{-10} \left(1 + \frac{m_e}{M}\right)$$

$$= 1215.68 \quad \text{for hydrogen}$$

$$= 1215.35 \quad \text{for deuterium}$$

$$= 2430.45 \quad \text{for positronium}$$

7. The ground state wave function of the electron in tritium ($Z = 1$) is

$$\psi_{100}(\mathbf{r}) = \frac{2}{\sqrt{4\pi}} \left(\frac{1}{a_0}\right)^{3/2} e^{-r/a_0}$$

This is to be expanded in a complete set of eigenstates of the $Z = 2$ hydrogenlike atom, and the probability that an energy measurement will yield the ground state energy of the $Z = 2$ atom is the square of the scalar product

$$\int d^3r \frac{2}{\sqrt{4\pi}} \left(\frac{1}{a_0}\right)^{3/2} e^{-r/a_0} \frac{2}{\sqrt{4\pi}} 2 \left(\frac{2}{a_0}\right)^{3/2} e^{-2r/a_0}$$

$$= \frac{8\sqrt{2}}{a_0^3} \int_0^\infty r^2 dr e^{-3r/a_0} = \frac{8\sqrt{2}}{a_0^3} \left(\frac{a_0}{3}\right)^3 2! = \frac{16\sqrt{2}}{27}$$

Thus the probability is $P = \frac{512}{729}$

8. The equation reads

$$-\nabla^2 \psi + \left(-\frac{E^2 - m^2 c^4}{\hbar^2 c^2} - \frac{2Z\alpha E}{\hbar c} \frac{1}{r} - \frac{(Z\alpha)^2}{r^2}\right) \psi(\mathbf{r}) = 0$$

Compare this with the hydrogenlike atom case

$$-\nabla^2 \psi(\mathbf{r}) + \left(\frac{2mE_B}{\hbar^2} - \frac{2mZe^2}{4\pi\epsilon_0 \hbar^2} \frac{1}{r}\right) \psi(\mathbf{r}) = 0$$

and recall that

$$-\nabla^2 = -\frac{d^2}{dr^2} - \frac{2}{r} \frac{d}{dr} + \frac{\ell(\ell+1)}{r^2}$$

We may thus make a translation

$$E^2 - m^2 c^4 \rightarrow -2mc^2 E_B$$

$$-\frac{2Z\alpha E}{\hbar c} \rightarrow -\frac{2mZe^2}{4\pi\epsilon_0 \hbar^2}$$

$$\ell(\ell+1) - Z^2 \alpha^2 \rightarrow \ell(\ell+1)$$

Thus in the expression for the hydrogenlike atom energy eigenvalue

$$2mE_B = -\frac{m^2 Z^2 e^2}{4\pi\epsilon_0 \hbar^2} \frac{1}{(n_r + \ell + 1)^2}$$

we replace ℓ by ℓ^* , where $\ell^*(\ell^*+1) = \ell(\ell+1) - (Z\alpha)^2$, that is,

$$\ell^* = -\frac{1}{2} + \left[\left(\ell + \frac{1}{2} \right)^2 - (Z\alpha)^2 \right]^{1/2}$$

We also replace $\frac{mZe^2}{4\pi\epsilon_0 \hbar}$ by $\frac{Z\alpha E}{c}$ and $2mE_B$ by $-\frac{E^2 - m^2 c^4}{c^2}$

We thus get

$$E^2 = m^2 c^4 \left[1 + \frac{Z^2 \alpha^2}{(n_r + \ell^* + 1)^2} \right]^{-1}$$

For $(Z\alpha) \ll 1$ this leads to

$$E - mc^2 = -\frac{1}{2} mc^2 (Z\alpha)^2 \frac{1}{(n_r + \ell^* + 1)^2}$$

This differs from the nonrelativistic result only through the replacement of ℓ by ℓ^* .

9. We use the fact that

$$\langle T \rangle_{nl} - \frac{Ze^2}{4\pi\epsilon_0} \langle \frac{1}{r} \rangle_{nl} = E_{nl} = -\frac{mc^2 (Z\alpha)^2}{2n^2}$$

Since

$$\frac{Ze^2}{4\pi\epsilon_0} \langle \frac{1}{r} \rangle_{nl} = \frac{Ze^2}{4\pi\epsilon_0} \frac{Z}{a_0 n^2} = \frac{Ze^2}{4\pi\epsilon_0} \frac{2mc\alpha}{\hbar n^2} = \frac{mc^2 Z^2 \alpha^2}{n^2}$$

we get

$$\langle T \rangle_{nl} = \frac{mc^2 Z^2 \alpha^2}{2n^2} = \frac{1}{2} \langle V(r) \rangle_{nl}$$

10. The expectation value of the energy is

$$\begin{aligned} \langle E \rangle &= \left(\frac{4}{6}\right)^2 E_1 + \left(\frac{3}{6}\right)^2 E_2 + \left(-\frac{1}{6}\right)^2 E_2 + \left(\frac{\sqrt{10}}{6}\right)^2 E_2 \\ &= -\frac{mc^2 \alpha^2}{2} \left[\frac{16}{36} + \frac{20}{36} \frac{1}{2^2} \right] = -\frac{mc^2 \alpha^2}{2} \frac{21}{36} \end{aligned}$$

Similarly

$$\langle \mathbf{L}^2 \rangle = \hbar^2 \left[\frac{16}{36} \times 0 + \frac{20}{36} \times 2 \right] = \frac{40}{36} \hbar^2$$

Finally

$$\begin{aligned} \langle L_z \rangle &= \hbar \left[\frac{16}{36} \times 0 + \frac{9}{36} \times 1 + \frac{1}{36} \times 0 + \frac{10}{36} \times (-1) \right] \\ &= -\frac{1}{36} \hbar \end{aligned}$$

11. We change notation from α to β to avoid confusion with the fine-structure constant that appears in the hydrogen atom wave function. The probability is the square of the integral

$$\begin{aligned} & \int d^3r \left(\frac{\beta}{\sqrt{\pi}} \right)^{3/2} e^{-\beta^2 r^2 / 2} \frac{2}{\sqrt{4\pi}} \left(\frac{Z}{a_0} \right)^{3/2} e^{-Zr/a_0} \\ &= \frac{4}{\pi^{1/4}} \left(\frac{Z\beta}{a_0} \right)^{3/2} \int_0^\infty r^2 dr e^{-\beta^2 r^2 / 2} e^{-Zr/a_0} \\ &= \frac{4}{\pi^{1/4}} \left(\frac{Z\beta}{a_0} \right)^{3/2} \left(-2 \frac{d}{d\beta^2} \right) \int_0^\infty dr e^{-\beta^2 r^2 / 2} e^{-Zr/a_0} \end{aligned}$$

The integral cannot be done in closed form, but it can be discussed for large and small $a_0\beta$.

12. It follows from $\langle \frac{d}{dt} (\mathbf{p} \bullet \mathbf{r}) \rangle = 0$ that $\langle [H, \mathbf{p} \bullet \mathbf{r}] \rangle = 0$

Now

$$\left[\frac{1}{2m} p_i p_i + V(r), x_j p_j \right] = \frac{1}{m} (-i\hbar) p^2 + i\hbar x_j \frac{\partial V}{\partial x_j} = -i\hbar \left(\frac{p^2}{m} - \mathbf{r} \bullet \nabla V(\mathbf{r}) \right)$$

As a consequence

$$\left\langle \frac{\mathbf{p}^2}{m} \right\rangle = \langle \mathbf{r} \bullet \nabla V(r) \rangle$$

If

$$V(r) = -\frac{Ze^2}{4\pi\epsilon_0 r}$$

then

$$\langle \mathbf{r} \bullet \nabla V(r) \rangle = \left\langle \frac{Ze^2}{4\pi\epsilon_0 r} \right\rangle$$

so that

$$\langle T \rangle = \frac{1}{2} \left\langle \frac{Ze^2}{4\pi\epsilon_0 r} \right\rangle = -\frac{1}{2} \langle V(r) \rangle$$

13. The radial equation is

$$\left(\frac{d^2}{dr^2} + \frac{2}{r} \frac{d}{dr}\right)R(r) + \frac{2m}{\hbar^2} \left(E - \frac{1}{2} m \omega^2 r^2 - \frac{l(l+1)\hbar^2}{2mr^2}\right)R(r) = 0$$

With a change of variables to $\rho = \sqrt{\frac{m\omega}{\hbar}} r$ and with $E = \lambda\hbar\omega/2$ this becomes

$$\left(\frac{d^2}{d\rho^2} + \frac{2}{\rho} \frac{d}{d\rho}\right)R(\rho) + \left(\lambda - \rho^2 - \frac{l(l+1)}{\rho^2}\right)R(\rho) = 0$$

We can easily check that the large ρ behavior is $e^{-\rho^2/2}$ and the small ρ behavior is ρ^l . The function $H(\rho)$ defined by

$$R(\rho) = \rho^l e^{-\rho^2/2} H(\rho)$$

obeys the equation

$$\frac{d^2 H(\rho)}{d\rho^2} + 2\left(\frac{l+1}{\rho} - \rho\right) \frac{dH(\rho)}{d\rho} + (\lambda - 3 - 2l)H(\rho) = 0$$

Another change of variables to $y = \rho^2$ yields

$$\frac{d^2 H(y)}{dy^2} + \left(\frac{l+3/2}{y} - 1\right) \frac{dH(y)}{dy} + \frac{\lambda - 2l - 3}{4y} H(y) = 0$$

This is the same as Eq. (8-27), if we make the replacement

$$\begin{aligned} 2l &\rightarrow 2l + 3/2 \\ \lambda - 1 &\rightarrow \frac{\lambda - 2l - 3}{4} \end{aligned}$$

This leads to the result that

$$\lambda = 4n_r + 2l + 3$$

or, equivalently

$$E = \hbar\omega(2n_r + l + 3/2)$$

While the solution is $L_a^{(b)}(y)$ with $a = n_r$ and $b = (2l + 3)/4$

CHAPTER 9

1. With
$$A^+ = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 \\ \sqrt{1} & 0 & 0 & 0 & 0 \\ 0 & \sqrt{2} & 0 & 0 & 0 \\ 0 & 0 & \sqrt{3} & 0 & 0 \\ 0 & 0 & 0 & \sqrt{4} & 0 \end{pmatrix}$$

we have

$$(A^+)^2 = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 \\ \sqrt{1} & 0 & 0 & 0 & 0 \\ 0 & \sqrt{2} & 0 & 0 & 0 \\ 0 & 0 & \sqrt{3} & 0 & 0 \\ 0 & 0 & 0 & \sqrt{4} & 0 \end{pmatrix} \begin{pmatrix} 0 & 0 & 0 & 0 & 0 \\ \sqrt{1} & 0 & 0 & 0 & 0 \\ 0 & \sqrt{2} & 0 & 0 & 0 \\ 0 & 0 & \sqrt{3} & 0 & 0 \\ 0 & 0 & 0 & \sqrt{4} & 0 \end{pmatrix} = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ \sqrt{2} & 0 & 0 & 0 & 0 \\ 0 & \sqrt{6} & 0 & 0 & 0 \\ 0 & 0 & \sqrt{12} & 0 & 0 \end{pmatrix}$$

It follows that

$$(A^+)^3 = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 \\ \sqrt{1} & 0 & 0 & 0 & 0 \\ 0 & \sqrt{2} & 0 & 0 & 0 \\ 0 & 0 & \sqrt{3} & 0 & 0 \\ 0 & 0 & 0 & \sqrt{4} & 0 \end{pmatrix} \begin{pmatrix} 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ \sqrt{2} & 0 & 0 & 0 & 0 \\ 0 & \sqrt{6} & 0 & 0 & 0 \\ 0 & 0 & \sqrt{12} & 0 & 0 \end{pmatrix} = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ \sqrt{3.2.1} & 0 & 0 & 0 & 0 \\ 0 & \sqrt{4.3.2} & 0 & 0 & 0 \end{pmatrix}$$

The next step is obvious: In the 5 x 5 format, there is only one entry in the bottom left-most corner, and it is $\sqrt{4.3.2.1}$.

2. [The reference should be to Eq. (6-36) instead of Eq. (6-4)]

$$x = \sqrt{\frac{\hbar}{2m\omega}} (A + A^+) = \sqrt{\frac{\hbar}{2m\omega}} \begin{pmatrix} 0 & \sqrt{1} & 0 & 0 & 0 \\ \sqrt{1} & 0 & \sqrt{2} & 0 & 0 \\ 0 & \sqrt{2} & 0 & \sqrt{3} & 0 \\ 0 & 0 & \sqrt{3} & 0 & \sqrt{4} \\ 0 & 0 & 0 & \sqrt{4} & 0 \end{pmatrix}$$

from which it follows that

$$x^2 = \left(\frac{\hbar}{2m\omega} \right) \begin{pmatrix} 1 & 0 & \sqrt{2.1} & 0 & 0 \\ 0 & 3 & 0 & \sqrt{3.2} & 0 \\ \sqrt{2.1} & 0 & 5 & 0 & \sqrt{4.3} \\ 0 & \sqrt{3.2} & 0 & 7 & 0 \\ 0 & 0 & \sqrt{4.3} & 0 & 9 \end{pmatrix}$$

3. The procedure here is exactly the same.

We have

$$p = i\sqrt{\frac{m\hbar\omega}{2}}(A^+ - A) = i\sqrt{\frac{m\hbar\omega}{2}} \begin{pmatrix} 0 & -\sqrt{1} & 0 & 0 & 0 \\ \sqrt{1} & 0 & -\sqrt{2} & 0 & 0 \\ 0 & \sqrt{2} & 0 & -\sqrt{3} & 0 \\ 0 & 0 & \sqrt{3} & 0 & -\sqrt{4} \\ 0 & 0 & 0 & \sqrt{4} & 0 \end{pmatrix}$$

from which it follows that

$$p^2 = \frac{m\hbar\omega}{2} \begin{pmatrix} 1 & 0 & -\sqrt{2.1} & 0 & 0 \\ 0 & 3 & 0 & -\sqrt{3.2} & 0 \\ -\sqrt{2.1} & 0 & 5 & 0 & -\sqrt{4.3} \\ 0 & -\sqrt{3.2} & 0 & 7 & 0 \\ 0 & 0 & -\sqrt{4.3} & 0 & 9 \end{pmatrix}$$

4. We have

$$u_1 = A^+ u_0 = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 \\ \sqrt{1} & 0 & 0 & 0 & 0 \\ 0 & \sqrt{2} & 0 & 0 & 0 \\ 0 & 0 & \sqrt{3} & 0 & 0 \\ 0 & 0 & 0 & \sqrt{4} & 0 \end{pmatrix} \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \\ 0 \end{pmatrix} = \begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \\ 0 \end{pmatrix}$$

5. We write

$$u_2 = \frac{1}{\sqrt{2!}} (A^+)^2 u_0 = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ \sqrt{2} & 0 & 0 & 0 & 0 \\ 0 & \sqrt{6} & 0 & 0 & 0 \\ 0 & 0 & \sqrt{12} & 0 & 0 \end{pmatrix} \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \\ 0 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 1 \\ 0 \\ 0 \end{pmatrix}$$

Similarly

$$u_3 = \frac{1}{\sqrt{3!}} (A^+)^3 u_0 = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ \sqrt{3 \cdot 2 \cdot 1} & 0 & 0 & 0 & 0 \\ 0 & \sqrt{4 \cdot 3 \cdot 2} & 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \\ 0 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \\ 0 \end{pmatrix}$$

and

$$u_4 = \frac{1}{\sqrt{4!}} (A^+)^4 u_0 = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ \sqrt{4 \cdot 3 \cdot 2 \cdot 1} & 0 & 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \\ 0 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 1 \end{pmatrix}$$

The pattern is clear. u_n is represented by a column vector with all zeros, except a 1 in the $(n+1)$ -th place.

6. (a)

$$\langle H \rangle = \frac{1}{\sqrt{6}} (1 \ 2 \ 1 \ 0) \hbar \omega \begin{pmatrix} 1/2 & 0 & 0 & 0 \\ 0 & 3/2 & 0 & 0 \\ 0 & 0 & 5/2 & 0 \\ 0 & 0 & 0 & 7/2 \end{pmatrix} \frac{1}{\sqrt{6}} \begin{pmatrix} 1 \\ 2 \\ 1 \\ 0 \end{pmatrix} = \frac{3}{2} \hbar \omega$$

$$(b) \langle x^2 \rangle = \frac{1}{\sqrt{6}} (1 \ 2 \ 1 \ 0) \frac{\hbar}{2m\omega} \begin{pmatrix} 1 & 0 & \sqrt{2} & 0 \\ 0 & 3 & 0 & \sqrt{6} \\ \sqrt{2} & 0 & 5 & 0 \\ 0 & 0 & 0 & 7 \end{pmatrix} \frac{1}{\sqrt{6}} \begin{pmatrix} 1 \\ 2 \\ 1 \\ 0 \end{pmatrix} = \frac{\hbar}{2m\omega} \left(3 + \frac{\sqrt{2}}{3} \right)$$

$$\langle x \rangle = \frac{1}{\sqrt{6}} (1 \ 2 \ 1 \ 0) \sqrt{\frac{\hbar}{2m\omega}} \begin{pmatrix} 0 & \sqrt{1} & 0 & 0 \\ \sqrt{1} & 0 & \sqrt{2} & 0 \\ 0 & \sqrt{2} & 0 & \sqrt{3} \\ 0 & 0 & \sqrt{3} & 0 \end{pmatrix} \frac{1}{\sqrt{6}} \begin{pmatrix} 1 \\ 2 \\ 1 \\ 0 \end{pmatrix} = \sqrt{\frac{\hbar}{2m\omega}} \frac{2}{3} (1 + \sqrt{2})$$

$$\langle p^2 \rangle = \frac{1}{\sqrt{6}} (1 \ 2 \ 1 \ 0) \frac{m\hbar\omega}{2} \begin{pmatrix} 1 & 0 & -\sqrt{2} & 0 \\ 0 & 3 & 0 & -\sqrt{6} \\ -\sqrt{2} & 0 & 5 & 0 \\ 0 & -\sqrt{6} & 0 & 7 \end{pmatrix} \frac{1}{\sqrt{6}} \begin{pmatrix} 1 \\ 2 \\ 1 \\ 0 \end{pmatrix} = \frac{m\hbar\omega}{2} \left(3 - \frac{\sqrt{2}}{3}\right)$$

$$\langle p \rangle = \frac{1}{\sqrt{6}} (1 \ 2 \ 1 \ 0) i \sqrt{\frac{m\hbar\omega}{2}} \begin{pmatrix} 0 & -\sqrt{1} & 0 & 0 \\ \sqrt{1} & 0 & -\sqrt{2} & 0 \\ 0 & \sqrt{2} & 0 & -\sqrt{3} \\ 0 & 0 & \sqrt{3} & 0 \end{pmatrix} \frac{1}{\sqrt{6}} \begin{pmatrix} 1 \\ 2 \\ 1 \\ 0 \end{pmatrix} = 0$$

(c) We get

$$(\Delta x)^2 = \frac{\hbar}{2m\omega} \frac{5}{3} \left(1 - \frac{\sqrt{2}}{3}\right); (\Delta p)^2 = \frac{\hbar}{2m\omega} \left(3 - \frac{\sqrt{2}}{3}\right)$$

$$(\Delta x)(\Delta p) = 2.23\hbar$$

7. Consider

$$\begin{pmatrix} -3 & \sqrt{19/4}e^{i\pi/3} \\ \sqrt{19/4}e^{-i\pi/3} & 6 \end{pmatrix} \begin{pmatrix} u_1 \\ u_2 \end{pmatrix} = \lambda \begin{pmatrix} u_1 \\ u_2 \end{pmatrix}$$

Suppose we choose $u_1=1$. The equations then lead to

$$(\lambda + 3) + \sqrt{19/4}e^{i\pi/3}u_2 = 0$$

$$\sqrt{19/4}e^{-i\pi/3} + (6 - \lambda)u_2 = 0$$

(a) Dividing one equation by the other leads to

$$(\lambda + 3)(\lambda - 6) = -19/4$$

The roots of this equation are $\lambda = -7/2$ and $\lambda = 13/2$. The values of u_2 corresponding to the two eigenvalues are

$$u_2(-7/2) = \frac{1}{\sqrt{19}} e^{-i\pi/3} ; u_2(13/2) = -\sqrt{19} e^{-i\pi/3}$$

(b) The normalized eigenvectors are

$$\frac{1}{\sqrt{20}} \begin{pmatrix} \sqrt{19} \\ -e^{-i\pi/3} \end{pmatrix} ; \frac{1}{\sqrt{20}} \begin{pmatrix} e^{i\pi/3} \\ \sqrt{19} \end{pmatrix}$$

It is easy to see that these are orthogonal.

(c) The matrix that diagonalizes the original matrix is, according to Eq. (9-55)

$$U = \frac{1}{\sqrt{20}} \begin{pmatrix} 1 & -\sqrt{19} e^{i\pi/3} \\ \sqrt{19} e^{-i\pi/3} & 1 \end{pmatrix}$$

It is easy to check that

$$U^+ A U = \begin{pmatrix} 13/2 & 0 \\ 0 & -7/2 \end{pmatrix}$$

8. We have, as a result of problem 7,

$$A = U A_{diag} U^+$$

From this we get

$$e^A = U e^{A_{diag}} U^+ = U \begin{pmatrix} e^{13/2} & 0 \\ 0 & e^{-7/2} \end{pmatrix} U^+$$

The rest is rather trivial matrix multiplication.

9, The solution of

$$\begin{pmatrix} 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 \end{pmatrix} \begin{pmatrix} a \\ b \\ c \\ d \end{pmatrix} = \lambda \begin{pmatrix} a \\ b \\ c \\ d \end{pmatrix}$$

is equivalent to solving

$$a + b + c + d = \lambda a = \lambda b = \lambda c = \lambda d$$

One solution is clearly $a = b = c = d$ with $\lambda = 4$. The eigenvector is $\frac{1}{2} \begin{pmatrix} 1 \\ 1 \\ 1 \\ 1 \end{pmatrix}$

We next observe that if any two (or more) of a, b, c, d are *not* equal, then $\lambda = 0$. These are the only possibilities, so that we have *three* eigenvalues all equal to zero. The Eigenvectors must satisfy $a + b + c + d = 0$, and they all must be mutually orthogonal. The following choices will work

$$\frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -1 \\ 0 \\ 0 \end{pmatrix}, \quad \frac{1}{\sqrt{2}} \begin{pmatrix} 0 \\ 0 \\ 1 \\ -1 \end{pmatrix}, \quad \frac{1}{2} \begin{pmatrix} 1 \\ 1 \\ -1 \\ -1 \end{pmatrix}$$

10. An hermitian matrix A can always be diagonalized by a particular unitary matrix U , such that

$$UAU^+ = A_{diag}$$

Let us now take traces on both sides: $TrUAU^+ = TrU^+UA = TrA$ while $TrA_{diag} = \sum_n a_n$

Where the a_n are the eigenvalues of A .

11. The product of two $N \times N$ matrices of the form $M = \begin{pmatrix} 1 & 1 & 1 & 1 & \dots \\ 1 & 1 & 1 & 1 & \dots \\ 1 & 1 & 1 & 1 & \dots \\ 1 & 1 & 1 & 1 & \dots \\ \dots & \dots & \dots & \dots & \dots \end{pmatrix}$ is

$$\begin{pmatrix} N & N & N & N & \dots \\ N & N & N & N & \dots \\ N & N & N & N & \dots \\ N & N & N & N & \dots \\ \dots & \dots & \dots & \dots & \dots \end{pmatrix}. \text{ Thus } M^2 = NM. \text{ This means that the eigenvalues can only be}$$

N or zero. Now the sum of the eigenvalues is the trace of M which is N (see problem 10). Thus there is one eigenvalue N and $(N-1)$ eigenvalues 0.

12. We found that the matrix $U = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 0 & 1 \\ i & 0 & -i \\ 0 & \sqrt{2} & 0 \end{pmatrix}$ has the property that

$M_3 = U(L_z / \hbar)U^+$. We may now calculate

$$\begin{aligned} M_1 &\equiv U(L_x / \hbar)U^+ = \\ &= \frac{1}{2} \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 0 & 1 \\ i & 0 & -i \\ 0 & \sqrt{2} & 0 \end{pmatrix} \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix} \begin{pmatrix} 1 & -i & 0 \\ 0 & 0 & \sqrt{2} \\ 1 & i & 0 \end{pmatrix} = \begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ 1 & 0 & 0 \end{pmatrix} \end{aligned}$$

and

$$\begin{aligned} M_2 &\equiv U(L_y / \hbar)U^+ = \\ &= \frac{1}{2} \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 0 & 1 \\ i & 0 & -i \\ 0 & \sqrt{2} & 0 \end{pmatrix} \begin{pmatrix} 0 & -i & 0 \\ i & 0 & -i \\ 0 & i & 0 \end{pmatrix} \begin{pmatrix} 1 & -i & 0 \\ 0 & 0 & \sqrt{2} \\ 1 & i & 0 \end{pmatrix} = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix} \end{aligned}$$

We can easily check that

$$\begin{aligned}
[M_1, M_2] &= \begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ 1 & 0 & 0 \end{pmatrix} \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix} - \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix} \begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ 1 & 0 & 0 \end{pmatrix} = \\
&= \begin{pmatrix} 0 & 1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} = iM_3
\end{aligned}$$

This was to be expected. The set M_1, M_2 and M_3 give us another representation of angular momentum matrices.

13. We have $AB = BA$. Now let U be a unitary matrix that diagonalizes A . In our case we have the additional condition that in

$$UAU^+ = A_{diag} = \begin{pmatrix} a_1 & 0 & 0 & 0 \\ 0 & a_2 & 0 & 0 \\ 0 & 0 & a_3 & 0 \\ 0 & 0 & 0 & a_4 \end{pmatrix}$$

all the diagonal elements are different. (We wrote this out for a 4 x 4 matrix)
Consider now

$$U[A, B]U^+ = UAU^+UBU^+ - UBU^+UAU^+ = 0$$

This reads as follows (for a 4 x 4 matrix)

$$\begin{pmatrix} a_1 & 0 & 0 & 0 \\ 0 & a_2 & 0 & 0 \\ 0 & 0 & a_3 & 0 \\ 0 & 0 & 0 & a_4 \end{pmatrix} \begin{pmatrix} b_{11} & b_{12} & b_{13} & b_{14} \\ b_{21} & b_{22} & b_{23} & b_{24} \\ b_{31} & b_{32} & b_{33} & b_{34} \\ b_{41} & b_{42} & b_{43} & b_{44} \end{pmatrix} = \begin{pmatrix} b_{11} & b_{12} & b_{13} & b_{14} \\ b_{21} & b_{22} & b_{23} & b_{24} \\ b_{31} & b_{32} & b_{33} & b_{34} \\ b_{41} & b_{42} & b_{43} & b_{44} \end{pmatrix} \begin{pmatrix} a_1 & 0 & 0 & 0 \\ 0 & a_2 & 0 & 0 \\ 0 & 0 & a_3 & 0 \\ 0 & 0 & 0 & a_4 \end{pmatrix}$$

If we look at the (12) matrix elements of the two products, we get, for example

$$a_1 b_{12} = a_2 b_{12}$$

and since we require that the eigenvalues are all different, we find that $b_{12} = 0$. This argument extends to all off-diagonal elements in the products, so that the only matrix elements in UBU^+ are the diagonal elements b_{ii} .

14. If M and M^+ commute, so do the *hermitian* matrices $(M + M^+)$ and $i(M - M^+)$.

Suppose we find the matrix U that diagonalizes $(M + M^+)$. Then that same matrix will diagonalize $i(M - M^+)$, provided that the eigenvalues of $M + M^+$ are all

different. This then shows that the same matrix U diagonalizes both M and M^+ separately.

(The problem is not really solved, till we learn how to deal with the situation when the eigenvalues of A in problem **13** are not all different).

CHAPTER 10

1. We need to solve
$$\frac{\hbar}{2} \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \begin{pmatrix} u \\ v \end{pmatrix} = \pm \frac{\hbar}{2} \begin{pmatrix} u \\ v \end{pmatrix}$$

For the + eigenvalue we have $u = -iv$, so that the normalized eigenstate is $\chi_+ = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ i \end{pmatrix}$

The – eigenstate can be obtained by noting that it must be orthogonal to the + state, and this leads to $\chi_- = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -i \end{pmatrix}$.

2, We note that the matrix has the form

$$\begin{aligned} \sigma_z \cos \alpha + \sigma_x \sin \alpha \cos \beta + \sigma_y \sin \alpha \sin \beta &\equiv \boldsymbol{\sigma} \cdot \mathbf{n} \\ \mathbf{n} &= (\sin \alpha \cos \beta, \sin \alpha \sin \beta, \cos \alpha) \end{aligned}$$

This implies that the eigenvalues must be ± 1 . We can now solve

$$\begin{pmatrix} \cos \alpha & \sin \alpha e^{-i\beta} \\ \sin \alpha e^{i\beta} & -\cos \alpha \end{pmatrix} \begin{pmatrix} u \\ v \end{pmatrix} = \pm \begin{pmatrix} u \\ v \end{pmatrix}$$

For the + eigenvalue we have $u \cos \alpha + v \sin \alpha e^{-i\beta} = u$. We may rewrite this in the form

$$2v \sin \frac{\alpha}{2} \cos \frac{\alpha}{2} e^{-i\beta} = 2u \sin^2 \frac{\alpha}{2}$$

From this we get

$$\chi_+ = \begin{pmatrix} \cos \frac{\alpha}{2} \\ e^{i\beta} \sin \frac{\alpha}{2} \end{pmatrix}$$

The – eigenstate can be obtained in a similar way, *or* we may use the requirement of orthogonality, which directly leads to

$$\chi_- = \begin{pmatrix} e^{-i\beta} \sin \frac{\alpha}{2} \\ -\cos \frac{\alpha}{2} \end{pmatrix}$$

The matrix $U = \begin{pmatrix} \cos \frac{\alpha}{2} & e^{-i\beta} \sin \frac{\alpha}{2} \\ e^{i\beta} \sin \frac{\alpha}{2} & -\cos \frac{\alpha}{2} \end{pmatrix}$

has the property that

$$U^+ \begin{pmatrix} \cos \alpha & \sin \alpha e^{-i\beta} \\ \sin \alpha e^{i\beta} & -\cos \alpha \end{pmatrix} U = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

as is easily checked.

The construction is quite simple.

$$S_z = \hbar \begin{pmatrix} 3/2 & 0 & 0 & 0 \\ 0 & 1/2 & 0 & 0 \\ 0 & 0 & -1/2 & 0 \\ 0 & 0 & 0 & -3/2 \end{pmatrix}$$

To construct S_+ we use $(S_+)_{mn} = \hbar \delta_{m,n+1} \sqrt{(l-m+1)(l+m)}$ and get

$$S_+ = \hbar \begin{pmatrix} 0 & \sqrt{3} & 0 & 0 \\ 0 & 0 & 2 & 0 \\ 0 & 0 & 0 & \sqrt{3} \\ 0 & 0 & 0 & 0 \end{pmatrix}$$

We can easily construct $S_- = (S_+)^+$. We can use these to construct

$$S_x = \frac{1}{2}(S_+ + S_-) = \frac{\hbar}{2} \begin{pmatrix} 0 & \sqrt{3} & 0 & 0 \\ \sqrt{3} & 0 & 2 & 0 \\ 0 & 2 & 0 & \sqrt{3} \\ 0 & 0 & \sqrt{3} & 0 \end{pmatrix}$$

and

$$S_y = \frac{i}{2}(S_- - S_+) = \frac{\hbar}{2} \begin{pmatrix} 0 & -i\sqrt{3} & 0 & 0 \\ i\sqrt{3} & 0 & -2i & 0 \\ 0 & 2i & 0 & -i\sqrt{3} \\ 0 & 0 & i\sqrt{3} & 0 \end{pmatrix}$$

The eigenstates in the above representation are very simple:

$$\chi_{3/2} = \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix}; \chi_{1/2} = \begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \end{pmatrix}; \chi_{-1/2} = \begin{pmatrix} 0 \\ 0 \\ 1 \\ 0 \end{pmatrix}; \chi_{-3/2} = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \end{pmatrix}$$

5. We first need the eigenstates of $(3S_x + 4S_y)/5$. The eigenvalues will be $\pm \hbar/2$ since the operator is of the form $\mathbf{S} \cdot \mathbf{n}$, where \mathbf{n} is a unit vector $(3/5, 4/5, 0)$. The equation to be solved is

$$\frac{\hbar}{2} \left(\frac{3}{5} \sigma_x + \frac{4}{5} \sigma_y \right) \chi_{\pm} = \pm \frac{\hbar}{2} \chi_{\pm}$$

In particular we want the eigenstate for the -ve eigenvalue, that is, we want to solve

$$\begin{pmatrix} 0 & \frac{3-4i}{5} \\ \frac{3+4i}{5} & 0 \end{pmatrix} \begin{pmatrix} u \\ v \end{pmatrix} = - \begin{pmatrix} u \\ v \end{pmatrix}$$

This is equivalent to $(3-4i)v = -5u$. A normalized state is $\frac{1}{\sqrt{50}} \begin{pmatrix} 3-4i \\ -5 \end{pmatrix}$.

The required probability is the square of

$$\frac{1}{\sqrt{5}} (2 \quad 1) \frac{1}{\sqrt{50}} \begin{pmatrix} 3-4i \\ -5 \end{pmatrix} = \frac{1}{\sqrt{250}} (6-8i-5) = \frac{1}{\sqrt{250}} (1-8i)$$

This number is $65/250 = 13/50$.

6. The normalized eigenspinor of S_y corresponding to the negative eigenvalue was found in problem 1. It is $\frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -i \end{pmatrix}$. The answer is thus the square of

$$\frac{1}{\sqrt{65}}(4 \quad 7) \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -i \end{pmatrix} = \frac{1}{\sqrt{130}}(4 - 7i)$$

which is $65/130 = 1/2$.

7. We make use of $\sigma_x \sigma_y = i\sigma_z = -\sigma_y \sigma_x$ and so on, as well as $\sigma_x^2 = 1$ and so on, to work out

$$\begin{aligned} & (\sigma_x A_x + \sigma_y A_y + \sigma_z A_z)(\sigma_x B_x + \sigma_y B_y + \sigma_z B_z) \\ &= A_x B_x + A_y B_y + A_z B_z + i\sigma_z (A_x B_y - A_y B_x) + i\sigma_y (A_z B_x - A_x B_z) + i\sigma_x (A_y B_z - A_z B_y) \\ &= \mathbf{A} \cdot \mathbf{B} + i\boldsymbol{\sigma} \cdot \mathbf{A} \times \mathbf{B} \end{aligned}$$

8. We may use the material in Eq. (10-26,27), so that at time T , we start with

$$\psi(T) = \frac{1}{\sqrt{2}} \begin{pmatrix} e^{-i\omega T} \\ e^{i\omega T} \end{pmatrix}$$

with $\omega = egB/4m_e$. This now serves as an initial state for a spin 1/2 particle placed in a magnetic field pointing in the y direction. The equation for ψ is according to Eq. (10-23)

$$i \frac{d\psi(t)}{dt} = \omega \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \psi(t)$$

Thus with $\psi(t) = \begin{pmatrix} a(t) \\ b(t) \end{pmatrix}$ we get $\frac{da}{dt} = -\omega b$; $\frac{db}{dt} = \omega a$. The solutions are in general

$$\begin{aligned} a(t) &= a(T) \cos \omega(t - T) - b(T) \sin \omega(t - T) \\ b(t) &= b(T) \cos \omega(t - T) + a(T) \sin \omega(t - T) \end{aligned}$$

We know that $a(T) = \frac{e^{-i\omega T}}{\sqrt{2}}$; $b(T) = \frac{e^{i\omega T}}{\sqrt{2}}$

So that

$$\psi(2T) = \frac{1}{\sqrt{2}} \begin{pmatrix} e^{-i\omega T} \cos \omega T - e^{i\omega T} \sin \omega T \\ e^{i\omega T} \cos \omega T + e^{-i\omega T} \sin \omega T \end{pmatrix}$$

The amplitude that a measurement of $S_{x_}$ yields $\hbar/2$ is

$$\frac{1}{\sqrt{2}}(1 \quad 1) \frac{1}{\sqrt{2}} \begin{pmatrix} e^{-i\omega T} \cos \omega T - e^{i\omega T} \sin \omega T \\ e^{i\omega T} \cos \omega T + e^{-i\omega T} \sin \omega T \end{pmatrix} = (\cos^2 \omega T - i \sin^2 \omega T)$$

Thus the probability is $P = \cos^4 \omega T + \sin^4 \omega T = \frac{1}{2}(1 + \cos^2 2\omega T)$

9. If we set an arbitrary matrix $\begin{pmatrix} \alpha & \beta \\ \gamma & \delta \end{pmatrix}$ equal to $A + \sigma \cdot \mathbf{B} = \begin{pmatrix} A + B_z & B_x - iB_y \\ B_x + iB_y & A - B_z \end{pmatrix}$

we see that allowing $A, B_x \dots$ to be complex we can match all of the α, β, \dots

(b) If the matrix $M = A + \sigma \cdot \mathbf{B}$ is to be unitary, then we require that

$$(A + \sigma \cdot \mathbf{B})(A^* + \sigma \cdot \mathbf{B}^*) = |A|^2 + A\sigma \cdot \mathbf{B}^* + A^*\sigma \cdot \mathbf{B} + \mathbf{B} \cdot \mathbf{B}^* + i\sigma \cdot \mathbf{B} \times \mathbf{B}^* = \mathbf{1}$$

which can be satisfied if

$$\begin{aligned} |A|^2 + |B_x|^2 + |B_y|^2 + |B_z|^2 &= 1 \\ AB_x^* + A^*B_x + i(B_yB_z^* - B_y^*B_z) &= 0 \\ \dots \end{aligned}$$

If the matrix M is to be hermitian, we must require that A and all the components of \mathbf{B} be real.

10. Here we make use of the fact that $(\sigma \cdot \mathbf{a})(\sigma \cdot \mathbf{a}) = \mathbf{a} \cdot \mathbf{a} \equiv a^2$ in the expansion

$$\begin{aligned} e^{i\sigma \cdot \mathbf{a}} &= 1 + i(\sigma \cdot \mathbf{a}) + \frac{i^2}{2!}(\sigma \cdot \mathbf{a})^2 + \frac{i^3}{3!}(\sigma \cdot \mathbf{a})^3 + \frac{i^4}{4!}(\sigma \cdot \mathbf{a})^4 + \dots \\ &= 1 - \frac{1}{2!}a^2 + \frac{1}{4!}(a^2)^2 + \dots + i\sigma \cdot \hat{\mathbf{a}}\left(a - \frac{a^3}{3!} + \dots\right) \\ &= \cos a + i\sigma \cdot \hat{\mathbf{a}} \sin a = \cos a + i\sigma \cdot \mathbf{a} \frac{\sin a}{a} \end{aligned}$$

11. We begin with the relation

$$\mathbf{S}^2 = \left(\frac{\hbar}{2} \sigma_1 + \frac{\hbar}{2} \sigma_2 \right)^2 = \frac{\hbar^2}{4} (\sigma_1^2 + \sigma_2^2 + 2\sigma_1 \cdot \sigma_2)$$

from which we obtain $\sigma_1 \bullet \sigma_2 = 2S(S+1) - 3$. This = -3 for a singlet and +1 for a triplet state.

We now choose \hat{e} to point in the z direction, so that the first term in S_{12} is equal to $3\sigma_{1z}\sigma_{2z}$.

(a) for a singlet state the two spins are always in opposite directions so that the first term is -6 and the second is $+3$. Thus

$$S_{12}X_{singlet} = 0$$

(b) For a triplet the first term is $+1$ when $S_z = 1$ and $S_z = -1$ and -1 when $S_z = 0$. This means that S_{12} acting on a triplet state in the first case is $3-1=2$, and in the second case it is $-3-1= -4$. Thus

$$(S_{12} - 2)(S_{12} + 4)X_{triplet} = 0$$

12. The potential may be written in the form

$$V(r) = V_1(r) + V_2(r)S_{12} + V_3(r)[2S(S+1) - 3]$$

For a singlet state S_{12} has expectation value zero, so that

$$V(r) = V_1(r) - 3V_3(r)$$

For the triplet state S_{12} has a value that depends on the z component of the total spin. What may be relevant

for a potential energy is an average, assuming that the two particles have equal probability of being in any one of the three S_z states. In that case the average value of S_z is $(2+2-4)/3= 0$

13. (a) It is clear that for the singlet state, $\psi_{singlet} = \frac{1}{\sqrt{2}}(\chi_+^{(1)}\chi_-^{(2)} - \chi_-^{(1)}\chi_+^{(2)})$, if one of the electrons is in the “up” state, the other must be in the “down” state.

(b). Suppose that we denote the eigenstates of S_y by ξ_{\pm} . These are, as worked out in problem 1,

$$\xi_+^{(1)} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ i \end{pmatrix}; \xi_-^{(1)} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -i \end{pmatrix}$$

The spinors for particle (1) may be expanded in terms of the ξ_{\pm} thus:

$$\chi_+ = \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \frac{1}{\sqrt{2}} \left(\frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ i \end{pmatrix} + \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -i \end{pmatrix} \right) = \frac{1}{\sqrt{2}} (\xi_+ + \xi_-)$$

$$\chi_- = \begin{pmatrix} 0 \\ 1 \end{pmatrix} = \frac{i}{\sqrt{2}} \left(\frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ i \end{pmatrix} - \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -i \end{pmatrix} \right) = \frac{i}{\sqrt{2}} (\xi_+ - \xi_-)$$

Similarly, for particle (2), we want to expand the spinors in terms of the η_{\pm} , the eigenstates of S_x

$$\eta_+^{(2)} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \end{pmatrix} ; \quad \eta_-^{(2)} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -1 \end{pmatrix}$$

thus

$$\chi_+ = \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \frac{1}{\sqrt{2}} \left(\frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \end{pmatrix} + \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -1 \end{pmatrix} \right) = \frac{1}{\sqrt{2}} (\eta_+ + \eta_-)$$

$$\chi_- = \begin{pmatrix} 0 \\ 1 \end{pmatrix} = \frac{1}{\sqrt{2}} \left(\frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \end{pmatrix} - \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -1 \end{pmatrix} \right) = \frac{1}{\sqrt{2}} (\eta_+ - \eta_-)$$

We now pick out, in the expansion of the singlet wave function the coefficient of $\xi_+^{(1)} \eta_+^{(2)}$ and take its absolute square. Some simple algebra shows that it is

$$\left| \frac{1}{\sqrt{2}} \frac{1}{\sqrt{2}} \frac{1-i}{\sqrt{2}} \right|^2 = \frac{1}{4}$$

9. The state is $(\cos \alpha_1 \chi_+^{(1)} + \sin \alpha_1 e^{i\beta_1} \chi_-^{(1)}) (\cos \alpha_2 \chi_+^{(2)} + \sin \alpha_2 e^{i\beta_2} \chi_-^{(2)})$. We need to calculate the scalar product of this with the three triplet wave functions of the two-electron system. It is easier to calculate the probability that the state is found in a singlet state, and then subtract that from unity.

The calculation is simple

$$\begin{aligned} & \left\langle \frac{1}{\sqrt{2}} (\chi_+^{(1)} \chi_-^{(2)} - \chi_-^{(1)} \chi_+^{(2)}) \mid (\cos \alpha_1 \chi_+^{(1)} + \sin \alpha_1 e^{i\beta_1} \chi_-^{(1)}) (\cos \alpha_2 \chi_+^{(2)} + \sin \alpha_2 e^{i\beta_2} \chi_-^{(2)}) \right\rangle \\ &= \frac{1}{\sqrt{2}} (\cos \alpha_1 \sin \alpha_2 e^{i\beta_2} - \sin \alpha_1 e^{i\beta_1} \cos \alpha_2) \end{aligned}$$

The absolute square of this is the singlet probability. It is

$$P_s = \frac{1}{2} (\cos^2 \alpha_1 \sin^2 \alpha_2 + \cos^2 \alpha_2 \sin^2 \alpha_1 + 2 \sin \alpha_1 \cos \alpha_1 \sin \alpha_2 \cos \alpha_2 \cos(\beta_1 - \beta_2))$$

and

$$P_t = 1 - P_s$$

14. We use $\mathbf{J} = \mathbf{L} + \mathbf{S}$ so that $\mathbf{J}^2 = \mathbf{L}^2 + \mathbf{S}^2 + 2\mathbf{L}\cdot\mathbf{S}$, from which we get

$$\mathbf{L} \cdot \mathbf{S} = \frac{1}{2}[J(J+1) - L(L+1) - 2]$$

since $S = 1$. Note that we have taken the division by \hbar^2 into account. For $J = L + 1$ this takes on the value L ; for $J = L$, it takes on the value -1 , and for $J = L - 1$ it is $-L - 1$. We therefore find

$$J = L + 1: \quad V = V_1 + LV_2 + L^2V_3$$

$$J = L \quad V = V_1 - V_2 + V_3$$

$$J = L - 1 \quad V = V_1 - (L+1)V_2 + (L+1)^2V_3$$

CHAPTER 11

1. The first order contribution is

$$E_n^{(1)} = \lambda \langle n | x^2 | n \rangle = \lambda \left(\sqrt{\frac{\hbar}{2m\omega}} \right)^2 \langle n | (A + A^+)(A + A^+) | n \rangle$$

To calculate the matrix element $\langle n | A^2 + AA^+ + A^+A + (A^+)^2 | n \rangle$ we note that

$$A^+ | n \rangle = \sqrt{n+1} | n+1 \rangle; \quad \langle n | A = \sqrt{n+1} \langle n+1 | \quad \text{so that (1) the first and last terms give}$$

zero, and the second and third terms yield $(n+1) + (n-1) = 2n$. Thus the first order shift is

$$E_n^{(1)} = \lambda \left(\frac{\hbar}{m\omega} n \right)$$

The second order calculation is quite complicated. What is involved is the calculation of

$$E_n^{(2)} = \lambda^2 \left(\frac{\hbar}{2m\omega} \right)^2 \sum_{m \neq n} \frac{\langle n | (A + A^+)^2 | m \rangle \langle m | (A + A^+)^2 | n \rangle}{\hbar\omega(n-m)}$$

This is manageable but quite messy. The suggestion is to write

$$H = \frac{p^2}{2m} + \frac{1}{2} m\omega^2 x^2 + \lambda x^2$$

This is just a simple harmonic oscillator with frequency

$$\omega^* = \sqrt{\omega^2 + 2\lambda/m} = \omega + \frac{\lambda}{\omega m} - \frac{1}{2} \frac{\lambda^2}{\omega^3 m^2} + \dots$$

Whose spectrum is

$$E_n = \hbar\omega^* \left(n + \frac{1}{2} \right) = \hbar\omega \left(n + \frac{1}{2} \right) + \frac{\lambda\hbar}{\omega m} \left(n + \frac{1}{2} \right) - \frac{\lambda^2\hbar}{2\omega^3 m^2} \left(n + \frac{1}{2} \right) + \dots$$

The extra factor of 1/2 that goes with each n is the zero-point energy. We are only interested in the change in energy of a given state $|n\rangle$ and thus subtract the zero-point energy to each order of λ . Note that the first order λ calculation is correct.

2. The eigenfunction of the rotator are the spherical harmonics. The first order energy shift for $l = 1$ states is given by

$$\Delta E = \langle 1, m | E \cos \theta | 1, m \rangle = E \int_0^{2\pi} d\phi \int_0^\pi \sin \theta d\theta \cos \theta |Y_{1,m}|^2$$

For $m = \pm 1$, this becomes

$$2\pi E \int_0^\pi \sin \theta d\theta \cos \theta \left(\frac{3}{8\pi}\right) \sin^2 \theta = \frac{3E}{4} \int_{-1}^1 duu(1-u^2) = 0$$

The integral for $m = 0$ is also zero. This result should have been anticipated. The eigenstates of \mathbf{L}^2 are also eigenstates of parity. The perturbation $\cos \theta$ is *odd* under the reflection $\mathbf{r} \rightarrow -\mathbf{r}$ and therefore the expectation value of an odd operator will always be zero. Since the perturbation represents the interaction with an electric field, our result states that a symmetric rotator does not have a permanent electric dipole moment.

The second order shift is more complicated. What needs to be evaluated is

$$\Delta E^{(2)} = E^2 \sum_{L, M (L \neq 1)} \frac{|\langle 1, m | \cos \theta | L, M \rangle|^2}{E_1 - E_L}$$

with $E_L = \frac{\hbar^2}{2I} L(L+1)$. The calculation is simplified by the fact that only $L = 0$ and $L = 2$ terms contribute. This can easily be seen from the table of spherical harmonics. For $L = 1$ we saw that the matrix element vanishes. For the higher values we see that $\cos \theta Y_{1,\pm 1} \propto Y_{2,\pm 1}$ and $\cos \theta Y_{1,0} \propto aY_{2,0} + bY_{0,0}$. The orthogonality of the spherical harmonics for different values of L takes care of the matter. Note that because of the ϕ integration, for $m = \pm 1$ only the $L = 2, M = \pm 1$ term contributes, while for the $m = 0$ term, there will be contributions from $L = 0$ and $L = 2, M = 0$. Some simple integrations lead to

$$\Delta E_{m=\pm 1}^{(2)} = -\frac{2IE^2}{\hbar^2} \frac{1}{15}; \quad \Delta E_{m=0}^{(2)} = -\frac{2IE^2}{\hbar^2} \frac{1}{60}$$

3. To lowest order in V_0 the shift is given by

$$\begin{aligned} \Delta E &= \left(\sqrt{\frac{2}{L}}\right)^2 \frac{V_0}{L} \int_0^L dx x \sin^2 \frac{n\pi x}{L} \\ &= \frac{2V_0}{L^2} \left(\frac{L}{\pi}\right)^2 \int_0^\pi duu \sin^2 nu = \frac{V_0}{\pi^2} \int_0^\pi duu(1 - \cos 2nu) = \frac{1}{2} V_0 \end{aligned}$$

The result that the energy shift is just the value of the perturbation at the mid-point is perhaps not surprising, given that the square of the eigenfunctions do not, on the average, favor one side of the potential over the other.

4. The matrix $\begin{pmatrix} E & \lambda & 0 & 0 \\ \lambda & E & 0 & 0 \\ 0 & 0 & 2E & \sigma \\ 0 & 0 & \sigma & 0 \end{pmatrix}$ consists of two boxes which can be diagonalized

separately. The upper left hand box involves solving $\begin{pmatrix} E & \lambda \\ \lambda & E \end{pmatrix} \begin{pmatrix} u \\ v \end{pmatrix} = \eta \begin{pmatrix} u \\ v \end{pmatrix}$

The result is that the eigenvalues are $\eta = E \pm \lambda$. The corresponding eigenstates are easily worked out and are $\frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ \pm 1 \end{pmatrix}$ for the two cases.

For the lower left hand box we have to solve $\begin{pmatrix} 2E & \sigma \\ \sigma & 0 \end{pmatrix} \begin{pmatrix} a \\ b \end{pmatrix} = \xi \begin{pmatrix} a \\ b \end{pmatrix}$. Here we find that the eigenvalues are $\xi = E \pm \sqrt{E^2 + \sigma^2}$. The corresponding eigenstates are

$$N \begin{pmatrix} \sigma \\ -E \pm \sqrt{E^2 + \sigma^2} \end{pmatrix} \text{ respectively, with } \frac{1}{N^2} = \sigma^2 + (-E \pm \sqrt{E^2 + \sigma^2})^2.$$

5. The *change* in potential energy is given by

$$V_1 = -\frac{3e^2}{8\pi\epsilon_0 R^3} \left(R^2 - \frac{1}{3} r^2 \right) + \frac{e^2}{4\pi\epsilon_0 r} \quad r \leq R$$

$$= 0 \quad \text{elsewhere}$$

Thus

$$\Delta E = \int d^3r \psi_{nl}^*(\mathbf{r}) V_1 \psi_{nl}(\mathbf{r}) = \int_0^R r^2 dr V_1 R_{nl}^2(r)$$

We may now calculate this for various states.

$$n = 1 \quad \Delta E_{10} = 4 \left(\frac{Z}{a_0} \right)^3 \int_0^R r^2 dr e^{-2Zr/a_0} \left(-\frac{3e^2}{8\pi\epsilon_0 R^3} \left(R^2 - \frac{1}{3} r^2 \right) + \frac{e^2}{4\pi\epsilon_0 r} \right)$$

With a change of variables to $x = r/Za_0$ and with $\rho = ZR/a_0$ this becomes

$$\Delta E_{10} = 4 \left(\frac{Ze^2}{4\pi\epsilon_0 a_0} \right) \int_0^\rho x^2 dx \left(-\frac{3}{2\rho} + \frac{x^2}{2\rho^3} + \frac{1}{x} \right) e^{-2x}$$

Since $x \ll 1$ we may approximate $e^{-2x} \approx 1 - 2x$, which simplifies the integrals. What results is

$$\Delta E_{10} = \left(\frac{Ze^2}{4\pi\epsilon_0 a_0} \right) \left(\frac{4}{10} \rho^2 + \dots \right)$$

A similar calculation yields

$$\Delta E_{20} = \frac{1}{2} \left(\frac{Ze^2}{4\pi\epsilon_0 a_0} \right) \int_0^\rho x^2 dx (1-x)^2 \left(-\frac{3}{2\rho} + \frac{x^2}{2\rho^3} + \frac{1}{x} \right) e^{-x} \approx \left(\frac{Ze^2}{4\pi\epsilon_0 a_0} \right) \left(\frac{1}{20} \rho^2 + \dots \right)$$

and

$$\Delta E_{21} = \frac{1}{24} \left(\frac{Ze^2}{4\pi\epsilon_0 a_0} \right) \int_0^\rho x^2 dx x^2 \left(-\frac{3}{2\rho} + \frac{x^2}{2\rho^3} + \frac{1}{x} \right) e^{-x} \approx \left(\frac{Ze^2}{4\pi\epsilon_0 a_0} \right) \left(\frac{1}{1120} \rho^4 + \dots \right)$$

6. We need to calculate $\lambda \langle 0 | x^4 | 0 \rangle$. One way of proceeding is to use the expression

$$x = \sqrt{\frac{\hbar}{2m\omega}} (A + A^\dagger)$$

Then

$$\lambda \langle 0 | x^4 | 0 \rangle = \lambda \left(\frac{\hbar}{2m\omega} \right)^2 \langle 0 | (A + A^\dagger)(A + A^\dagger)(A + A^\dagger)(A + A^\dagger) | 0 \rangle$$

The matrix element is

$$\begin{aligned} & \langle 0 | (A + A^\dagger)(A + A^\dagger)(A + A^\dagger)(A + A^\dagger) | 0 \rangle = \\ & \langle 0 | A^\dagger (A + A^\dagger)(A + A^\dagger) A^\dagger | 0 \rangle = \\ & \langle 1 | (A + A^\dagger)(A + A^\dagger) | 1 \rangle = \\ & \left[\langle 0 | + \sqrt{2} \langle 2 | \right] \left[| 0 \rangle + \sqrt{2} | 2 \rangle \right] = 3 \end{aligned}$$

Thus the energy shift is $\Delta E = 3\lambda \left(\frac{\hbar}{2m\omega} \right)^2$

It is easy to see that the same result is obtained from

$$\int_{-\infty}^{\infty} dx (\lambda x^4) \left[\left(\frac{m\omega}{\hbar\pi} \right)^{1/4} e^{-m\omega x^2/2\hbar} \right]^2$$

7. The first order perturbation shift is

$$\begin{aligned}\Delta E_n &= \frac{2\varepsilon}{b} \int_0^b dx \sin \frac{\pi x}{b} \left(\sin \frac{n\pi x}{b} \right)^2 \\ &= \frac{2\varepsilon}{\pi} \int_0^\pi du \sin u (\sin nu)^2 \\ &= \frac{2\varepsilon}{\pi} \left(1 + \frac{1}{4n^2 - 1} \right)\end{aligned}$$

8. It follows from $[p, x] = -i\hbar$ that

$$\begin{aligned}-i\hbar &= \langle a | px - xp | a \rangle = \\ &= \sum_n \{ \langle a | p | n \rangle \langle n | x | a \rangle - \langle a | x | n \rangle \langle n | p | a \rangle \}\end{aligned}$$

Now

$$\langle a | p | n \rangle = m \langle a | \frac{dx}{dt} | n \rangle = \frac{im}{\hbar} \langle a | Hx - xH | n \rangle = \frac{im}{\hbar} (E_a - E_n) \langle a | x | n \rangle$$

Consequently

$$\langle n | p | a \rangle = \langle a | p | n \rangle^* = -\frac{im}{\hbar} (E_a - E_n) \langle n | x | a \rangle$$

Thus

$$-i\hbar = \sum_n \frac{2im}{\hbar} (E_a - E_n) \langle a | x | n \rangle \langle n | x | a \rangle$$

from which it follows that

$$\sum_n (E_n - E_a) |\langle a | x | n \rangle|^2 = \frac{\hbar^2}{2m}$$

9. For the harmonic oscillator, with $|a\rangle = |0\rangle$, we have

$$\langle n | x | 0 \rangle = \sqrt{\frac{\hbar}{2m\omega}} \langle n | A^+ | 0 \rangle = \sqrt{\frac{\hbar}{2m\omega}} \delta_{n,1}$$

This means that in the sum rule, the left hand side is

$$\hbar\omega\left(\frac{\hbar}{2m\omega}\right) = \frac{\hbar^2}{2m}$$

as expected.

10. For the $n = 3$ Stark effect, we need to consider the following states:

$$l = 2 : m_l = 2, 1, 0, -1, -2$$

$$l = 1 : m_l = 1, 0, -1$$

$$l = 0 : m_l = 0$$

In calculating matrix element of z we have selection rules $\Delta l = 1$ (parity forbids $\Delta l = 0$) and, since we are dealing with z , also $\Delta m_l = 0$. Thus the possible matrix elements that enter are

$$\langle 2, 1 | z | 1, 1 \rangle = \langle 2, -1 | z | 1, -1 \rangle \equiv A$$

$$\langle 2, 0 | z | 1, 0 \rangle \equiv B$$

$$\langle 1, 0 | z | 0, 0 \rangle \equiv C$$

The matrix to be diagonalized is

$$\begin{pmatrix} 0 & A & 0 & 0 & 0 & 0 & 0 & 0 \\ A & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ \hline 0 & 0 & 0 & B & 0 & 0 & 0 & 0 \\ 0 & 0 & B & 0 & C & 0 & 0 & 0 \\ 0 & 0 & 0 & C & 0 & 0 & 0 & 0 \\ \hline 0 & 0 & 0 & 0 & 0 & 0 & 0 & A \\ 0 & 0 & 0 & 0 & 0 & 0 & A & 0 \end{pmatrix}$$

The columns and rows are labeled by $(2, 1), (1, 1), (2, 0), (1, 0), (0, 0), (2, -1), (1, -1)$.

The problem therefore separates into three different matrices. The eigenvalues of the submatrices that couple the $(2, 1)$ and $(1, 1)$ states, as well as those that couple the $(2, -1)$ and $(1, -1)$ states are

$$\lambda = \pm A$$

where

$$A = \int d\Omega Y_{21}^* \cos \theta Y_{11} \int_0^\infty r^2 dr R_{32}(r) r R_{31}(r)$$

The mixing among the $m_l = 0$ states involves the matrix $\begin{pmatrix} 0 & B & 0 \\ B & 0 & C \\ 0 & C & 0 \end{pmatrix}$

Whose eigenvalues are $\lambda = 0, \pm \sqrt{B^2 + C^2}$.. Here

$$B = \int d\Omega Y_{20}^* \cos \theta Y_{10} \int_0^\infty r^2 dr R_{32}(r) r R_{31}(r)$$

$$C = \int d\Omega Y_{10}^* \cos \theta Y_{00} \int_0^\infty r^2 dr R_{31}(r) r R_{30}(r)$$

The eigenstates of the A submatrices are those of σ_x , that is $\frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ \pm 1 \end{pmatrix}$. The eigenstates of the central 3 x 3 matrix are

$$\frac{1}{\sqrt{B^2 + C^2}} \begin{pmatrix} C \\ 0 \\ -B \end{pmatrix}; \frac{1}{\sqrt{2(B^2 + C^2)}} \begin{pmatrix} B \\ \pm \sqrt{B^2 + C^2} \\ C \end{pmatrix}$$

with the first one corresponding to the $\lambda = 0$ eigenvalue.

11. For a one-dimensional operator (labeled by the x variable) we introduced the raising and lowering operators A^+ and A . We were able to write the Hamiltonian in the form

$$H_x = \hbar\omega(A^+A + \frac{1}{2})$$

We now do the same thing for the harmonic oscillator labeled by the y variable. The raising and lowering operators will be denoted by B^+ and B , with

$$H_y = \hbar\omega(B^+B + \frac{1}{2})$$

The eigenstates of $H_x + H_y$ are

$$|m, n\rangle = \frac{(A^+)^n (B^+)^m}{\sqrt{n!} \sqrt{m!}} |0, 0\rangle$$

where the ground state has the property that $A|0, 0\rangle = B|0, 0\rangle = 0$

The perturbation may be written in the form

$$H_1 = 2\lambda xy = \frac{\hbar\lambda}{m\omega} (A + A^+)(B + B^+)$$

(a) The first order shift of the ground state is

$$\langle 0,0 | H_1 | 0,0 \rangle = 0$$

since every single of the operators A, \dots, B^+ has zero expectation value in the ground state.

(b) Consider the two degenerate states $|1,0\rangle$ and $|0,1\rangle$. The matrix elements of interest to us are

$$\langle 1,0 | (A+A^+)(B + B^+) | 1,0 \rangle = \langle 0,1 | (A+A^+)(B + B^+) | 0,1 \rangle = 0$$

$$\langle 1,0 | (A+A^+)(B + B^+) | 0,1 \rangle = \langle 0,1 | (A+A^+)(B + B^+) | 1,0 \rangle = \langle 1,0 | (A+A^+)(B + B^+) | 1,0 \rangle = 1$$

Thus in degenerate perturbation theory we must diagonalize the matrix

$$\begin{pmatrix} 0 & h \\ h & 0 \end{pmatrix}$$

where $h = \frac{\lambda\hbar}{m\omega}$. The eigenvalues are $\pm h$, and the degenerate levels are split to

$$E = \hbar\omega(1 \pm \frac{\lambda}{m\omega^2})$$

(c) The second order expression is

$$\begin{aligned} & \left(\frac{\lambda\hbar}{m\omega} \right)^2 \sum_{k,n} \frac{|\langle 0,0 | (A + A^+)(B + B^+) | k,n \rangle|^2}{-\hbar\omega(k+n)} = \\ & - \frac{\lambda^2\hbar}{m\omega^3} \sum_{k,n} \frac{|\langle 1,1 | k,n \rangle|^2}{(k+n)} = - \frac{\lambda^2\hbar}{2m\omega^3} \end{aligned}$$

The exact solution to this problem may be found by working with the potential at a classical level. The potential energy is

$$\frac{1}{2} m\omega^2(x^2 + y^2) + \lambda xy$$

Let us carry out a rotation in the $x - y$ plane. The kinetic energy does not change since \mathbf{p}^2 is unchanged under rotations. If we let

$$\begin{aligned} x &= x' \cos\theta + y' \sin\theta \\ y &= -x' \sin\theta + y' \cos\theta \end{aligned}$$

then the potential energy, after a little rearrangement, takes the form

$$\left(\frac{1}{2}m\omega^2 - \lambda \sin 2\theta\right)x'^2 + \left(\frac{1}{2}m\omega^2 + \lambda \sin 2\theta\right)y'^2 + 2\lambda \cos 2\theta x' y'$$

If we choose $\cos 2\theta = 0$, so that $\sin 2\theta = 1$, this reduces to two decoupled harmonic oscillators. The energy is the sum of the two energies. Since

$$\begin{aligned}\frac{1}{2}m\omega_x^2 &= \frac{1}{2}m\omega^2 - \lambda \\ \frac{1}{2}m\omega_y^2 &= \frac{1}{2}m\omega^2 + \lambda\end{aligned}$$

the total energy for an arbitrary excited state is

$$E_{k,n} = \hbar\omega_x\left(k + \frac{1}{2}\right) + \hbar\omega_y\left(n + \frac{1}{2}\right)$$

where

$$\begin{aligned}\hbar\omega_x &= \hbar\omega(1 - 2\lambda/m\omega^2)^{1/2} = \hbar\omega - \frac{\hbar\lambda}{m\omega} - \frac{\hbar\lambda^2}{2m^2\omega^3} + \dots \\ \hbar\omega_y &= \hbar\omega(1 + 2\lambda/m\omega^2)^{1/2} = \hbar\omega + \frac{\hbar\lambda}{m\omega} - \frac{\hbar\lambda^2}{2m^2\omega^3} + \dots\end{aligned}$$

12. The spectral line corresponds to the transition $(n = 4, l = 3) \rightarrow (n = 3, l = 2)$. We must therefore examine what happens to these energy levels under the perturbation

$$H_1 = \frac{e}{2m} \mathbf{L} \cdot \mathbf{B}$$

We define the z axis by the direction of \mathbf{B} , so that the perturbation is $\frac{eB}{2m} L_z$.

In the absence of the perturbation the initial state is $(2l + 1) = 7$ -fold degenerate, with the L_z level unchanged, and the others moved up and down in intervals of $eB/2m$.

The final state is 5-fold degenerate, and the same splitting occurs, with the same intervals. If transitions with zero or ± 1 change in L_z/\hbar , the lines are as shown in the figure on the right.

What will be the effect of a constant electric field parallel to \mathbf{B} ?
The additional perturbation is therefore

$$H_2 = -e\mathbf{E}_0 \cdot \mathbf{r} = -eE_0z$$

and we are only interested in what this does to the energy level structure. The perturbation acts as in the Stark effect. The effect of H_1 is to mix up levels that are degenerate, corresponding to a given m_l value with *different values of l* . For example, the $l = 3, m_l = 2$ and the $l = 2, m_l = 2$ degeneracy (for $n = 4$) will be split. There will be a further breakdown of degeneracy.

13. The eigenstates of the unperturbed Hamiltonian are eigenstates of σ_z . They are

$$\begin{pmatrix} 1 \\ 0 \end{pmatrix} \text{ corresponding to } E = E_0 \text{ and } \begin{pmatrix} 0 \\ 1 \end{pmatrix} \text{ corresponding to } E = -E_0.$$

The first order shifts are given by

$$\begin{aligned} (1 \ 0)\lambda \begin{pmatrix} \alpha & u \\ u^* & \beta \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix} &= \lambda\alpha \\ (0 \ 1)\lambda \begin{pmatrix} \alpha & u \\ u^* & \beta \end{pmatrix} \begin{pmatrix} 0 \\ 1 \end{pmatrix} &= \lambda\beta \end{aligned}$$

for the two energy levels.

The second order shift for the upper state involves summing over intermediate states that differ from the initial state. Thus, for the upper state, the intermediate state is just the lower one, and the energy denominator is $E_0 - (-E_0) = 2E_0$. Thus the second order shift is

$$\frac{\lambda^2}{2E_0} (1 \ 0) \begin{pmatrix} \alpha & u \\ u^* & \beta \end{pmatrix} \begin{pmatrix} 0 \\ 1 \end{pmatrix} (1 \ 0) \begin{pmatrix} \alpha & u \\ u^* & \beta \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \frac{\lambda^2 |u|^2}{2E_0}$$

For the lower state we get

$$\frac{\lambda^2}{-2E_0} (0 \ 1) \begin{pmatrix} \alpha & u \\ u^* & \beta \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix} (0 \ 1) \begin{pmatrix} \alpha & u \\ u^* & \beta \end{pmatrix} \begin{pmatrix} 0 \\ 1 \end{pmatrix} = -\frac{\lambda^2 |u|^2}{2E_0}$$

The exact eigenvalues can be obtained from

$$\det \begin{vmatrix} E_0 + \alpha - \varepsilon & u \\ u^* & -E_0 + \beta - \varepsilon \end{vmatrix} = 0$$

This leads to

$$\begin{aligned}\varepsilon &= \lambda \frac{\alpha + \beta}{2} \pm \sqrt{\left(E_0 - \lambda \frac{\alpha - \beta}{2}\right)^2 + \lambda^2 |u|^2} \\ &= \lambda \frac{\alpha + \beta}{2} \pm \left(E_0 - \lambda \frac{\alpha - \beta}{2}\right) \left(1 + \frac{1}{2} \frac{\lambda^2 |u|^2}{E_0^2} + \dots\right)\end{aligned}$$

(b) Consider now

$$H = \begin{pmatrix} E_0 & u \\ v & -E_0 \end{pmatrix}$$

where we have dropped the α and β terms. The eigenvalues are easy to determine, and they are

$$\varepsilon = \pm \sqrt{E_0^2 + \lambda^2 uv}$$

The eigenstates are written as $\begin{pmatrix} a \\ b \end{pmatrix}$ and they satisfy

$$\begin{pmatrix} E_0 & u \\ v & -E_0 \end{pmatrix} \begin{pmatrix} a \\ b \end{pmatrix} = \pm \sqrt{E_0^2 + \lambda^2 uv} \begin{pmatrix} a \\ b \end{pmatrix}$$

For the upper state we find that the un-normalized eigenstate is

$$\begin{pmatrix} \lambda u \\ \sqrt{E_0^2 + \lambda^2 uv} - E_0 \end{pmatrix}$$

For the lower state it is

$$\begin{pmatrix} -\lambda u \\ \sqrt{E_0^2 + \lambda^2 uv} + E_0 \end{pmatrix}$$

The scalar product

$$-\lambda^2 |u|^2 + \left[(E_0^2 + \lambda^2 uv) - E_0^2 \right] = \lambda^2 u(u^* - v) \neq 0$$

which shows that the eigenstates are not orthogonal unless $v = u^*$.

CHAPTER 12.

1. With a potential of the form

$$V(r) = \frac{1}{2} m \omega^2 r^2$$

the perturbation reduces to

$$\begin{aligned} H_1 &= \frac{1}{2m^2c^2} \mathbf{S} \cdot \mathbf{L} \frac{1}{r} \frac{dV(r)}{dr} = \frac{\omega^2}{4mc^2} (\mathbf{J}^2 - \mathbf{L}^2 - \mathbf{S}^2) \\ &= \frac{(\hbar\omega)^2}{4mc^2} (j(j+1) - l(l+1) - s(s+1)) \end{aligned}$$

where l is the orbital angular momentum, s is the spin of the particle in the well (e.g. $1/2$ for an electron or a nucleon) and j is the total angular momentum. The possible values of j are $l + s, l + s - 1, l + s - 2, \dots, |l - s|$.

The unperturbed energy spectrum is given by $E_{n_r, l} = \hbar\omega(2n_r + l + \frac{3}{2})$. Each of the levels characterized by l is $(2l + 1)$ -fold degenerate, but there is an additional degeneracy, not unlike that appearing in hydrogen. For example $n_r=2, l=0$, $n_r=1, l=2$, $n_r=0, l=4$ all have the same energy.

A picture of the levels and their spin-orbit splitting is given below.

2. The effects that enter into the energy levels corresponding to $n = 2$, are (I) the basic Coulomb interaction, (ii) relativistic and spin-orbit effects, and (iii) the hyperfine structure which we are instructed to ignore. Thus, in the absence of a magnetic field, the levels under the influence of the Coulomb potential consist of $2n^2 = 8$ degenerate levels. Two of the levels are associated with $l = 0$ (spin up and spin down) and six

levels with $l = 0$, corresponding to $m_l = 1, 0, -1$, spin up and spin down. The latter can be rearranged into states characterized by \mathbf{J}^2 , \mathbf{L}^2 and J_z . There are two levels characterized by $j = l - 1/2 = 1/2$ and four levels with $j = l + 1/2 = 3/2$. These energies are split by relativistic effects and spin-orbit coupling, as given in Eq. (12-16). We ignore reduced mass effects (other than in the original Coulomb energies). We therefore have

$$\begin{aligned}\Delta E &= -\frac{1}{2} m_e c^2 \alpha^4 \frac{1}{n^3} \left(\frac{1}{j+1/2} - \frac{3}{4n} \right) \\ &= -\frac{1}{2} m_e c^2 \alpha^4 \left(\frac{5}{64} \right) \quad j = 1/2 \\ &= -\frac{1}{2} m_e c^2 \alpha^4 \left(\frac{1}{64} \right) \quad j = 3/2\end{aligned}$$

(b) The Zeeman splittings for a given j are

$$\begin{aligned}\Delta E_B &= \frac{e\hbar B}{2m_e} m_j \left(\frac{2}{3} \right) \quad j = 1/2 \\ &= \frac{e\hbar B}{2m_e} m_j \left(\frac{4}{3} \right) \quad j = 3/2\end{aligned}$$

Numerically $\frac{1}{128} m_e c^2 \alpha^4 \approx 1.132 \times 10^{-5} eV$, while for $B = 2.5T$ $\frac{e\hbar B}{2m_e} = 14.47 \times 10^{-5} eV$,

so under these circumstances the magnetic effects are a factor of 13 larger than the relativistic effects. Under these circumstances one could neglect these and use Eq. (12-26).

3. The unperturbed Hamiltonian is given by Eq. (12-34) and the magnetic field interacts both with the spin of the electron and the spin of the proton. This leads to

$$H = A \frac{\mathbf{S} \cdot \mathbf{I}}{\hbar^2} + a \frac{S_z}{\hbar} + b \frac{I_z}{\hbar}$$

Here

$$\begin{aligned}A &= \frac{4}{3} \alpha^4 m_e c^2 g_p \left(\frac{m_e}{M_p} \right) \frac{\mathbf{I} \cdot \mathbf{S}}{\hbar^2} \\ a &= 2 \frac{e\hbar B}{2m_e} \\ b &= -g_p \frac{e\hbar B}{2M_p}\end{aligned}$$

Let us now introduce the total spin $\mathbf{F} = \mathbf{S} + \mathbf{I}$. It follows that

$$\begin{aligned}\frac{\mathbf{S} \cdot \mathbf{I}}{\hbar^2} &= \frac{1}{2\hbar^2} \left(\hbar^2 F(F+1) - \frac{3}{4} \hbar^2 - \frac{3}{4} \hbar^2 \right) \\ &= \frac{1}{4} \quad \text{for } F=1 \\ &= -\frac{3}{4} \quad \text{for } F=0\end{aligned}$$

We next need to calculate the matrix elements of $aS_z + bI_z$ for eigenstates of \mathbf{F}^2 and F_z . These will be exactly like the spin triplet and spin singlet eigenstates. These are

$$\langle 1,1 | aS_z + bI_z | 1,1 \rangle = \langle \chi_+ \xi_+ | aS_z + bI_z | \chi_+ \xi_+ \rangle = \frac{1}{2}(a+b)$$

$$\langle 1,0 | aS_z + bI_z | 1,0 \rangle = \left(\frac{1}{\sqrt{2}} \right)^2 \langle \chi_+ \xi_- + \chi_- \xi_+ | aS_z + bI_z | \chi_+ \xi_- + \chi_- \xi_+ \rangle = 0$$

$$\langle 1,-1 | aS_z + bI_z | 1,-1 \rangle = \langle \chi_- \xi_- | aS_z + bI_z | \chi_- \xi_- \rangle = -\frac{1}{2}(a+b)$$

And for the singlet state ($F=0$)

$$\langle 1,0 | aS_z + bI_z | 0,0 \rangle = \left(\frac{1}{\sqrt{2}} \right)^2 \langle \chi_+ \xi_- - \chi_- \xi_+ | aS_z + bI_z | \chi_+ \xi_- - \chi_- \xi_+ \rangle = \frac{1}{2}(a-b)$$

$$\langle 0,0 | aS_z + bI_z | 0,0 \rangle = \left(\frac{1}{\sqrt{2}} \right)^2 \langle \chi_+ \xi_- - \chi_- \xi_+ | aS_z + bI_z | \chi_+ \xi_- - \chi_- \xi_+ \rangle = 0$$

Thus the magnetic field introduces mixing between the $|1,0\rangle$ state and the $|0,0\rangle$ state. We must therefore diagonalize the submatrix

$$\begin{pmatrix} A/4 & (a-b)/2 \\ (a-b)/2 & -3A/4 \end{pmatrix} = \begin{pmatrix} -A/4 & 0 \\ 0 & -A/4 \end{pmatrix} + \begin{pmatrix} A/2 & (a-b)/2 \\ (a-b)/2 & -A/2 \end{pmatrix}$$

The second submatrix commutes with the first one. Its eigenvalues are easily determined to be $\pm \sqrt{A^2/4 + (a-b)^2/4}$ so that the overall eigenvalues are

$$-A/4 \pm \sqrt{A^2/4 + (a-b)^2/4}$$

Thus the spectrum consists of the following states:

$$F = 1, F_z = 1 \quad E = A/4 + (a + b)/2$$

$$F = 1, F_z = -1 \quad E = A/4 - (a + b)/2$$

$$F = 1, 0; F_z = 0 \quad E = -A/4 \pm \sqrt{(A^2/4 + (a - b)^2/4}$$

We can now put in numbers.

For $B = 10^{-4}$ T, the values, in units of 10^{-6} eV are 1.451, 1.439, $0(10^{-10})$, -2.89

For $B = 1$ T, the values in units of 10^{-6} eV are 57.21, -54.32, 54.29 and 7×10^{-6} .

4. According to Eq. (12-17) the energies of hydrogen-like states, including relativistic + spin-orbit contributions is given by

$$E_{n,j} = -\frac{1}{2} \frac{m_e c^2 (Z\alpha)^2}{(1 + m_e/M_p)} \frac{1}{n^2} - \frac{1}{2} m_e c^2 (Z\alpha)^4 \frac{1}{n^3} \left(\frac{1}{j + 1/2} - \frac{3}{4n} \right)$$

The wavelength in a transition between two states is given by

$$\lambda = \frac{2\pi\hbar c}{\Delta E}$$

where ΔE is the change in energy in the transition. We now consider the transitions $n=3, j=3/2 \rightarrow n=1, j=1/2$ and $n=3, j=1/2 \rightarrow n=1, j=1/2$. The corresponding energy differences (neglecting the reduced mass effect) is

$$(3, 3/2 \rightarrow 1, 1/2) \quad \Delta E = \frac{1}{2} m_e c^2 (Z\alpha)^2 \left(1 - \frac{1}{9}\right) + \frac{1}{2} m_e c^2 (Z\alpha)^4 \frac{1}{4} \left(1 - \frac{1}{27}\right)$$

$$(3, 1/2 \rightarrow 1, 1/2) \quad \frac{1}{2} m_e c^2 (Z\alpha)^2 \left(1 - \frac{1}{9}\right) + \frac{1}{2} m_e c^2 (Z\alpha)^4 \frac{1}{4} \left(1 - \frac{3}{27}\right)$$

We can write these in the form

$$(3, 3/2 \rightarrow 1, 1/2) \quad \Delta E_0 \left(1 + \frac{13}{48} (Z\alpha)^2\right)$$

$$(3, 1/2 \rightarrow 1, 1/2) \quad \Delta E_0 \left(1 + \frac{1}{18} (Z\alpha)^2\right)$$

where

$$\Delta E_0 = \frac{1}{2} m_e c^2 (Z\alpha)^2 \frac{8}{9}$$

The corresponding wavelengths are

$$(3,3/2 \rightarrow 1,1/2) \quad \lambda_0 \left(1 - \frac{13}{48} (Z\alpha)^2\right) = 588.995 \times 10^{-9} m$$

$$(3,1/2 \rightarrow 1,1/2) \quad \lambda_0 \left(1 - \frac{1}{18} (Z\alpha)^2\right) = 589.592 \times 10^{-9} m$$

We may use the two equations to calculate λ_0 and Z . Dividing one equation by the other we get, after a little arithmetic $Z = 11.5$, which fits with the $Z = 11$ for Sodium.

(Note that if we take for λ_0 the average of the two wavelengths, then, using $\lambda_0 = 2\pi\hbar c / \Delta E_0 = 9\pi\hbar / 2mc(Z\alpha)^2$, we get a seemingly unreasonably small value of $Z = 0.4$! This is not surprising. The ionization potential for sodium is 5.1 eV instead of $Z^2(13.6 \text{ eV})$, for reasons that will be discussed in Chapter 14)

4. The relativistic correction to the kinetic energy term is $-\frac{1}{2mc^2} \left(\frac{\mathbf{p}^2}{2m}\right)^2$. The energy shift in the ground state is therefore

$$\Delta E = -\frac{1}{2mc^2} \langle 0 | \left(\frac{\mathbf{p}^2}{2m}\right)^2 | 0 \rangle = -\frac{1}{2mc^2} \langle 0 | \left(H - \frac{1}{2} m \omega^2 r^2\right)^2 | 0 \rangle$$

To calculate $\langle 0 | r^2 | 0 \rangle$ and $\langle 0 | r^4 | 0 \rangle$ we need the ground state wave function. We know that for the one-dimensional oscillator it is

$$u_0(x) = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} e^{-m\omega x^2/2\hbar}$$

so that for the three dimensional oscillator it is

$$u_0(r) = u_0(x)u_0(y)u_0(z) = \left(\frac{m\omega}{\pi\hbar}\right)^{3/4} e^{-m\omega r^2/2\hbar}$$

It follows that

$$\begin{aligned} \langle 0 | r^2 | 0 \rangle &= \int_0^\infty 4\pi r^2 dr \left(\frac{m\omega}{\pi\hbar}\right)^{3/2} r^2 e^{-m\omega r^2/\hbar} = \\ &= 4\pi \left(\frac{m\omega}{\pi\hbar}\right)^{3/2} \left(\frac{\hbar}{m\omega}\right)^{5/2} \int_0^\infty dy y^4 e^{-y^2} \\ &= \frac{3\hbar}{2m\omega} \end{aligned}$$

We can also calculate

$$\begin{aligned}\langle 0 | r^4 | 0 \rangle &= \int_0^\infty 4\pi r^2 dr \left(\frac{m\omega}{\pi\hbar} \right)^{3/2} r^4 e^{-m\omega r^2/\hbar} = \\ &= 4\pi \left(\frac{m\omega}{\pi\hbar} \right)^{3/2} \left(\frac{\hbar}{m\omega} \right)^{7/2} \int_0^\infty dy y^6 e^{-y^2} \\ &= \frac{15}{4} \left(\frac{\hbar}{m\omega} \right)^2\end{aligned}$$

We made use of $\int_0^\infty dz z^n e^{-z} = \Gamma(n+1) = n\Gamma(n)$ and $\Gamma\left(\frac{1}{2}\right) = \sqrt{\pi}$

Thus

$$\begin{aligned}\Delta E &= -\frac{1}{2mc^2} \left(\left(\frac{3}{2} \hbar\omega \right)^2 - \left(\frac{3}{2} \hbar\omega \right) \left(m\omega^2 \frac{3\hbar}{2m\omega} \right) + \frac{1}{4} m^2 \omega^4 \left(\frac{15}{4} \right) \left(\frac{\hbar}{m\omega} \right)^2 \right) \\ &= -\frac{15}{32} \frac{(\hbar\omega)^2}{mc^2}\end{aligned}$$

6. (a) With $J = 1$ and $S = 1$, the possible values of the orbital angular momentum, such that $j = L + S, L + S - 1, \dots, |L - S|$ can only be $L = 0, 1, 2$. Thus the possible states are ${}^3S_1, {}^3P_1, {}^3D_1$. The parity of the deuteron is $(-1)^L$ assuming that the intrinsic parities of the proton and neutron are taken to be $+1$. Thus the S and D states have positive parity and the P state has opposite parity. Given parity conservation, the only possible admixture can be the 3D_1 state.

(b) The interaction with a magnetic field consists of three contributions: the interaction of the spins of the proton and neutron with the magnetic field, and the $\mathbf{L} \cdot \mathbf{B}$ term, if L is not zero. We write

$$H = -\mathbf{M}_p \cdot \mathbf{B} - \mathbf{M}_n \cdot \mathbf{B} - \mathbf{M}_L \cdot \mathbf{B}$$

$$\mathbf{M}_p = \frac{eg_p}{2M} \mathbf{S}_p = (5.5792) \frac{e\hbar}{2M} \left(\frac{\mathbf{S}_p}{\hbar} \right)$$

$$\text{where } \mathbf{M}_n = \frac{eg_n}{2M} \mathbf{S}_n = (-3.8206) \frac{e\hbar}{2M} \left(\frac{\mathbf{S}_n}{\hbar} \right)$$

$$\mathbf{M}_L = \frac{e}{2M_{red}} \mathbf{L}$$

We take the neutron and proton masses equal ($= M$) and the reduced mass of the two-particle system for equal masses is $M/2$. For the 3S_1 state, the last term does not contribute.

If we choose \mathbf{B} to define the z axis, then the energy shift is

$$-\frac{eB\hbar}{2M} \langle {}^3S_1 | g_p \left(\frac{S_{pz}}{\hbar} \right) + g_n \left(\frac{S_{nz}}{\hbar} \right) | {}^3S_1 \rangle$$

We write

$$g_p \left(\frac{S_{pz}}{\hbar} \right) + g_n \left(\frac{S_{nz}}{\hbar} \right) = \frac{g_p + g_n}{2} \frac{S_{pz} + S_{nz}}{\hbar} + \frac{g_p - g_n}{2} \frac{S_{pz} - S_{nz}}{\hbar}$$

It is easy to check that the last term has zero matrix elements in the triplet states, so that we are left with $\frac{1}{2}(g_p + g_n) \frac{S_z}{\hbar}$, where S_z is the z -component of the total spin.. Hence

$$\langle {}^3S_1 | H_1 | {}^3S_1 \rangle = -\frac{3B\hbar}{2M} \frac{g_p + g_n}{2} m_s$$

where m_s is the magnetic quantum number ($m_s = 1, 0, -1$) for the total spin. We may therefore write the magnetic moment of the deuteron as

$$\mu_{eff} = -\frac{e}{2M} \frac{g_p + g_n}{2} \mathbf{S} = -(0.8793) \frac{e}{2M} \mathbf{S}$$

The experimental measurements correspond to $g_d = 0.8574$ which suggests a small admixture of the 3D_1 to the deuteron wave function.

CHAPTER 13

1. (a) electron-proton system $m_r = \frac{m_e}{1 + m_e / M_p} = (1 - 5.45 \times 10^{-4})m_e$
- (b) electron-deuteron system $m_r = \frac{m_e}{1 + m_e / M_d} = (1 - 2.722 \times 10^{-4})m_e$
- (c) For two identical particles of mass m , we have $m_r = \frac{m}{2}$

2. One way to see that P_{12} is hermitian, is to note that the eigenvalues ± 1 are both real. Another way is to consider

$$\begin{aligned} \sum_{i,j} \int dx_1 dx_2 \psi_{ij}^*(x_1, x_2) P_{12} \psi_{ij}(x_1, x_2) &= \\ \sum_{i,j} \int dx_1 dx_2 \psi_{ij}^*(x_1, x_2) \psi_{ji}(x_2, x_1) &= \\ \sum_{j,i} \int dy_1 dy_2 \psi_{ji}^*(y_2, y_1) \psi_{ij}(y_1, y_2) &= \sum_{j,i} \int dy_1 dy_2 (P_{12} \psi_{ij}(y_1, y_2))^* \psi_{ij}(y_1, y_2) \end{aligned}$$

3. If the two electrons are in the same spin state, then the spatial wave function must be antisymmetric. One of the electrons can be in the ground state, corresponding to $n = 1$, but the other must be in the next lowest energy state, corresponding to $n = 2$. The wave function will be

$$\psi_{ground}(x_1, x_2) = \frac{1}{\sqrt{2}} (u_1(x_1)u_2(x_2) - u_2(x_1)u_1(x_2))$$

4. The energy for the n -th level is $E_n = \frac{\hbar^2 \pi^2}{2ma^2} n^2 \equiv \varepsilon n^2$

Only two electrons can go into a particular level, so that with N electrons, the lowest $N/2$ levels must be filled. The energy thus is

$$E_{tot} = \sum_{n=1}^{N/2} 2\varepsilon n^2 \approx 2\varepsilon \frac{1}{3} \left(\frac{N}{2}\right)^3 = \frac{\varepsilon N^3}{12}$$

If N is odd, then the above is uncertain by a factor of εN^2 which differs from the above by $(12/N)\varepsilon$, a small number if N is very large.

5. The problem is one of two electrons interacting with each other. The form of the interaction is a square well potential. The reduction of the two-body problem to a one-particle system is straightforward. With the notation

$x = x_1 - x_2; X = \frac{x_1 + x_2}{2}; P = p_1 + p_2$, the wave function has the form $\psi(x_1, x_2) = e^{iPx} u(x)$, where $u(x)$ is a solution of

$$-\frac{\hbar^2}{m} \frac{d^2 u(x)}{dx^2} + V(x)u(x) = Eu(x)$$

Note that we have taken into account the fact that the reduced mass is $m/2$. The spatial interchange of the two electrons corresponds to the exchange $x \rightarrow -x$. Let us denote the lowest bound state wave function by $u_0(x)$ and the next lowest one by $u_1(x)$. We know that the lowest state has even parity, that means, it is even under the above interchange, while the next lowest state is odd under the interchange. Hence, for the two electrons in a spin singlet state, the spatial symmetry must be even, and therefore the state is $u_0(x)$, while for the spin triplet states, the spatial wave function is odd, that is, $u_1(x)$.

6. With $P = p_1 + p_2; p = \frac{1}{2}(p_1 - p_2); X = \frac{1}{2}(x_1 + x_2); x = x_1 - x_2$, the Hamiltonian becomes

$$H = \frac{P^2}{2M} + \frac{1}{2} M\omega^2 X^2 + \frac{p^2}{2\mu} + \frac{1}{2} \mu\omega^2 x^2$$

with $M = 2m$ the total mass of the system, and $\mu = m/2$ the reduced mass. The energy spectrum is the sum of the energies of the oscillator describing the motion of the center of mass, and that describing the relative motion. Both are characterized by the same angular frequency ω so that the energy is

$$E = \hbar\omega(N + \frac{1}{2}) + \hbar\omega(n + \frac{1}{2}) = \hbar\omega(N + n + 1) \equiv \hbar\omega(\nu + 1)$$

The degeneracy is given by the number of ways the integer ν can be written as the sum of two non-negative integers. Thus, for a given ν we can have

$$(N, n) = (\nu, 0), (\nu-1, 1), (\nu-2, 2), \dots, (1, \nu-1), (0, \nu)$$

so that the degeneracy is $\nu + 1$.

Note that if we treat the system as two independent harmonic oscillators characterized by the same frequency, then the energy takes the form

$$E = \hbar\omega(n_1 + \frac{1}{2}) + \hbar\omega(n_2 + \frac{1}{2}) = \hbar\omega(n_1 + n_2 + 1) \equiv \hbar\omega(\nu + 1)$$

which is the same result, as expected.

7. When the electrons are in the same spin state, the spatial two-electron wave function must be antisymmetric under the interchange of the electrons. Since the two electrons do not interact, the wave function will be a product of the form

$$\frac{1}{\sqrt{2}}(u_n(x_1)u_k(x_2) - u_k(x_1)u_n(x_2))$$

with energy $E = E_n + E_k = \frac{\hbar^2 \pi^2}{2ma^2}(n^2 + k^2)$. The lowest state corresponds to $n = 1$, $k = 2$, with $n^2 + k^2 = 5$. The first excited state would normally be the (2,2) state, but this is not antisymmetric, so that we must choose (1,3) for the quantum numbers.

8. The antisymmetric wave function is of the form

$$\begin{aligned} N \frac{\pi}{\mu^2} & \left(e^{-\mu^2(x_1-a)^2/2} e^{-\mu^2(x_2+a)^2/2} - e^{-\mu^2(x_1+a)^2/2} e^{-\mu^2(x_2-a)^2/2} \right) \\ & = N \frac{\pi}{\mu^2} e^{-\mu^2 a^2} e^{-\mu^2(x_1^2+x_2^2)/2} \left(e^{-\mu^2(x_2-x_1)a} - e^{-\mu^2(x_1-x_2)a} \right) \end{aligned}$$

Let us introduce the center of mass variable X and the separation x by

$$x_1 = X + \frac{x}{2}; \quad x_2 = X - \frac{x}{2}$$

The wave function then becomes

$$\psi = 2N \frac{\pi}{\mu^2} e^{-\mu^2 a^2} e^{-\mu^2 X^2} e^{-\mu^2 x^2/4} \sinh \mu^2 a x$$

To normalize, we require

$$\int_{-\infty}^{\infty} dX \int_{-\infty}^{\infty} dx |\psi|^2 = 1$$

Some algebra leads to the result that

$$N \frac{\pi}{\mu^2} = \frac{1}{\sqrt{2}} \frac{1}{\sqrt{1 - e^{-2\mu^2 a^2}}}$$

The second factor is present because of the overlap. If we want this to be within 1 part in a 1000 away from 1, then we require that $e^{-2(\mu a)^2} \approx 1/500$, i.e. $\mu a = 1.76$, or $a = 0.353$

$$\text{nm } R_{fi} = \frac{4}{\pi} (Z\alpha)^3 \frac{d^2}{a_0^2} \sqrt{\frac{mc^2}{2\Delta E}} \frac{mc^2}{\hbar}.$$

.

9. Since

$$\psi = \sqrt{2} \frac{e^{-(\mu a)^2}}{\sqrt{1 - e^{-2(\mu a)^2}}} e^{-(\mu X)^2} e^{-(\mu a)^2/4} \sinh \mu^2 ax$$

the probability density for x is obtained by integrating the square of ψ over all X . This is a simple Gaussian integral, and it leads to

$$P(x)dx = \frac{2e^{-2(\mu a)^2}}{1 - e^{-2(\mu a)^2}} \sqrt{\frac{\pi}{2}} \frac{1}{\mu} e^{-(\mu x)^2/2} \sinh^2(\mu^2 ax) dx$$

It is obvious that

$$\langle X \rangle = \int_{-\infty}^{\infty} dX X e^{-2(\mu X)^2} = 0$$

since the integrand is an odd function of X .

10. If we denote μx by y , then the relevant quantities in the plot are $e^{-y^2/2} \sinh^2 2y$ and $e^{-y^2/2} \sinh^2(y/2)$.

11. Suppose that the particles are bosons. Spin is irrelevant, and the wave function for the two particles is symmetric. The changes are minimal. The wave function is

$$\psi = 2N \frac{\pi}{\mu^2} e^{-\mu^2 a^2} e^{-\mu^2 X^2} e^{-\mu^2 x^2/4} \cosh \mu^2 xa$$

with

$$N \frac{\mu^2}{\pi} = \frac{1}{\sqrt{2}} \frac{1}{\sqrt{1 + e^{-2\mu^2 a^2}}}$$

and

$$P(x) = \frac{2e^{-2\mu^2 a^2}}{1 + e^{-2\mu^2 a^2}} \frac{\sqrt{\pi}}{\mu\sqrt{2}} e^{-\mu^2 x^2/2} \cosh^2(\mu^2 ax)$$

The relevant form is now $P(y) = e^{-y^2/2} \cosh^2 \kappa y$ which peaks at $y = 0$ and has extrema at

$-y \cosh \kappa y + 2\kappa \sinh \kappa y = 0$, that is, when

$$\tanh \kappa y = y / 2\kappa$$

which only happens if $2\kappa^2 > 1$. Presumably, when the two centers are close together, then the peak occurs in between; if they are far apart, there is a slight rise in the middle, but most of the time the particles are around their centers at $\pm a$.

12. The calculation is almost unchanged. The energy is given by

$$E = pc = \frac{\hbar \pi c}{L} \sqrt{n_1^2 + n_2^2 + n_3^2}$$

so that in Eq. (13-58)

$$R^2 = \sqrt{n_1^2 + n_2^2 + n_3^2} = (E_F / \hbar c \pi)^2 L^2$$

Thus

$$N = \frac{\pi}{3} \left(\frac{E_F L}{\pi \hbar c} \right)^3$$

and

$$E_F = \pi \hbar c \left(\frac{3n}{\pi} \right)^{1/3}$$

13. The number of triplets of positive integers $\{n_1, n_2, n_3\}$ such that

$$n_1^2 + n_2^2 + n_3^2 = R^2 = \frac{2mE}{\hbar^2 \pi^2} L^2$$

is equal to the numbers of points that lie on an octant of a sphere of radius R , within a thickness of $\Delta n = 1$. We therefore need $\frac{1}{8} 4\pi R^2 dR$. To translate this into E we use $2RdR = (2mL^2 / \hbar^2 \pi^2) dE$. Hence the degeneracy of states is

$$N(E)dE = 2 \times \frac{1}{8} 4\pi R(RdR) = L^3 \frac{m\sqrt{2m}}{\hbar^3 \pi^2} \sqrt{E} dE$$

To get the electron density we had to multiply by 2 to take into account that there are two electrons per state.

14. Since the photons are massless, and there are two photon states per energy state, this problem is identical to problem 12. We thus get

$$n_1^2 + n_2^2 + n_3^2 = R^2 = \left(\frac{E}{\hbar\pi c} \right)^2 L^2$$

or $R = EL / \hbar\pi c$. Hence

$$N(E)dE = \frac{1}{8} 4\pi R^2 dE = L^3 \frac{E^2}{\hbar^3 c^3 \pi^2} dE$$

15. The eigenfunctions for a particle in a box of sides L_1, L_2, L_3 are of the form of a product

$$u(x, y, z) = \sqrt{\frac{8}{L_1 L_2 L_3}} \sin \frac{n_1 \pi x}{L_1} \sin \frac{n_2 \pi y}{L_2} \sin \frac{n_3 \pi z}{L_3}$$

and the energy for a massless particle, for which $E = pc$ is

$$E = \hbar c \pi \sqrt{\frac{n_1^2}{L_1^2} + \frac{n_2^2}{L_2^2} + \frac{n_3^2}{L_3^2}} = \hbar c \pi \sqrt{\frac{n_1^2 + n_2^2}{a^2} + \frac{n_3^2}{L^2}}$$

Note that $a \ll L$. thus the low-lying states will have $n_1 = n_2 = 1$, with n_3 ranging from 1 upwards. At some point the two levels $n_1 = 2, n_2 = 1$ and $n_1 = 1, n_2 = 2$ will provide a new “platform” upon which $n_3 = 1, 2, 3, \dots$ are stacked. With $a = 1$ nm and $L = 10^3$ nm, for $n_1 = n_2 = 1$ the n_3 values can go up to 10^3 before the new platform starts.

16. For nonrelativistic particles we have

$$E = \frac{\hbar^2}{2m} \left(\frac{n_1^2 + n_2^2}{a^2} + \frac{n_3^2}{L^2} \right)$$

17. We have

$$E_F = \frac{\hbar^2 \pi^2}{2M} \left(\frac{3n}{\pi} \right)^{2/3}$$

where M is the nucleon mass, taken to be the same for protons and for neutrons, and where n is the *number density*. Since there are Z protons in a volume $\frac{4\pi}{3} r_0^3 A$, the number densities for protons and neutrons are

$$n_p = \frac{3}{4\pi r_0^3} \frac{Z}{A}; \quad n_n = \frac{3}{4\pi r_0^3} \frac{A-Z}{A}$$

Putting in numbers, we get

$$E_{Fp} = 65 \left(\frac{Z}{A} \right)^{2/3} \text{ MeV}; \quad E_{Fn} = 65 \left(1 - \frac{Z}{A} \right)^{2/3} \text{ MeV}$$

For $A = 208$, $Z = 82$ these numbers become $E_{Fp} = 35 \text{ MeV}$; $E_{Fn} = 47 \text{ MeV}$.

CHAPTER 14

1. The spin-part of the wave function is the triplet

$$\begin{aligned} m_s = 1 & \quad \chi_+^{(1)} \chi_+^{(2)} \\ m_s = 0 & \quad \frac{1}{\sqrt{2}} (\chi_+^{(1)} \chi_-^{(2)} + \chi_-^{(1)} \chi_+^{(2)}) \\ m_s = -1 & \quad \chi_-^{(1)} \chi_-^{(2)} \end{aligned}$$

This implies that the spatial part of the wave function must be antisymmetric under the interchange of the coordinates of the two particles. For the lowest energy state, one of the electrons will be in an $n = 1, l = 0$ state. The other will be in an $n = 2, l = 1$, or $l = 0$ state. The possible states are

$$\begin{aligned} & \frac{1}{\sqrt{2}} (u_{100}(\mathbf{r}_1) u_{21m}(\mathbf{r}_2) - u_{100}(\mathbf{r}_2) u_{21m}(\mathbf{r}_1)) \quad m = 1, 0, -1 \\ & \frac{1}{\sqrt{2}} (u_{100}(\mathbf{r}_1) u_{200}(\mathbf{r}_2) - u_{100}(\mathbf{r}_2) u_{200}(\mathbf{r}_1)) \end{aligned}$$

Thus the total number of states with energy $E_2 + E_1$ is $3 \times 4 = 12$

2. For the triplet state, the first order perturbation energy shifts are given by

$$\begin{aligned} \Delta E_{21m} &= \iint d^3 r_1 d^3 r_2 \left| \frac{1}{\sqrt{2}} (u_{100}(\mathbf{r}_1) u_{21m}(\mathbf{r}_2) - u_{100}(\mathbf{r}_2) u_{21m}(\mathbf{r}_1)) \right|^2 \frac{e^2}{4\pi\epsilon_0 |\mathbf{r}_1 - \mathbf{r}_2|} \\ \Delta E_{200} &= \iint d^3 r_1 d^3 r_2 \left| \frac{1}{\sqrt{2}} (u_{100}(\mathbf{r}_1) u_{200}(\mathbf{r}_2) - u_{100}(\mathbf{r}_2) u_{200}(\mathbf{r}_1)) \right|^2 \frac{e^2}{4\pi\epsilon_0 |\mathbf{r}_1 - \mathbf{r}_2|} \end{aligned}$$

The $l = 1$ energy shift uses two-electron wave functions that have an orbital angular momentum 1. There is no preferred direction in the problem, so that there cannot be any dependence on the eigenvalue of L_z . Thus all three m values have the same energy. The $l = 0$ energy shift uses different wave functions, and thus the degeneracy will be split. Instead of a 12-fold degeneracy we will have a splitting into $9 + 3$ states.

The simplification of the energy shift integrals reduces to the simplification of the integrals in the second part of Eq. (14-29). The working out of this is messy, and we only work out the $l = 1$ part.

The integrals $\iint d^3 r_1 d^3 r_2 \rightarrow \int_0^\infty r_1^2 dr_1 \int_0^\infty r_2^2 dr_2 \int d\Omega_1 \int d\Omega_2$ and the angular parts only come through the u_{210} wave function and through the $1/r_{12}$ term. We use Eqs. (14-26) – (14-29) to get, for the direct integral

$$\frac{e^2}{4\pi\epsilon_0} \int_0^\infty r_1^2 dr_1 \int_0^\infty r_2^2 dr_2 R_{10}(r_1)^2 R_{21}(r_2)^2$$

$$\int d\Omega_1 \int d\Omega_2 \left(\frac{1}{\sqrt{4\pi}} \right)^2 \left(\sqrt{\frac{3}{4\pi}} \cos\theta_2 \right)^2 \sum_L P_L(\cos\theta_{12}) \frac{r_{<}^L}{r_{>}^{L+1}}$$

where θ_{12} is the angle between \mathbf{r}_1 and \mathbf{r}_2 . We make use of an addition theorem which reads

$$P_L(\cos\theta_{12}) = P_L(\cos\theta_1)P_L(\cos\theta_2)$$

$$+ 2 \sum_{m=1}^L \frac{(L-m)!}{(L+m)!} P_L^m(\cos\theta_1)P_L^m(\cos\theta_2) \cos m\phi_2 \frac{r_{<}^L}{r_{>}^{L+1}}$$

Since the sum is over $m = 1, 2, 3, \dots$ the integration over ϕ_2 eliminates the sum, and for all practical purposes we have

$$\sum_L P_L(\cos\theta_{12}) \frac{r_{<}^L}{r_{>}^{L+1}} = \sum_L P_L(\cos\theta_1)P_L(\cos\theta_2) \frac{r_{<}^L}{r_{>}^{L+1}}$$

The integration over $d\Omega_1$ yields $4\pi\delta_{L0}$ and in our integral we are left with

$\int d\Omega_2 (\cos\theta_2)^2 = 4\pi/3$. The net effect is to replace the sum by $1/r_{>}$ to be inserted into the radial integral.

(b) For the exchange integral has the following changes have to be made: In the radial integral,

$$R_{10}(r_1)^2 R_{21}(r_2)^2 \rightarrow R_{10}(r_1)R_{21}(r_1)R_{10}(r_2)R_{21}(r_2)$$

In the angular integral

$$\frac{1}{4\pi} \frac{3}{4\pi} (\cos\theta_2)^2 \rightarrow \frac{3}{(4\pi)^2} \cos\theta_1 \cos\theta_2$$

In the azimuthal integration again the $m \neq 0$ terms disappear, and in the rest there is a product of two integrals of the form

$$\int d\Omega \sqrt{\frac{3}{4\pi}} \cos\theta P_L(\cos\theta) = \sqrt{\frac{4\pi}{3}} \delta_{L1}$$

The net effect is that the sum is replaced by $\frac{1}{3} \frac{r_{<}}{r_{>}^2}$ inserted into the radial integral.

For the $l = 0$ case the same procedure will work, leading to

$$\frac{e^2}{4\pi\epsilon_0} \int_0^\infty r_1^2 dr_1 \int_0^\infty r_2^2 dr_2 \frac{1}{r_>} [R_{10}(r_1)R_{20}(r_2) \mathbf{I} [R_{10}(r_1)R_{20}(r_2) - R_{10}(r_2)R_{20}(r_1)]]$$

The radial integrals are actually quite simple, but there are many terms and the calculation is tedious, without teaching us anything about physics.

To estimate which of the $(l=0, l=0)$ or the $(l=0, l=1)$ antisymmetric combinations has a lower energy we approach the problem physically. In the two-electron wave function, one of the electrons is in the $n=1, l=0$ state. The other electron is in an $n=2$ state. Because of this, the wave function is pushed out somewhat. There is nevertheless some probability that the electron can get close to the nucleus. This probability is larger for the $l=0$ state than for the $l=1$ state. We thus expect that the state in which both electrons have zero orbital angular momentum is the lower-lying state.

3. In the ground state of ortho-helium, both electrons have zero orbital angular momentum. Thus the only contributions to the magnetic moment come from the electron spin. An electron interacts with the magnetic field according to

$$H = -\frac{ge}{2m_e} \mathbf{s}_1 \cdot \mathbf{B} - \frac{ge}{2m_e} \mathbf{s}_2 \cdot \mathbf{B} = -\frac{ge}{2m_e} \mathbf{S} \cdot \mathbf{B}$$

The value of g is 2, and thus coefficient of B takes on the values $-\frac{e\hbar}{2m_e} m_1$, where $m_1 = 1, 0, -1$.

4. We assume that ψ is properly normalized, and is of the form

$$|\psi\rangle = |\psi_0\rangle + \varepsilon |\chi\rangle$$

The normalization condition implies that

$$\langle \psi | \psi \rangle = 1 = \langle \psi_0 | \psi_0 \rangle + \varepsilon^* \langle \chi | \psi_0 \rangle + \varepsilon \langle \psi_0 | \chi \rangle + \varepsilon \varepsilon^* \langle \chi | \chi \rangle$$

so that

$$\varepsilon^* \langle \chi | \psi_0 \rangle + \varepsilon \langle \psi_0 | \chi \rangle + \varepsilon \varepsilon^* \langle \chi | \chi \rangle = 0$$

Now

$$\begin{aligned} \langle \psi | H | \psi \rangle &= \langle \psi_0 + \varepsilon \chi | H | \psi_0 + \varepsilon \chi \rangle \\ &= E_0 + \varepsilon^* E_0 \langle \chi | \psi_0 \rangle + \varepsilon E_0 \langle \psi_0 | \chi \rangle + |\varepsilon|^2 \langle \chi | H | \chi \rangle \\ &= E_0 + |\varepsilon|^2 \langle \chi | H - E_0 | \chi \rangle \end{aligned}$$

where use has been made of the normalization condition. Thus the expectation value of H differs from the exact value by terms of order $|\epsilon|^2$.

5. We need to calculate

$$E(\alpha) = \frac{\int_0^\infty 4\pi r^2 dr e^{-\alpha r} \left[-\frac{\hbar^2}{2m} \left(\frac{d^2}{dr^2} + \frac{2}{r} \frac{d}{dr} \right) + \frac{1}{2} m\omega^2 r^2 \right] e^{-\alpha r}}{\int_0^\infty 4\pi r^2 dr e^{-2\alpha r}}$$

With a little algebra, and using $\int_0^\infty dy y^n e^{-y} = n!$, we end up with

$$E(\alpha) = \frac{\hbar^2 \alpha^2}{2m} + \frac{3m\omega^2}{2\alpha^2}$$

This takes its minimum value when $dE(\alpha)/d\alpha = 0$. This is easily worked out, and leads to $\alpha^2 = \sqrt{3}m\omega/\hbar$. When this is substituted into $E(\alpha)$ we get

$$E_{min} = \sqrt{3}\hbar\omega$$

The true ground state energy is bound to lie below this value. The true value is $\frac{3}{2}\hbar\omega$ so that our result is pretty good.

4. The Schrodinger equation for a bound state in an attractive potential, with $l = 0$ reads

$$-\frac{\hbar^2}{2m} \left(\frac{d^2}{dr^2} + \frac{2}{r} \frac{d}{dr} \right) \psi(r) - |V_0| f\left(\frac{r}{r_0}\right) \psi(r) = -E_B \psi(r)$$

With the notation $x = r/r_0$, $u_0(x) = x \psi(x)$, $\lambda = 2m|V_0|r_0^2/\hbar^2$; $\alpha^2 = 2mE_B r_0^2/\hbar^2$ this becomes

$$\frac{d^2 u_0(x)}{dx^2} - \alpha^2 u_0(x) + \lambda f(x) u_0(x) = 0$$

Consider, now an arbitrary function $w(x)$ which satisfies $w(0) = 0$ (like $u_0(0)$), and define

$$\eta[w] = \frac{\int_0^\infty dx \left(\left(\frac{dw(x)}{dx} \right)^2 + \alpha^2 w^2(x) \right)}{\int_0^\infty dx f(x) w^2(x)}$$

We are asked to prove that if $\eta = \lambda + \delta\lambda$ and $w(x) = u_0(x) + \delta u(x)$, then as $\delta u(x) \rightarrow 0$, $\delta\lambda \rightarrow 0$. We work to first order in $\delta u(x)$ only. Then the right hand side of the above equation, written in abbreviated form becomes

$$\frac{\int (u_0'^2 + \alpha^2 u_0^2) + 2 \int (u_0' \delta u' + \alpha^2 u_0 \delta u)}{\int f(u_0^2 + 2u_0 \delta u)} =$$

$$= \frac{\int (u_0'^2 + \alpha^2 u_0^2)}{\int f u_0^2} - 2 \frac{\int (u_0' \delta u' + \alpha^2 u_0 \delta u)}{\int f u_0^2} \frac{\int (u_0'^2 + \alpha^2 u_0^2)}{\int f u_0^2}$$

In the above, the first term is just $\eta[u_0]$, and it is easy to show that this is just λ . The same form appears in the second term. For the first factor in the second term we use

$$\int dx (u_0' \delta u') = \int dx \frac{d}{dx} (u_0' \delta u) - \int dx u_0'' \delta u$$

The first term on the right vanishes because the eigenfunction vanishes at infinity and because $\delta u(0) = 0$. Thus the second term in the equation for $\eta[w]$ becomes

$$\frac{2}{\int f u_0^2} \int \delta u [-u_0'' + \alpha^2 u_0 - \lambda f u_0]$$

Thus $\eta \rightarrow \lambda$ as $\delta u \rightarrow 0$.

5. We want to minimize $\langle \psi | H | \psi \rangle = \sum_{i,j} a_i^* H_{ij} a_j$ subject to the condition that $\langle \psi | \psi \rangle = \sum_i a_i^* a_i = 1$. The method of Lagrange multipliers instructs us to minimize

$$F(a_i^*, a_i) = \sum_{ij} a_i^* H_{ij} a_j - \lambda \sum_i a_i^* a_i$$

The condition is that $\partial F / \partial a_i^* = 0$. The condition implies that

$$\sum_j H_{ij} a_j = \lambda a_i$$

Similarly $\partial F / \partial a_i = 0$ implies that

$$\sum_i a_i^* H_{ij} = \lambda a_j^*$$

Thus the minimization condition yields solutions of an eigenvalue equation for H .

6. Consider the expectation value of H evaluated with the normalized trial wave function

$$\psi(x) = \left(\frac{\beta}{\sqrt{\pi}} \right)^{1/2} e^{-\beta^2 x^2 / 2}$$

Then an evaluation of the expectation value of H yields, after some algebra,

$$\begin{aligned} E(\beta) &= \int_{-\infty}^{\infty} dx \psi^*(x) \left(-\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + V(x) \right) \psi(x) \\ &= \frac{\beta}{\sqrt{\pi}} \int_{-\infty}^{\infty} dx \left(\frac{\hbar^2}{2m} (\beta^2 - \beta^4 x^2) e^{-\beta^2 x^2} \right) + \frac{\beta}{\sqrt{\pi}} \int_{-\infty}^{\infty} dx V(x) e^{-\beta^2 x^2} \\ &= \frac{\hbar^2 \beta^2}{2m} + \frac{\beta}{\sqrt{\pi}} \int_{-\infty}^{\infty} dx V(x) e^{-\beta^2 x^2} \end{aligned}$$

The question is: can we find a value of β such that this is negative. If so, then the true value of the ground state energy will necessarily be more negative. We are given the fact that the potential is attractive, that is, $V(x)$ is never positive. We write $V(x) = -|V(x)|$ and ask whether we can find a value of β such that

$$\frac{\beta}{\sqrt{\pi}} \int_{-\infty}^{\infty} dx |V(x)| e^{-\beta^2 x^2} > \frac{\hbar^2 \beta^2}{2m}$$

For any given $|V(x)|$ we can always find a square “barrier” that is contained in the positive form of $|V(x)|$. If the height of that barrier is V_0 and it extends from $-a$ to $+a$, for example, then the left side of the above equation is always *larger than*

$$L(\beta) = \frac{\beta}{\sqrt{\pi}} V_0 \int_{-a}^a dx e^{-\beta^2 x^2}$$

Our question becomes: Can we find a β such that

$$\frac{4m}{\hbar^2} L(\beta) > \beta^2$$

It is clear that for small β such that $\beta^2 a^2 \ll 1$, the left hand side is approximated by $2a \frac{\beta}{\sqrt{\pi}} \frac{4mV_0}{\hbar^2}$. This is linear in β so that we can always find a β small enough so that the left hand side is larger than the right hand side.

7. The data indicates a resonance corresponding to a wavelength of 20.61 nm. This corresponds to an energy of

$$h \frac{c}{\lambda} = \frac{2\pi(1.054 \times 10^{-34} \text{ J s})(3 \times 10^8 \text{ m/s})}{(20.61 \times 10^{-9} \text{ m})(1.602 \times 10^{-19} \text{ J/eV})} = 60.17 \text{ eV}$$

above the ground state. The ground state has energy -78.98 eV , while the ground state of He^+ has a binding energy of a hydrogenlike atom with $Z=2$, that is, 54.42 eV . This means that the ionization energy of He is $(78.98-54.42)\text{eV} = 24.55 \text{ eV}$ above the ground state. Thus when the $(2s)(2p)$ state decays into He^+ and an electron, the electron has an energy of $(60.17 - 24.55)\text{eV} = 35.62 \text{ eV}$. This translates into

$$v = \sqrt{2E / m} = 3.54 \times 10^6 \text{ m/s}.$$

The first excited state of the He^+ ion lies $54.42(1-1/4)=40.82 \text{ eV}$ above the ground state of He^+ , and this is *above* the $(2s)(2p)$ state.

8. To calculate the minimum of

$$E(\alpha_1, \alpha_2, \dots) = \frac{\langle \psi(\alpha_1, \alpha_2, \dots) | H | \psi(\alpha_1, \alpha_2, \dots) \rangle}{\langle \psi(\alpha_1, \alpha_2, \dots) | \psi(\alpha_1, \alpha_2, \dots) \rangle}$$

we set $\partial E / \partial \alpha_i = 0$, $i = 1, 2, 3, \dots$. This implies that

$$\frac{\langle \frac{\partial \psi}{\partial \alpha_i} | H | \psi \rangle + \langle \psi | H | \frac{\partial \psi}{\partial \alpha_i} \rangle}{\langle \psi | \psi \rangle} - \frac{\langle \psi | H | \psi \rangle \left(\langle \frac{\partial \psi}{\partial \alpha_i} | \psi \rangle + \langle \psi | \frac{\partial \psi}{\partial \alpha_i} \rangle \right)}{\langle \psi | \psi \rangle^2} = 0$$

This is equivalent to

$$\begin{aligned} \langle \frac{\partial \psi}{\partial \alpha_i} | H | \psi \rangle + \langle \psi | H | \frac{\partial \psi}{\partial \alpha_i} \rangle = \\ E(\alpha_1, \alpha_2, \dots) \left(\langle \frac{\partial \psi}{\partial \alpha_i} | \psi \rangle + \langle \psi | \frac{\partial \psi}{\partial \alpha_i} \rangle \right) \end{aligned}$$

Let us now assume that H depends on some parameter λ . To calculate the minimum we must choose our parameters α_i to depend on λ_i . We may rewrite the starting equation by emphasizing the dependence of everything on λ , as follows

$$E(\lambda) \langle \psi(\lambda) | \psi(\lambda) \rangle = \langle \psi(\lambda) | H | \psi(\lambda) \rangle$$

Let us now differentiate with respect to λ , noting that $\frac{\partial}{\partial \lambda} = \sum_i \frac{\partial \alpha_i}{\partial \lambda} \frac{\partial}{\partial \alpha_i}$

We get

$$\begin{aligned} & \frac{dE(\lambda)}{d\lambda} \langle \psi(\lambda) | \psi(\lambda) \rangle + E(\lambda) \sum_i \frac{\partial \alpha_i}{\partial \lambda} \left(\left\langle \frac{\partial \psi}{\partial \alpha_i} | \psi(\lambda) \right\rangle + \left\langle \psi(\lambda) | \frac{\partial \psi(\lambda)}{\partial \alpha_i} \right\rangle \right) = \\ & = \left\langle \psi(\lambda) | \frac{\partial H}{\partial \lambda} | \psi(\lambda) \right\rangle + \sum_i \frac{\partial \alpha_i}{\partial \lambda} \left(\left\langle \frac{\partial \psi}{\partial \alpha_i} | H | \psi(\lambda) \right\rangle + \left\langle \psi(\lambda) | H | \frac{\partial \psi(\lambda)}{\partial \alpha_i} \right\rangle \right) \end{aligned}$$

Since we have shown that

$$\begin{aligned} & \left\langle \frac{\partial \psi}{\partial \alpha_i} | H | \psi \right\rangle + \left\langle \psi | H | \frac{\partial \psi}{\partial \alpha_i} \right\rangle = \\ & E(\alpha_1, \alpha_2, \dots) \left(\left\langle \frac{\partial \psi}{\partial \alpha_i} | \psi \right\rangle + \left\langle \psi | \frac{\partial \psi}{\partial \alpha_i} \right\rangle \right) \end{aligned}$$

we obtain the result that

$$\frac{dE(\lambda)}{d\lambda} \langle \psi(\lambda) | \psi(\lambda) \rangle = \left\langle \psi(\lambda) | \frac{\partial H}{\partial \lambda} | \psi(\lambda) \right\rangle$$

With normalized trial wave functions we end up with

$$\frac{dE(\lambda)}{d\lambda} = \left\langle \psi(\alpha_1, \alpha_2, \dots) | \frac{\partial H}{\partial \lambda} | \psi(\alpha_1, \alpha_2, \dots) \right\rangle$$

A comment: The Pauli theorem in Supplement 8-A has the same form, but it deals with exact eigenvalues and exact wave functions. Here we find that the same form applies to approximate values of the eigenvalue and eigenfunctions, provided that these are chosen to depend on parameters $\{\alpha\}$ which minimize the expectation value of the Hamiltonian (which does not depend on these parameters).

9. With the trial wave function

$$\psi(x) = \left(\frac{\beta}{\sqrt{\pi}} \right)^{1/2} e^{-\beta^2 x^2 / 2}$$

we can calculate

$$\begin{aligned}
E(\beta) &= \frac{\beta}{\sqrt{\pi}} \int_{-\infty}^{\infty} dx e^{-\beta^2 x^2 / 2} \left(-\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + \lambda x^4 \right) e^{-\beta^2 x^2 / 2} \\
&= \frac{\beta}{\sqrt{\pi}} \int_{-\infty}^{\infty} dx e^{-\beta^2 x^2} \left(\frac{\hbar^2}{2m} (\beta^2 - \beta^4 x^2) + \lambda x^4 \right) \\
&= \frac{\hbar^2 \beta^2}{2m} + \frac{3\lambda}{4\beta^4}
\end{aligned}$$

We minimize this by setting $\partial E / \partial \beta = 0$, which leads to $\beta^2 = \left(\frac{6m\lambda}{\hbar^2} \right)^{1/3}$. When this is inserted into the expression for E , we get

$$E_{min} = \left(\frac{\hbar^2}{2m} \right)^{2/3} (4\lambda)^{1/3} \left(\frac{6^{1/3}}{4} + \frac{3}{4} \frac{1}{6^{2/3}} \right) = 1.083 \left(\frac{\hbar^2}{2m} \right)^{2/3} \lambda^{1/3}$$

This is quite close to the exact value, for which the coefficient is 1.060

10. With the Hamiltonian

$$H = \frac{p^2}{2m} + \lambda x^4$$

we first choose $(1/2m)$ as the parameter in the Feynman-Hellmann theorem. This leads to

$$\langle 0 | p^2 | 0 \rangle = \frac{\partial E_{min}}{\partial (1/m)} = 0.890 (\hbar^4 m \lambda)^{1/3}$$

If we choose λ as the parameter, then

$$\langle 0 | x^4 | 0 \rangle = \frac{\partial E_{min}}{\partial \lambda} = 0.353 \left(\frac{\hbar^2}{2m\lambda} \right)^{2/3}$$

11. We start from

$$E_0 \leq \frac{\langle \psi | H | \psi \rangle}{\langle \psi | \psi \rangle} = \frac{\sum_{ij} a_i^* H_{ij} a_j}{\sum_i a_i^* a_i}$$

We now choose for the trial vector one in which all the entries are zero, except that at the k -th position there is 1, so that $a_i = \delta_{ik}$. This leads to

$$E_0 \leq H_{kk} \quad (k \text{ is not summed over})$$

We may choose $k = 1, 2, 3, \dots$. Thus the lowest eigenvalue is always smaller than the smallest of the diagonal elements.

12. With the system's center of mass at rest, the two-body problem reduces to a one-body problem, whose Hamiltonian is

$$H = \frac{\mathbf{p}^2}{2\mu} + \frac{1}{2}\mu\omega^2 r^2$$

where μ is the reduced mass, whose value is $m/2$.

(a) The two particles are in an $l = 0$ state which means that the ground state wave function only depends on r , which is symmetric under the interchange of the two particles (Recall that $r = |\mathbf{r}_1 - \mathbf{r}_2|$). Thus the electrons must be in a spin-singlet state, and the ground state wave function is

$$\psi(\mathbf{r}) = u_0(r)X_{\text{singlet}}$$

where

$$u_0(r) = u_0(x)u_0(y)u_0(z) = \left(\frac{\mu\omega}{\hbar\pi}\right)^{3/4} e^{-\mu\omega r^2/2\hbar}$$

(We use $u_0(x)$ from Eq. (6-55)).

(b) To proceed with this we actually have to know something about the solutions of the simple harmonic oscillator in three dimensions. The solution of this was required by Problem 13 in Chapter 8. We recall that the solutions are very similar to the hydrogen atom problem. There are two quantum numbers, n_r and l . Here $l = 0$, so that the first excited *singlet* state must correspond to $n_r = 1$. In the spin triplet state, the spin-wave function is symmetric, so that the spatial wave function must be *antisymmetric*. This is not possible with $l = 0$!

To actually obtain the wave function for the first excited singlet state, we look at the equation for $H(\rho)$, with $H(\rho)$ of the form $a + b\rho^2$. Since

$$\frac{d^2 H}{d\rho^2} + 2\left(\frac{1}{\rho} - \rho\right)\frac{dH}{d\rho} + 4H = 0$$

We get $H(\rho) = 1 - 2\rho^2/3$ and the solution is

$$u_1(r) = N\left(1 - \frac{2}{3}\rho^2\right)e^{-\rho^2/2}$$

where $\rho = \left(\frac{\mu\omega}{\hbar}\right)^{1/2} r$. The normalization constant is obtained from the requirement that

$$N^2 \int_0^\infty r^2 dr \left(1 - \frac{2\mu\omega}{3\hbar} r^2\right)^2 e^{-\mu\omega r^2/\hbar} = 1$$

so that

$$N^2 = \frac{6}{\sqrt{\pi}} \left(\frac{\mu\omega}{\hbar}\right)^{3/2}$$

(c) The energy shift to lowest order is

$$\Delta E = \int_0^\infty r^2 dr \left[C \frac{\delta(r)}{r^2} \right] N^2 \left(1 - \frac{2\mu\omega}{3\hbar} r^2\right)^2 e^{-\mu\omega r^2/\hbar} = CN^2$$

13. The energy is given by

$$E = \frac{1}{2} M_{red} \omega^2 (R - R_0)^2 + \frac{\hbar^2 J(J+1)}{2M_{red} R^2}$$

If we treat the vibrational potential classically, then the lowest state of energy is characterized by $R = R_0$. The vibrational motion changes the separation of the nuclei in the molecule. The new equilibrium point is given by R_1 , which is determined by the solution of

$$\left(\frac{\partial E}{\partial R}\right)_{R_1} = 0 = M_{red} \omega^2 (R_1 - R_0) - \frac{J(J+1)\hbar^2}{M_{red} R_1^3}$$

Let $R_1 = R_0 + \Delta$. Then to first order in Δ ,

$$\Delta = \frac{J(J+1)\hbar^2}{M_{red}^2 \omega^2 R_0^3}$$

If we now insert the new value of R_1 into the energy equation, we find that only the rotational energy is changed (since the vibrational part is proportional to Δ^2). The rotational energy is now

$$\begin{aligned} E_{rot} &= \frac{J(J+1)\hbar^2}{2M_{red} R_0^2 (1 + 2\Delta/R_0)} \\ &= \frac{J(J+1)\hbar^2}{2M_{red} R_0^2} - (J(J+1))^2 \frac{\hbar^4}{M_{red}^3 \omega^2 R_0^6} \end{aligned}$$

The sign of the second term is negative. The sign is dictated by the fact that the rotation stretches the molecule and effectively increases its moment of inertia.

14. In the transition $J = 1 \rightarrow J = 0$ we have

$$\Delta E = \frac{\hbar^2}{2M_{red}R^2}(2-0) = \frac{2\pi\hbar c}{\lambda}$$

so that

$$\begin{aligned} R^2 &= \frac{\hbar\lambda}{2\pi c} \frac{1}{M_{red}} = \frac{\hbar\lambda}{2\pi c} \frac{1}{M_{nucleon}} \left(\frac{1}{12} + \frac{1}{16} \right) = \\ &= (1.127 \times 10^{-10} \text{ m})^2 \end{aligned}$$

The internuclear separation is therefore 0.113 nm, and the moment of inertia is

$$M_{red}R^2 = 1.45 \times 10^{-46} \text{ kg}\cdot\text{m}^2$$

15. (a) The two nuclei are identical. Since the two-electron state is a spatially symmetric spin 0 state, we can ignore the electrons in discussing the lowest energy states of the molecule. In the ground state, the two protons will be in the symmetric $L = 0$ state, so that they must be in a spin-antisymmetric $S = 0$ state.

For the spin-symmetric $S = 1$ state, the spatial wave function must be antisymmetric, so that the lowest energy state will have $L = 1$.

(b) The lowest energy state that lies above the ground state of $L = 0$, and is also a spin $S = 0$ state must have $L = 2$. Thus the change in energy in the transition is

$$\Delta E = \frac{\hbar^2}{M_p R^2} (2(2+1) - 0) = \frac{6\hbar^2}{M_p R^2} = \frac{2\pi\hbar c}{\lambda_s}$$

We have used the fact that the reduced mass of the two-proton system is $M_p/2$.

For the $S = 1$ system, the state above the lowest $L = 1$ state is the $L = 3$ state, and here

$$\Delta E = \frac{\hbar^2}{M_p R^2} (3(3+1) - 1(1+1)) = \frac{10\hbar^2}{M_p R^2} = \frac{2\pi\hbar c}{\lambda_t}$$

The singlet and triplet wavelengths are easily calculated once we know R . Note that these are not exactly the same, but can be looked up.

CHAPTER 15

1. With the perturbing potential given, we get

$$C(1s \rightarrow 2p) = \frac{eE_0}{i\hbar} \langle \phi_{210} | z | \phi_{100} \rangle \int_0^\infty dt e^{i\omega t} e^{-\gamma t}$$

where $\omega = (E_{21} - E_{10})$. The integral yields $1/(\gamma - i\omega)$ so that the absolute square of $C(1s \rightarrow 2p)$ is

$$P(1s \rightarrow 2p) = e^2 E_0^2 \frac{|\langle \phi_{210} | z | \phi_{100} \rangle|^2}{\hbar^2 (\omega^2 + \gamma^2)}$$

We may use $|\langle \phi_{210} | z | \phi_{100} \rangle|^2 = \frac{2^{15}}{3^{10}} a_0^2$ to complete the calculation.

2. Here we need to calculate the absolute square of

$$\frac{1}{i\hbar} \int_0^T dt e^{i\omega_{21}t} \sin \omega t \times \frac{2}{a} \lambda \int_0^a dx \sin \frac{2\pi x}{a} \left(x - \frac{a}{2}\right) \sin \frac{\pi x}{a}$$

Let us first consider the time integral. We will assume that at $t = 0$ the system starts in the ground state. The time integral then becomes

$$\int_0^\infty dt e^{i\omega_{21}t} \sin \omega t = \frac{1}{2i} \int_0^\infty dt \{e^{i(\omega_{21} + \omega)t} - e^{i(\omega_{21} - \omega)t}\} = \frac{\omega}{\omega^2 - \omega_{21}^2}$$

We have used the fact that an finitely rapidly oscillating function is zero on the average. In the special case that ω matches the transition frequency, one must deal with this integral in a more delicate manner. We shall exclude this possibility.

The spatial integral involves

$$\begin{aligned} & \frac{2}{a} \int_0^a dx \sin \frac{2\pi x}{a} \sin \frac{\pi x}{a} \left(x - \frac{a}{2}\right) = \\ & \frac{1}{a} \int_0^a \left(\cos \frac{\pi x}{a} - \cos \frac{3\pi x}{a} \right) \left(x - \frac{a}{2}\right) \\ & = \frac{1}{a} \int_0^a dx \left[\frac{d}{dx} \left\{ \left(\frac{a}{\pi} \sin \frac{\pi x}{a} - \frac{a}{3\pi} \sin \frac{3\pi x}{a} \right) \left(x - \frac{a}{2}\right) \right\} - \left(\frac{a}{\pi} \sin \frac{\pi x}{a} - \frac{a}{3\pi} \sin \frac{3\pi x}{a} \right) \right] \\ & = \frac{1}{a} \left[\frac{a^2}{\pi^2} \cos \frac{\pi x}{a} - \frac{a^2}{9\pi^2} \cos \frac{3\pi x}{a} \right]_0^a = -2 \frac{a}{\pi^2} \frac{8}{9} \end{aligned}$$

The probability is therefore

$$P_{12} = \left(\frac{\lambda}{\hbar}\right)^2 \left(\frac{16a}{9\pi^2}\right)^2 \frac{\omega^2}{(\omega_{21}^2 - \omega^2)^2}$$

(b) The transition from the $n = 1$ state to the $n = 3$ state is *zero*. The reason is that the eigenfunctions for all the odd values of n are all symmetric about $x = a/2$, while the potential $(x - a/2)$ is antisymmetric about that axis, so that the integral vanishes. In fact, quite generally all transition probabilities (even \rightarrow even) and (odd \rightarrow odd) vanish.

(c) The probability goes to zero as $\omega \rightarrow 0$.

3. The only change occurs in the absolute square of the time integral. The relevant one is

$$\int_{-\infty}^{\infty} dt e^{i\omega_{21}t} e^{-t^2/\tau^2} = \sqrt{\pi} e^{-\omega^2\tau^2/4}$$

which has to be squared.

When $\tau \rightarrow \infty$ this vanishes, showing that the transition rate vanishes for a very slowly varying perturbation.

4. The transition amplitude is

$$\begin{aligned} C_{n \rightarrow m} &= \frac{\lambda}{i\hbar} \langle m | \sqrt{\frac{\hbar}{2M\omega}} (A + A^+) | n \rangle \int_0^{\infty} dt e^{i\omega(m-n)t} e^{-\alpha t} \cos \omega_1 t \\ &= -i\lambda \sqrt{\frac{1}{2M\hbar\omega}} \left(\delta_{m,n-1} \sqrt{n} + \delta_{m,n+1} \sqrt{n+1} \right) \frac{\alpha - i\omega(m-n)}{(\alpha - i\omega(m-n))^2 + \omega_1^2} \end{aligned}$$

(a) Transitions are only allowed for $m = n \pm 1$.

(b) The absolute square of the amplitude is, taking into account that $(m - n)^2 = 1$,

$$\frac{\lambda^2}{2M\hbar\omega} (n\delta_{m,n-1} + (n+1)\delta_{m,n+1}) \frac{\alpha^2 + \omega^2}{(\alpha^2 + \omega_1^2 - \omega^2)^2 + 4\alpha^2\omega^2}$$

When $\omega_1 \rightarrow \omega$, nothing special happens, except that the probability appears to exceed unity when α^2 gets to be small enough. This is not possible physically, and what this suggests is that when the external frequency ω_1 matches the oscillator frequency, we get a resonance condition as α approaches zero. Under those circumstances first order perturbation theory is not applicable.

When $\alpha \rightarrow 0$, then we get a frequency dependence similar to that in problem 2.

5. The two particles have equal and opposite momenta, so that

$$E_i = \sqrt{(pc)^2 + m_i^2 c^4}$$

The integral becomes

$$\frac{1}{(2\pi\hbar)^6} \int d\Omega \int_0^\infty p^2 dp \delta(Mc^2 - E_1(p) - E_2(p))$$

and it is only the second integral that is of interest to us. Let us change variables to

$$u = E_1(p) + E_2(p)$$

then

$$du = \frac{pc^2}{E_1} dp + \frac{pc^2}{E_2} dp = (E_1 + E_2) \frac{p dp}{E_1 E_2}$$

and the momentum integral is

$$\begin{aligned} \int_0^\infty p^2 dp \delta(Mc^2 - E_1(p) - E_2(p)) &= \int_{(m_1+m_2)c^2}^\infty p \frac{E_1 E_2 du}{uc^2} \delta(Mc^2 - u) \\ &= p \frac{E_1 E_2}{Mc^4} \end{aligned}$$

To complete the expression we need to express p in terms of the masses.

We have

$$\begin{aligned} (m_2 c^2)^2 + p^2 c^2 &= (Mc^2 - \sqrt{(m_1 c^2)^2 + p^2 c^2})^2 \\ &= (Mc^2)^2 - 2Mc^2 E_1(p) + (m_1 c^2)^2 + p^2 c^2 \end{aligned}$$

This yields

$$E_1(p) = \frac{(Mc^2)^2 + (m_1 c^2)^2 - (m_2 c^2)^2}{2Mc^2}$$

and in the same way

$$E_2(p) = \frac{(Mc^2)^2 + (m_2 c^2)^2 - (m_1 c^2)^2}{2Mc^2}$$

By squaring both sides of either of these we may find an expression for p^2 . The result of a short algebraic manipulation yields

$$p^2 = \frac{c^2}{4M^2} (M - m_1 - m_2)(M - m_1 + m_2)(M + m_1 - m_2)(M + m_1 + m_2)$$

6. The wave function of a system subject to the perturbing potential

$$\lambda V(t) = V f(t)$$

where $f(0) = 0$ and $\lim_{t \rightarrow \infty} f(t) = 1$, with $df(t)/dt \ll \omega f(t)$, is given by

$$|\psi(t)\rangle = \sum_m C_m(t) e^{-iE_m^0 t/\hbar} |\phi_m\rangle$$

and to lowest order in V , we have

$$C_m(t) = \frac{1}{i\hbar} \int_0^t dt' e^{i\omega t'} f(t') \langle \phi_m | V | \phi_0 \rangle$$

where $\omega = (E_m^0 - E_0^0) / \hbar$ and at time $t = 0$ the system is in the ground state. The time integral is

$$\int_0^t dt' e^{i\omega t'} f(t') = \int_0^t dt' f(t') \frac{d}{dt'} \frac{e^{i\omega t'}}{i\omega} = \frac{1}{i\omega} \int_0^t dt' \frac{d}{dt'} (e^{i\omega t'} f(t')) - \frac{1}{i\omega} \int_0^t dt' e^{i\omega t'} df(t') / dt'$$

The second term is much smaller than the term we are trying to evaluate, so that we are left with the first term. Using $f(0) = 0$ we are left with $e^{i\omega t} / i\omega$, since for large times $f(t) = 1$. When this is substituted into the expression for $C_m(t)$ we get

$$C_m(t) = -\frac{e^{i\omega t}}{(E_m^0 - E_0^0)} \langle \phi_m | V | \phi_0 \rangle \quad m \neq 0$$

Insertion of this into the expression for $|\psi(t)\rangle$ yields

$$|\psi(t)\rangle = |\phi_0\rangle + e^{-iE_0^0 t/\hbar} \sum_{m \neq 0} \frac{\langle \phi_m | V | \phi_0 \rangle}{E_0^0 - E_m^0} |\phi_m\rangle$$

On the other hand the ground state wave function, to first order in V is

$$|w_0\rangle = |\phi_0\rangle + \sum_{n \neq 0} \frac{\langle \phi_n | V | \phi_0 \rangle}{E_0^0 - E_n^0} |\phi_n\rangle$$

It follows that

$$\langle w_0 | \psi(t) \rangle = 1 + e^{-iE_0^0 t/\hbar} \sum_{m \neq 0} \frac{\langle \phi_0 | V | \phi_m \rangle \langle \phi_m | V | \phi_0 \rangle}{(E_0^0 - E_m^0)^2}$$

Thus to order V the right side is just one.

A fuller discussion may be found in D.J.Griffiths *Introduction to Quantum Mechanics.i*

7. The matrix element to be calculated is

$$M_{fi} = -\frac{e^2}{4\pi\epsilon_0} \int d^3r_1 \int d^3r_2 \dots \int d^3r_A \Phi_f^*(r_1, r_2, \dots, r_A) \int d^3r \frac{e^{-ip \cdot r/\hbar}}{\sqrt{V}} \sum_{i=1}^Z \frac{1}{|\mathbf{r} - \mathbf{r}_i|} \psi_{100}(\mathbf{r}) \Phi_i(r_1, r_2, \dots, r_A)$$

The summation is over $I = 1, 2, 3, \dots, Z$, that is, only over the proton coordinates. The outgoing electron wave function is taken to be a plane wave, and the Φ are the nuclear wave functions. Now we take advantage of the fact that the nuclear dimensions are tiny compared to the electronic ones. Since $|\mathbf{r}_I| \ll |\mathbf{r}|$, we may write

$$\frac{1}{|\mathbf{r} - \mathbf{r}_i|} = \frac{1}{r} + \frac{\mathbf{r} \cdot \mathbf{r}_i}{r^3} + \dots$$

The $1/r$ term gives no contribution because $\langle \Phi_f | \Phi_i \rangle = 0$. This is a short-hand way of saying that the initial and final nuclear states are orthogonal to each other, because they have different energies. Let us now define

$$\mathbf{d} = \sum_{j=1}^Z \int d^3r_1 \int d^3r_2 \dots \int d^3r_A \Phi_f^*(r_1, r_2, \dots) \mathbf{r}_j \Phi_i(r_1, r_2, \dots)$$

The matrix element then becomes

$$M_{fi} = -\frac{e^2}{4\pi\epsilon_0} \int d^3r \frac{e^{-ip \cdot r/\hbar}}{\sqrt{V}} \frac{\mathbf{d} \cdot \mathbf{r}}{r^3} \psi_{100}(\mathbf{r})$$

The remaining task is to evaluate this integral.

First of all note that the free electron energy is given by

$$\frac{p^2}{2m} = \Delta E + |E_{100}|$$

where ΔE is the change in the nuclear energy. Since nuclear energies are significantly larger than atomic energy, we may take for p the value $p = \sqrt{2m\Delta E}$.

To proceed with the integral we choose \mathbf{p} to define the z axis, and write $p/\hbar = k$. We write the \mathbf{r} coordinate in terms of the usual angles θ and ϕ . We thus have

$$\int d^3r e^{-i\mathbf{p}\cdot\mathbf{r}/\hbar} \frac{d\mathbf{r}}{r^3} \psi_{100}(\mathbf{r}) =$$

$$\int d\Omega \int_0^\infty dr e^{-ikr \cos\theta} (d_x \sin\theta \cos\phi + d_y \sin\theta \sin\phi + d_z \cos\theta) \frac{2}{\sqrt{4\pi}} \left(\frac{Z}{a_0}\right)^{3/2} e^{-Zr/a_0}$$

The solid angle integration involves $\int_0^{2\pi} d\phi$, so that the first two terms above disappear. We are thus left with

$$\frac{1}{\sqrt{\pi}} \left(\frac{Z}{a_0}\right)^{3/2} 2\pi d_z \int_{-1}^1 d(\cos\theta) \int_0^\infty dr \cos\theta e^{-ikr \cos\theta} e^{-Zr/a_0} =$$

$$\frac{1}{\sqrt{\pi}} \left(\frac{Z}{a_0}\right)^{3/2} 2\pi (\mathbf{d}\cdot\hat{\mathbf{p}}) \int_{-1}^1 d(\cos\theta) \frac{\cos\theta}{(Z/a_0 + ik \cos\theta)}$$

The integral, with the change of variables $\cos\theta = u$ becomes

$$\int_{-1}^1 du \frac{u}{Z/a_0 + iku} =$$

$$\int_{-1}^1 du \frac{u(Z/a_0 - iku)}{(Z/a_0)^2 + k^2 u^2} =$$

$$-ik \int_{-1}^1 du \frac{u^2}{(Z/a_0)^2 + k^2 u^2}$$

$$\frac{-i}{k^2} \int_{-k}^k dw \frac{w^2}{(Z/a_0)^2 + w^2} = -\frac{2i}{k^2} \left[k - \frac{a_0}{Z} \arctan\left(\frac{a_0 k}{Z}\right) \right]$$

Note now that $\frac{ka_0}{Z} = \frac{k\hbar}{mcZ\alpha} = \sqrt{\frac{2\Delta E}{Z^2 mc^2 \alpha^2}} = \frac{1}{Z} \sqrt{\frac{\Delta E}{(13.6eV)}}$. If Z is not too large, then the factor is quite large, because nuclear energies are in the thousands or millions of electron volts. In that case the integral is simple: it is just

$$\frac{1}{\sqrt{\pi}} \left(\frac{Z}{a_0}\right)^{3/2} (2\pi) \frac{\mathbf{d}\cdot\mathbf{p}}{p^2} (-2i\hbar) \left[1 - \frac{\pi\hbar Z}{2a_0 p} \right]$$

We evaluate the rate using only the first factor in the square bracket. We need the absolute square of the matrix element which is

$$\left(-\frac{e^2}{4\pi\epsilon_0\sqrt{V}}\right)^2 16\pi\hbar^2 \left(\frac{Z}{a_0}\right)^3 \frac{(\mathbf{d}\cdot\mathbf{p})^2}{p^4}$$

The transition rate per nucleus is

$$\begin{aligned}
R_{fi} &= \frac{2\pi}{\hbar} \int \frac{d^3 p V}{(2\pi\hbar)^3} \delta\left(\frac{p^2}{2m} - \Delta E\right) |M_{fi}|^2 \\
&= \frac{2\pi}{\hbar} \int \frac{d^3 p V}{(2\pi\hbar)^3} \delta\left(\frac{p^2}{2m} - \Delta E\right) \frac{1}{V} \left(\frac{e^2}{4\pi\epsilon_0}\right)^2 16\pi\hbar^2 \left(\frac{Z}{a_0}\right)^3 \frac{(\mathbf{d}\cdot\mathbf{p})^2}{p^4}
\end{aligned}$$

In carrying out the solid angle integration we get

$$\int d\Omega (\mathbf{d}\cdot\mathbf{p})^2 = \frac{4\pi}{3} |\mathbf{d}|^2 p^2$$

so that we are left with some numerical factors times $\int dp \delta(p^2/2m - \Delta E) = \sqrt{\frac{m}{2\Delta E}}$

Putting all this together we finally get

$$R_{fi} = \frac{16}{3} (Z\alpha)^3 \frac{d^2}{a_0^2} \sqrt{\frac{mc^2}{2\Delta E}} \frac{mc^2}{\hbar}$$

We write this in a form that makes the dimension of the rate manifest.

CHAPTER 16.

1. The perturbation caused by the magnetic field changes the simple harmonic oscillator Hamiltonian H_0 to the new Hamiltonian H

$$H = H_0 + \frac{q}{2m} \mathbf{B} \cdot \mathbf{L}$$

If we choose \mathbf{B} to define the direction of the z axis, then the additional term involves $B L_z$. When H acts on the eigenstates of the harmonic oscillator, labeled by $|n_r, l, m_l\rangle$, we get

$$H |n_r, l, m_l\rangle = \left(\hbar\omega(2n_r + l + \frac{3}{2}) + \frac{qB\hbar}{2m} m_l \right) |n_r, l, m_l\rangle$$

Let us denote $qB/2m$ by ω_B . Consider the three lowest energy states:

$n_r = 0, l = 0$, the energy is $3\hbar\omega/2$.

$n_r = 0, l = 1$ This three-fold degenerate level with unperturbed energy $5\hbar\omega/2$, splits into three nondegenerate energy levels with energies

$$E = 5\hbar\omega/2 + \hbar\omega_B \begin{pmatrix} 1 \\ 0 \\ -1 \end{pmatrix}$$

The next energy level has quantum numbers $n_r = 2, l = 0$ or $n_r = 0, l = 2$. We thus have a four-fold degeneracy with energy $7\hbar\omega/2$. The magnetic field splits these into the levels according to the m_l value. The energies are

$$E = 7\hbar\omega/2 + \hbar\omega_B \begin{pmatrix} 2 \\ 1 \\ 0,0 \\ -1 \\ -2 \end{pmatrix} \quad n_r = 1,0$$

2, The system has only one degree of freedom, the angle of rotation θ . In the absence of torque, the angular velocity $\omega = d\theta/dt$ is constant. The kinetic energy is

$$E = \frac{1}{2} Mv^2 = \frac{1}{2} \frac{(M^2 v^2 R^2)}{MR^2} = \frac{1}{2} \frac{L^2}{I}$$

where $L = MvR$ is the angular momentum, and I the moment of inertia. Extending this to a quantum system implies the replacement of L^2 by the corresponding operator. This suggests that

$$H = \frac{\mathbf{L}^2}{2I}$$

(b) The operator \mathbf{L} can also be written as $\mathbf{p} \times \mathbf{R}$.

When the system is placed in a constant magnetic field, we make the replacement

$$\mathbf{p} \rightarrow \mathbf{p} - q\mathbf{A} = \mathbf{p} - q\left(-\frac{1}{2}\mathbf{r} \times \mathbf{B}\right) = \mathbf{p} + \frac{q}{2}\mathbf{r} \times \mathbf{B}$$

The operator \mathbf{r} represents the position of the particle relative to the axis of rotation, and this is equal to \mathbf{R} . We may therefore write

$$\mathbf{L} = \mathbf{R} \times \mathbf{p} \rightarrow \mathbf{R} \times \left(\mathbf{p} + \frac{q}{2}\mathbf{R} \times \mathbf{B}\right) = \mathbf{L} + \frac{q}{2}(\mathbf{R}(\mathbf{R} \cdot \mathbf{B}) - R^2\mathbf{B})$$

If we square this, and only keep terms linear in \mathbf{B} , then it follows from $(\mathbf{R} \cdot \mathbf{B}) = 0$, that

$$H = \frac{1}{2I}(\mathbf{L}^2 - qR^2\mathbf{L} \cdot \mathbf{B}) = \frac{\mathbf{L}^2}{2I} - \frac{q}{2M}\mathbf{L} \cdot \mathbf{B} = \frac{\mathbf{L}^2}{2I} - \frac{qB}{2M}L_z$$

The last step is taken because we choose the direction of \mathbf{B} to define the z axis.

The energy eigenvalues are therefore

$$E = \frac{\hbar^2 l(l+1)}{2I} - \frac{qB\hbar}{2M}m_l$$

where $m_l = l, l-1, l-2, \dots, -l$. Note that the lowest of the levels corresponds to $m_l = l$.

3. In the absence of a magnetic field, the frequency for the transition $n = 3$ to $n = 2$ is determined by

$$2\pi\hbar\nu = \frac{1}{2}mc^2\alpha^2\left(\frac{1}{4} - \frac{1}{9}\right)$$

so that

$$\nu = \frac{mc^2\alpha^2}{4\pi\hbar} \frac{5}{36}$$

The lines with $\Delta m_l = \pm 1$ are shifted upward (and downward) relative to the $\Delta m_l = 0$ (unperturbed) line. The amount of the shift is given by

$$h\Delta\nu = \frac{e\hbar B}{2mc}$$

so that

$$\Delta\nu = \frac{eB}{4\pi mc}$$

Numerically $\nu = 0.4572 \times 10^{15}$ Hz and with $B = 1$ T, $\Delta\nu = 1.40 \times 10^{10}$ Hz. Thus the frequencies are ν and $\nu(1 \pm \Delta\nu/\nu)$. Thus the wavelengths are c/ν and $(c/\nu)(1 \mp \Delta\nu/\nu)$. This leads to the three values $\lambda = 655.713$ nm, with the other lines shifted down/up by 0.02 nm.

4. The Hamiltonian is

$$H = \frac{1}{2m} (\mathbf{p} - q\mathbf{A})^2 - q\mathbf{E} \cdot \mathbf{r}$$

Let us choose $\mathbf{E} = (E, 0, 0)$ and $\mathbf{B} = (0, 0, B)$, but now we choose the gauge such that $\mathbf{A} = (0, Bx, 0)$. This leads to

$$\begin{aligned} H &= \frac{1}{2m} (p_x^2 + (p_y - qBx)^2 + p_z^2) - qEx = \\ &= \frac{1}{2m} (p_x^2 + p_y^2 + p_z^2 - 2qBp_y x + q^2 B^2 x^2 - 2mqEx) \end{aligned}$$

Let us now choose the eigenstate to be a simultaneous eigenstate of H, p_z (with eigenvalue zero) and p_y (with eigenvalue $\hbar k$). Then the Hamiltonian takes the form

$$H = \frac{\hbar^2 k^2}{2m} + \frac{1}{2m} p_x^2 + \frac{1}{2m} (qBx - \hbar k - mE/B)^2 - \frac{1}{2m} (\hbar k + mE/B)^2$$

This is the Hamiltonian for a shifted harmonic oscillator with a constant energy added on. We may write this in the form

$$H = -\frac{\hbar k E}{B} - \frac{mE^2}{2B^2} + \frac{1}{2} m \left(\frac{q^2 B^2}{m^2} \right) \left(x - \frac{\hbar k - mE/B}{qB} \right)^2$$

Thus the energy is

$$E = -\frac{\hbar k E}{B} - \frac{m E^2}{2 B^2} + \hbar \left(\frac{q B}{m} \right) \left(n + \frac{1}{2} \right)$$

with $n = 0, 1, 2, 3, \dots$

5. We first need to express everything in cylindrical coordinates. Since we are dealing with an infinite cylinder which we choose to be aligned with the z axis, nothing depends on z , and we only deal with the ρ and ϕ coordinates. We only need to consider the Schrodinger equation in the region $a \leq \rho \leq b$.

$$\text{We start with } H = \frac{1}{2m_e} (\Pi_x^2 + \Pi_y^2)$$

where

$$\Pi_x = -i\hbar \frac{\partial}{\partial x} + eA_x; \quad \Pi_y = -i\hbar \frac{\partial}{\partial y} + eA_y$$

To write this in cylindrical coordinates we use Eq. (16-33) and the fact that for the situation at hand

$$A_x = -\sin\phi \frac{\Phi}{2\pi\rho}; \quad A_y = \cos\phi \frac{\Phi}{2\pi\rho}; \quad A_\phi = \frac{\Phi}{2\pi\rho}$$

where Φ is the magnetic flux in the interior region. When all of this is put together, the equation

$$H\psi(\rho, \phi) = E\psi(\rho, \phi)$$

takes the form

$$E\psi = -\frac{\hbar^2}{2m_e} \left(\frac{\partial^2 \psi}{\partial \rho^2} + \frac{1}{\rho} \frac{\partial \psi}{\partial \rho} + \frac{1}{\rho^2} \frac{\partial^2 \psi}{\partial \phi^2} \right) - 2i\hbar e \frac{\Phi}{2\pi\rho^2} \frac{\partial \psi}{\partial \phi} + \frac{e^2}{\rho^2} \left(\frac{\Phi}{2\pi} \right)^2 \psi$$

To solve this, we use the separation of variables technique. Based on previous experience, we write

$$\psi(\rho, \phi) = f(\rho) e^{im\phi}$$

The single-valuedness of the solution implies that $m = 0, \pm 1, \pm 2, \pm 3, \dots$

With the notation $k^2 = 2m_e E / \hbar^2$ the equation for $f(\rho)$ becomes

$$-k^2 f(\rho) = \frac{d^2 f}{d\rho^2} + \frac{1}{\rho} \frac{df}{d\rho} - \left(m + \frac{e\Phi}{2\pi\hbar} \right)^2 f$$

If we now introduce $z = k\rho$ and $\nu = m + \frac{e\Phi}{2\pi\hbar}$ the equation takes the form

$$\frac{d^2 f(z)}{dz^2} + \frac{1}{z} \frac{df(z)}{dz} + \left(1 - \frac{\nu^2}{z^2}\right) f(z) = 0$$

This is Bessel's equation. The most general solution has the form

$$f(\rho) = AJ_\nu(k\rho) + BN_\nu(k\rho)$$

If we now impose the boundary conditions $f(ka) = f(kb) = 0$ we end up with

$$AJ_\nu(ka) + BN_\nu(ka) = 0$$

and

$$AJ_\nu(kb) + BN_\nu(kb) = 0$$

The two equations can only be satisfied if

$$J_\nu(ka)N_\nu(kb) - J_\nu(kb)N_\nu(ka) = 0$$

This is the *eigenvalue equation*, and the solution k clearly depends on the order ν of the Bessel functions, that is, on the flux enclosed in the interior cylinder.

CHAPTER 17

1. We start with Eq. (17-19). We define \mathbf{k} as the z axis. This means that the polarization vector, which is perpendicular to \mathbf{k} has the general form

$$\boldsymbol{\varepsilon}^{(\lambda)} = \hat{\mathbf{i}} \cos \varphi + \hat{\mathbf{j}} \sin \varphi$$

This leads to

$$\mathbf{B} = \nabla \times \mathbf{A} = -i \sqrt{\frac{\hbar}{2\varepsilon_0 \omega V}} k \hat{\mathbf{k}} \times (\hat{\mathbf{i}} \cos \varphi + \hat{\mathbf{j}} \sin \varphi) = B_0 (\hat{\mathbf{j}} \cos \varphi - \hat{\mathbf{i}} \sin \varphi)$$

We are now interested in

$$M = B_0 \frac{g_p - g_n}{2} \frac{\hbar}{2} \bar{X}_0 \{ (\sigma_y^{(p)} - \sigma_y^{(n)}) \cos \varphi - (\sigma_x^{(p)} - \sigma_x^{(n)}) \sin \varphi \} X_1^m$$

The operators are of the form

$$\sigma_y \cos \varphi - \sigma_x \sin \varphi = \begin{pmatrix} 0 & -i \cos \varphi \\ i \cos \varphi & 0 \end{pmatrix} - \begin{pmatrix} 0 & \sin \varphi \\ \sin \varphi & 0 \end{pmatrix} = \begin{pmatrix} 0 & -ie^{-i\varphi} \\ ie^{i\varphi} & 0 \end{pmatrix}$$

It is simple to work out the “bra” part of the scalar product

$$\frac{1}{\sqrt{2}} (\bar{\chi}_+^{(p)} \bar{\chi}_-^{(n)} - \bar{\chi}_-^{(p)} \bar{\chi}_+^{(n)}) \left[\begin{pmatrix} 0 & -ie^{-i\varphi} \\ ie^{i\varphi} & 0 \end{pmatrix}_p - \begin{pmatrix} 0 & -ie^{-i\varphi} \\ ie^{i\varphi} & 0 \end{pmatrix}_n \right]$$

with the help of

$$\bar{\chi}_+ \begin{pmatrix} 0 & -ie^{-i\varphi} \\ ie^{i\varphi} & 0 \end{pmatrix} = (1 \ 0) \begin{pmatrix} 0 & -ie^{-i\varphi} \\ ie^{i\varphi} & 0 \end{pmatrix} = (0 \ -ie^{-i\varphi}) = -ie^{-i\varphi} \bar{\chi}_-$$

and

$$\bar{\chi}_- \begin{pmatrix} 0 & -ie^{-i\varphi} \\ ie^{i\varphi} & 0 \end{pmatrix} = (0 \ 1) \begin{pmatrix} 0 & -ie^{-i\varphi} \\ ie^{i\varphi} & 0 \end{pmatrix} = (ie^{i\varphi} \ 0) = ie^{i\varphi} \bar{\chi}_+$$

This implies that the “bra” part is

$$\begin{aligned}
& \frac{1}{\sqrt{2}} (\bar{\chi}_+^{(p)} \bar{\chi}_-^{(n)} - \bar{\chi}_-^{(p)} \bar{\chi}_+^{(n)}) \left[\begin{pmatrix} 0 & -ie^{-i\varphi} \\ ie^{i\varphi} & 0 \end{pmatrix}_p - \begin{pmatrix} 0 & -ie^{-i\varphi} \\ ie^{i\varphi} & 0 \end{pmatrix}_n \right] = \\
& = -\sqrt{2}i(e^{-i\varphi} \bar{\chi}_-^{(p)} \bar{\chi}_-^{(n)} + e^{i\varphi} \bar{\chi}_+^{(p)} \bar{\chi}_+^{(n)}) \\
& = -\sqrt{2}i(e^{-i\varphi} \bar{X}_1^{-1} + e^{i\varphi} \bar{X}_1^1)
\end{aligned}$$

For the “ket” state we may choose $X_{\text{triplet}} = \alpha X_1^1 + \beta X_1^0 + \gamma X_1^{-1}$, and then the matrix element is

$$M = -i\sqrt{2}B_0 \frac{g_p - g_n}{2} \frac{\hbar}{2} (e^{i\varphi} \alpha + e^{-i\varphi} \gamma)$$

2. We are interested in finding out for what values of l, m , the matrix element

$$\frac{1}{2} \langle \ell, m | (\boldsymbol{\varepsilon} \cdot \mathbf{p})(\mathbf{k} \cdot \mathbf{r}) + (\boldsymbol{\varepsilon} \cdot \mathbf{r})(\mathbf{p} \cdot \mathbf{k}) | 0, 0 \rangle$$

does not vanish. We use the technique used in Eq. (17-22) to rewrite this in the form

$$\begin{aligned}
& \frac{1}{2} \frac{im_e}{\hbar} \langle \ell, m | [H_0, \boldsymbol{\varepsilon} \cdot \mathbf{r}](\mathbf{k} \cdot \mathbf{r}) + (\boldsymbol{\varepsilon} \cdot \mathbf{r})[H_0, \mathbf{k} \cdot \mathbf{r}] | 0, 0 \rangle = \\
& \frac{im_e}{2\hbar} \langle \ell, m | H_0(\boldsymbol{\varepsilon} \cdot \mathbf{r})(\mathbf{k} \cdot \mathbf{r}) - (\boldsymbol{\varepsilon} \cdot \mathbf{r})H_0(\mathbf{k} \cdot \mathbf{r}) + (\boldsymbol{\varepsilon} \cdot \mathbf{r})H_0(\mathbf{k} \cdot \mathbf{r}) - (\boldsymbol{\varepsilon} \cdot \mathbf{r})(\mathbf{k} \cdot \mathbf{r})H_0 | 0, 0 \rangle = \\
& \frac{im_e}{2\hbar} (E_{\ell, m} - E_{0, 0}) \langle \ell, m | (\boldsymbol{\varepsilon} \cdot \mathbf{r})(\mathbf{k} \cdot \mathbf{r}) | 0, 0 \rangle
\end{aligned}$$

Let us now choose \mathbf{k} to define the z axis, so that $\mathbf{k} = (0, 0, k)$. Since $\boldsymbol{\varepsilon}$ is perpendicular to \mathbf{k} , we may choose it to be represented by $\boldsymbol{\varepsilon} = (\cos \alpha, \sin \alpha, 0)$. Then, with the usual polar coordinates, we have

$$\begin{aligned}
(\boldsymbol{\varepsilon} \cdot \mathbf{r})(\mathbf{k} \cdot \mathbf{r}) &= k(\cos \alpha \sin \theta \cos \phi + \sin \alpha \sin \theta \sin \phi) \cos \theta = \\
&= k \sin \theta \cos \theta \cos(\phi - \alpha)
\end{aligned}$$

This is a linear combination of $Y_{21}(\theta, \phi)$ and $Y_{2,-1}(\theta, \phi)$. Thus the angular integral is of

the form $\int d\Omega Y_{\ell, m}^* Y_{2, \pm 1} Y_{0, 0}$, and since $Y_{0, 0}$ is just a number, the integral is proportional to $\delta_{\ell, 2}$.

There is also a selection rule that requires $m = \pm 1$. This comes about because of our choice of axes.

3. In the transition under consideration, the radial part of the transition rate is unchanged. The only change has to do with the part of the matrix element that deals with the dependence on the polarization of the photon emitted in the transition. Eq. (17-44), for example shows that $\delta_{m,1}$ is multiplied by $\varepsilon_x^2 + \varepsilon_y^2 = 1 - \varepsilon_z^2$ and this factor carries some information about the direction of the photon momentum, even though that does not appear explicitly in the matrix element. We proceed as follows: The direction of the polarization of the initial atomic state defines the z axis. Let the photon momentum direction be given by

$$\hat{\mathbf{d}} = \hat{\mathbf{i}} \sin\Theta \cos\Phi + \hat{\mathbf{j}} \sin\Theta \sin\Phi + \hat{\mathbf{k}} \cos\Theta$$

We may define two unit vectors perpendicular to this. For the first one we take $\hat{\mathbf{d}} \times \hat{\mathbf{k}}$, which, after being divided by the sine of the angle between these two vectors, i.e. by $\sin\Theta$, yields

$$\hat{\varepsilon}_1 = -\hat{\mathbf{i}} \sin\Phi + \hat{\mathbf{j}} \cos\Phi$$

The other one is $\hat{\varepsilon}_2 = \hat{\mathbf{d}} \times \hat{\varepsilon}_1$ (two vectors perpendicular to each other), which leads to

$$\hat{\varepsilon}_2 = \hat{\mathbf{i}} \cos\Theta \cos\Phi + \hat{\mathbf{j}} \cos\Theta \sin\Phi - \hat{\mathbf{k}} \sin\Theta$$

In the coordinate system in which $\hat{\mathbf{d}}$ represents the z axis, the ε_i vectors represent the x and y axes, and since the photon polarization must lie in that new $x - y$ plane, we see that the polarization vector has the form

$$\varepsilon = \cos\chi \hat{\varepsilon}_1 + \sin\chi \hat{\varepsilon}_2$$

Thus

$$\begin{aligned} \varepsilon_z &= \hat{\mathbf{k}} \cdot \varepsilon = -\sin\chi \sin\Theta, \\ \varepsilon_x &= \hat{\mathbf{i}} \cdot \varepsilon = \cos\chi \sin\Phi + \sin\chi \cos\Theta \cos\Phi, \\ \varepsilon_y &= \hat{\mathbf{j}} \cdot \varepsilon = -\cos\chi \cos\Phi + \sin\chi \cos\Theta \sin\Phi \end{aligned}$$

and

$$\varepsilon_x^2 + \varepsilon_y^2 = 1 - \varepsilon_z^2 = 1 - \sin^2\chi \sin^2\Theta$$

Thus the final answer (using Eq. (17-44)) is

$$d\Gamma = \frac{\alpha}{2\pi} \frac{\omega^3}{c^2} \frac{2^{15}}{3^{10}} \left(\frac{1}{2} \delta_{m,1} \right) (1 - \sin^2\chi \sin^2\Theta) d(\cos\Theta) d\Phi$$

The dependence on the polarization appears in the $\sin^2\chi$ term.

4. First of all, we need to recognize what $2p \rightarrow 1s$ means for the harmonic oscillator in three dimensions. The numbers “2” and “1” usually refer to the principal quantum number, e.g. $n = n_r + \ell + 1$ for the hydrogen atom. Here the energy spectrum is characterized by $2n_r + \ell + 1$, and it is this combination that we call the principal quantum number. Thus we take the $2p \rightarrow 1s$ transition to mean $(n_r = 0, \ell = 1) \rightarrow (n_r = 0, \ell = 0)$.

To solve this problem we recognized that nothing changes in the angular integration that was done for the $2p \rightarrow 1s$ transition in hydrogen. The only change in the matrix element involves the radial functions. In hydrogen we calculated

$$\int_0^\infty r^3 R_{21}(r) R_{10}(r) dr$$

using the radial functions for hydrogen. Here the same integral appears, except that the radial functions are those of the three-dimensional harmonic oscillator. Here, the properly normalized eigenfunctions are

$$R_{10}(r) = \frac{2}{\pi^{1/4}} \left(\frac{m\omega}{\hbar} \right)^{3/2} e^{-m\omega^2 r^2 / 2\hbar}$$

and

$$R_{21}(r) = \left(\frac{8}{3} \right)^{1/2} \frac{1}{\pi^{1/4}} \left(\frac{m\omega}{\hbar} \right)^{5/4} r e^{-m\omega^2 r^2 / 2\hbar}$$

Note that these functions appear in the solution to problem 8-13. Given these, the integral that yields the matrix element is straightforward. We have

$$\begin{aligned} M &= \left(\frac{8}{3} \right)^{1/2} \frac{2}{\pi^{1/2}} \left(\frac{m\omega}{\hbar} \right)^2 \int_0^\infty dr r^4 e^{-m\omega^2 r^2 / \hbar} = \\ &= \frac{4}{\pi^{1/2}} \left(\frac{2}{3} \right)^{1/2} \left(\frac{m\omega}{\hbar} \right)^2 \left(\frac{\hbar}{m\omega} \right)^{5/2} \frac{1}{2} \int_0^\infty dx x^3 e^{-x} \\ &= \frac{4}{\pi^{1/2}} \left(\frac{2}{3} \right)^{1/2} \left(\frac{m\omega}{\hbar} \right)^2 \left(\frac{\hbar}{m\omega} \right)^{5/2} \frac{1}{2} \frac{3\pi^{1/2}}{4} \end{aligned}$$

The square of this is $\frac{3\hbar}{2m\omega}$. We check that this has the dimensions of a (length)² as required. To get the decay rate, we just take the hydrogen result and make the substitution

$$|M_{hydrogen}|^2 = \frac{2^{15}}{3^9} a_0^2 \rightarrow |M|^2 = \frac{3\hbar}{2m\omega}$$

This then leads to the rate

$$R = \frac{4}{9} \alpha \frac{\omega^3}{c^2} |M|^2 = \frac{2\alpha}{3} \left(\frac{\hbar\omega}{mc^2} \right) \omega$$

CHAPTER 19

1. We have

$$M_{fi} = \frac{1}{V} \int d^3r e^{-i\Delta \cdot \mathbf{r}} V(\mathbf{r})$$

If $V(\mathbf{r}) = V(r)$, that is, if the potential is central, we may work out the angular integration as follows:

$$M_{fi} = \frac{1}{V} \int_0^\infty r^2 V(r) dr \int_0^{2\pi} d\phi \int_0^\pi \sin\theta d\theta e^{-i\Delta r \cos\theta}$$

with the choice of the vector Δ as defining the z axis. The angular integration yields

$$\int_0^{2\pi} d\phi \int_0^\pi \sin\theta d\theta e^{-i\Delta r \cos\theta} = 2\pi \int_{-1}^1 d(\cos\theta) e^{-i\Delta r \cos\theta} = \frac{4\pi}{\Delta r} \sin\Delta r$$

so that

$$M_{fi} = \frac{1}{V} \frac{4\pi}{\Delta} \int_0^\infty r dr V(r) \sin\Delta r$$

Note that this is an even function of Δ that is, it is a function of $\Delta^2 = (\mathbf{p}_f - \mathbf{p}_i)^2 / \hbar^2$

2. For the gaussian potential

$$M_{fi} = \frac{1}{V} \frac{4\pi V_0}{\Delta} \int_0^\infty r dr \sin\Delta r e^{-r^2/a^2}$$

Note that the integrand is an even function of r . We may therefore rewrite it as

$$\int_0^\infty r dr \sin\Delta r e^{-r^2/a^2} = \frac{1}{2} \int_{-\infty}^\infty r dr \sin\Delta r e^{-r^2/a^2}$$

The integral on the right may be rewritten as

$$\frac{1}{2} \int_{-\infty}^\infty r dr \sin\Delta r e^{-r^2/a^2} = \frac{1}{4i} \int_{-\infty}^\infty r dr \left(e^{-r^2/a^2 + i\Delta r} - c.c. \right)$$

Now

$$\frac{1}{4i} \int_{-\infty}^\infty r dr e^{-r^2/a^2 + i\Delta r} = \frac{1}{i} \frac{\partial}{\partial \Delta} \int_{-\infty}^\infty dr e^{-r^2/a^2 + i\Delta r} = -i \frac{\partial}{\partial \Delta} a \sqrt{\pi} e^{-a^2 \Delta^2 / 4} = i \frac{\Delta a^3 \sqrt{\pi}}{2} e^{-a^2 \Delta^2 / 4}$$

Subtracting the complex conjugate and dividing by $4i$ gives

$$M_{fi} = \frac{1}{V} (a\sqrt{\pi})^3 V_0 e^{-a^2 \Delta^2 / 4}$$

The comparable matrix element for the Yukawa potential is

$$\bar{M}_{fi} = \frac{1}{V} \frac{4\pi}{\Delta} V_Y b \int_0^\infty dr e^{-r/b} \sin \Delta r = \frac{1}{V} 4\pi V_Y \frac{b^3}{1 + b^2 \Delta^2}$$

We can easily check that the matrix elements and their derivatives with respect to Δ^2 at $\Delta = 0$ will be equal if $a = 2b$ and $V_Y = 2\sqrt{\pi} V_0$.

The differential cross section takes its simplest form if the scattering involves the same particles in the final state as in the initial state. The differential cross section is

$$\frac{d\sigma}{d\Omega} = \frac{\mu^2}{4\pi^2 \hbar^4} |U(\Delta)|^2$$

where μ is the reduced mass and $U(\Delta) = VM_{fi}$.

We are interested in the comparison

$$\frac{(d\sigma / d\Omega)_{\text{gauss}}}{(d\sigma / d\Omega)_{\text{Yukawa}}} = \frac{e^{-2b^2 \Delta^2}}{(1 + b^2 \Delta^2)^{-2}} = (1 + X)^2 e^{-2X}$$

where we have introduced the notation $X = b^2 \Delta^2$. This ratio, as a function of X , starts out at $X = 0$ with the value of 1, and zero slope, but then it drops rapidly, reaching less than 1% of its initial value when $X = 4$, that is, at $\Delta = 2/b$.

3. We use the hint to write

$$\frac{d\sigma}{d\Omega} = \frac{p^2}{\pi \hbar^2} \frac{d\sigma}{d\Delta^2} = \frac{\mu^2}{4\pi^2 \hbar^4} \left| 4\pi V_0 \frac{b^3}{1 + b^2 \Delta^2} \right|^2$$

The total cross section may be obtained by integrating this over Δ^2 with the range given by $0 \leq \Delta^2 \leq 4p^2 / \hbar^2$, corresponding to the values of $\cos\theta$ between -1 and $+1$. The integral can actually be done analytically. With the notation $k^2 = p^2 / \hbar^2$ the integral is

$$\int_0^{4k^2} d\Delta^2 \frac{1}{(1 + b^2 \Delta^2)^2} = \frac{1}{b^2} \int_0^{4k^2 b^2} \frac{dx}{(1 + x)^2} = \frac{4k^2}{1 + 4k^2 b^2}$$

This would immediately lead to the cross section if the particles were *not* identical. For identical particles, there are symmetry problems caused by the Pauli Exclusion Principle and the fact that the protons have spin $1/2$. The matrix elements are not affected by the

spin because there is no spin-orbit coupling or any other spin dependence in the potential. However:

In the spin *triplet* state, the spatial wave function of the proton is antisymmetric, while for the spin *singlet* state, the spatial wave function is symmetric. This means that in the original Born approximation we have

$$\int d^3r \frac{e^{-ik'r} \mp e^{ik'r}}{\sqrt{2}} V(r) \frac{e^{ik.r} \mp e^{-ik.r}}{\sqrt{2}} = \int d^3r V(r) e^{-i(k'-k).r} \mp \int d^3r V(r) e^{-i(k+k').r}$$

The first term has the familiar form

$$4\pi V_0 \frac{b^3}{1+b^2\Delta^2} = 4\pi V_0 \frac{b^3}{1+2b^2k^2(1-\cos\theta)}$$

and the second term is obtained by changing $\cos\theta$ to $-\cos\theta$. Thus the cross section involves

$$\begin{aligned} & \int_{-1}^1 d(\cos\theta) \left(\frac{1}{1+2b^2k^2-2b^2k^2\cos\theta} \mp \frac{1}{1+2b^2k^2+2b^2k^2\cos\theta} \right)^2 \\ & \rightarrow \int_{-1}^1 dz \left(\frac{1}{1+a-az} \mp \frac{1}{1+a+az} \right)^2 \\ & = \frac{4}{1+2a} \mp \frac{2}{a(1+a)} \ln(1+2a) \end{aligned}$$

where $a = 2b^2k^2$.

Thus the total cross section is

$$\sigma = \frac{8\pi\mu^2 b^6}{\hbar^4} V_0^2 \left[\left(\frac{4}{1+4k^2b^2} \right) \mp \frac{1}{k^2b^2(1+2k^2b^2)} \ln(1+4k^2b^2) \right]$$

The relation to the center of mass energy follows from $E = p^2/2\mu = \hbar^2k^2/2\mu$, so that

$$k^2 = \frac{2\mu E}{\hbar^2} = \frac{(1.67 \times 10^{-27} \text{ kg})(100 \times 1.6 \times 10^{-13} \text{ J})}{(1.054 \times 10^{-34} \text{ J}\cdot\text{s})^2}$$

With $b = 1.2 \times 10^{-15} \text{ m}$, we get $(kb)^2 = 3.5$, so that $\sigma = 4.3 \times 10^{-28} \text{ m}^2 = 4.3 \times 10^{-24} \text{ cm}^2 = 3.4 \text{ barns}$.

4. To make the table, we first of all make a change of notation: we will represent the proton spinors by χ_{\pm} and the neutron spinors by η_{\pm} . To work out the action of

$$\sigma_p \bullet \sigma_n = \sigma_{pz} \sigma_{nz} + 2(\sigma_{p+} \sigma_{n-} + \sigma_{p-} \sigma_{n+})$$

on the four initial combinations, we will use $\sigma_+ \chi_+ = \sigma_- \chi_- = 0$; $\sigma_+ \chi_- = \chi_+$; $\sigma_- \chi_+ = \chi_-$ and similarly for the neutron spinors. Thus

$$\begin{aligned} [\sigma_{pz} \sigma_{nz} + 2(\sigma_{p+} \sigma_{n-} + \sigma_{p-} \sigma_{n+})] \chi_+ \eta_+ &= \chi_+ \eta_+ \\ [\sigma_{pz} \sigma_{nz} + 2(\sigma_{p+} \sigma_{n-} + \sigma_{p-} \sigma_{n+})] \chi_+ \eta_- &= -\chi_+ \eta_- + 2\chi_- \eta_+ \\ [\sigma_{pz} \sigma_{nz} + 2(\sigma_{p+} \sigma_{n-} + \sigma_{p-} \sigma_{n+})] \chi_- \eta_+ &= -\chi_- \eta_+ + 2\chi_+ \eta_- \\ [\sigma_{pz} \sigma_{nz} + 2(\sigma_{p+} \sigma_{n-} + \sigma_{p-} \sigma_{n+})] \chi_- \eta_- &= \chi_- \eta_- \end{aligned}$$

From this we get for the matrix $A + B\sigma_p \bullet \sigma_n$, with rows and columns labeled by (++) , (+-), (-+), (--) the following

$$A + B\sigma_p \bullet \sigma_n = \begin{pmatrix} A+B & 0 & 0 & 0 \\ 0 & A-B & 2B & 0 \\ 0 & 2B & A-B & 0 \\ 0 & 0 & 0 & A+B \end{pmatrix}$$

The cross sections will form a similar matrix, with the amplitudes replaced by the absolute squares, i.e. $|A+B|^2$, $|2B|^2$, and $|A-B|^2$.

5. Consider $n-p$ scattering again. If the initial proton spin is not specified, then we must add the cross sections for all the possible initial proton states and divide by 2, since *a priori* there is no reason why in the initial state there should be more or less of up-spin protons. We also need to sum over the final states. Note that we do not sum amplitudes because the spin states of the proton are distinguishable.

Thus, for initial neutron spin up and final neutron spin up we have

$$\sigma(+|+) = \frac{1}{2} (\sigma(++ ,++) + \sigma(++ , -+) + \sigma(-+ ,++) + \sigma(-+ , -+))$$

where on the r.h.s. the first label on each side refers to the proton and the second to the neutron. We thus get

$$\sigma(+|+) = \frac{1}{2} (|A+B|^2 + |A-B|^2) = |A|^2 + |B|^2$$

Similarly

$$\begin{aligned}\sigma(-|+) &= \frac{1}{2}(\sigma(+-,++) + \sigma(+-, -+) + \sigma(--,++) + \sigma(--, -+)) \\ &= \frac{1}{2}(2|B|^2) = 2|B|^2\end{aligned}$$

Thus

$$P = \frac{|A|^2 + |B|^2 - 2|B|^2}{|A|^2 + |B|^2 + 2|B|^2} = \frac{|A|^2 - |B|^2}{|A|^2 + 3|B|^2}$$

6. For triplet \rightarrow triplet scattering we have (with the notation (S, S_z))

$$(1,1) \rightarrow (1,1) \quad \langle \chi_+ \eta_+ | \chi_+ \eta_+ \rangle = A + B$$

$$(1,-1) \rightarrow (1,-1) \quad \langle \chi_- \eta_- | \chi_- \eta_- \rangle = A + B$$

$$(1,0) \rightarrow (1,0) \quad \left\langle \frac{\chi_+ \eta_- + \chi_- \eta_+}{\sqrt{2}} \middle| \frac{\chi_+ \eta_- + \chi_- \eta_+}{\sqrt{2}} \right\rangle = \frac{1}{2}(A - B + 2B + 2B + A - B) = A + B$$

$$(0,0) \rightarrow (0,0) \quad \left\langle \frac{\chi_+ \eta_- - \chi_- \eta_+}{\sqrt{2}} \middle| \frac{\chi_+ \eta_- - \chi_- \eta_+}{\sqrt{2}} \right\rangle = \frac{1}{2}(A - B - 2B - 2B + A - B) = A - 3B$$

$$(0,0) \rightarrow (1,0) \quad \left\langle \frac{\chi_+ \eta_- - \chi_- \eta_+}{\sqrt{2}} \middle| \frac{\chi_+ \eta_- + \chi_- \eta_+}{\sqrt{2}} \right\rangle = \frac{1}{2}(A - B + 2B - 2B - A + B) = 0$$

We can check this by noting that (in units of \hbar ,

$$\begin{aligned}A + B \sigma_p \cdot \sigma_n &= A + 4B \mathbf{s}_p \cdot \mathbf{s}_n = A + 2B(\mathbf{S}^2 - \mathbf{s}_p^2 - \mathbf{s}_n^2) \\ &= A + 2B \left[S(S+1) - \frac{3}{2} \right]\end{aligned}$$

For $S = 1$ this is $A + B$, For $S = 0$, it is $A - B$, and since $\langle S = 1 | \mathbf{S}^2 - 3/2 | S = 0 \rangle = 0$ by orthogonality of the triplet to singlet states, we get the same result as above.

7. We have, with $x = kr$ and $\cos \theta = u$,

$$\begin{aligned}I(x) &= \int_{-1}^1 du g(u) e^{-iux} = \int_{-1}^1 du g(u) \frac{i}{x} \frac{d}{dx} e^{-iux} \\ &= \frac{i}{x} \int_{-1}^1 du \frac{d}{du} (g(u) e^{-iux}) - \frac{i}{x} \int_{-1}^1 du \left(\frac{dg}{du} \right) e^{-iux}\end{aligned}$$

The first term vanishes since $g(\pm 1) = 0$. We can proceed once more, and using the fact that the derivatives of $g(u)$ also vanish at $u = \pm 1$, we find

$$I(x) = \left(\frac{-i}{x}\right)^2 \int_{-1}^1 du \left(\frac{d^2 g}{du^2}\right) e^{-ixu}$$

and so on. We can always go beyond any pre-determined power of $1/x$ so that $I(x)$ goes to zero faster than any power of $(1/x)$.

7. We proceed as in the photoelectric effect. There the rate, as given in Eq.(19-111) is

$$R = \frac{2\pi V}{\hbar} \int d\Omega \frac{mp_e}{(2\pi\hbar)^3} |M_{fi}|^2$$

Here m is the electron mass, and p_e is the momentum of the outgoing electron. The factor arose out of the phase space integral

$$\int dp p^2 \delta\left(\frac{p^2}{2m} - E_\gamma\right) = \int d\left(\frac{p^2}{2m}\right) mp \delta\left(\frac{p^2}{2m} - E_\gamma\right) = mp_e$$

with p_e determined by the photon energy, as shown in the delta function. In the deuteron photodisintegration process, the energy conservation is manifest in $\delta\left(\frac{p^2}{M} - E_\gamma + E_B\right)$.

The delta function differs in two respects: first, some of the photon energy goes into dissociating the deuteron, which takes an energy E_B ; second, in the final state two particles of equal mass move in equal and opposite directions, both with momentum of magnitude p , so that the reduced mass $M_{red} = M/2$ appears. Thus the factor mp_e will be replaced by $Mp/2$, where the momentum of the particle is determined by the delta function.

Next, we consider the matrix element. The final state is the same as given in Eq. (19-114) with p_e replaced by p , and with the hydrogen-like wave function replaced by the deuteron ground state wave function. We thus have

$$\frac{d\sigma}{d\Omega} = \frac{2\pi}{\hbar} \frac{(VMp/2)}{(2\pi\hbar)^3} \frac{V}{c} \left(\frac{e}{M}\right)^2 \frac{\hbar}{2\varepsilon_0\omega V} \frac{1}{V} (\boldsymbol{\varepsilon} \cdot \mathbf{p})^2 \left| \int d^3r e^{i(\mathbf{k}-\mathbf{p}/\hbar) \cdot \mathbf{r}} \psi_d(\mathbf{r}) \right|^2$$

We need to determine the magnitude of the factor $e^{i\mathbf{k} \cdot \mathbf{r}}$. The integral is over the wave function of the deuteron. If the ground state wave function behaves as $e^{-\alpha r}$, then the probability distribution goes as $e^{-2\alpha r}$, and we may roughly take $1/2\alpha$ as the "size" of the deuteron. Note that $\alpha^2 = ME_B / \hbar^2$. As far as k is concerned, it is given by

$$k = \frac{p_\gamma}{\hbar} = \frac{E_\gamma}{\hbar c}$$

Numerically we get, with $E_B = 2.2$ MeV, and $E_\gamma = 10$ MeV, $k/2\alpha = 0.11$, which means that we can neglect the oscillating factor. Thus in the matrix element we just need $\int d^3r e^{i\mathbf{k}\cdot\mathbf{r}} \psi_d(\mathbf{r})$. The wave function to be used is

$$\psi_d(r) = \frac{N}{\sqrt{4\pi}} \frac{e^{-\alpha(r-r_0)}}{r} \quad r > r_0$$

N is determined by the normalization condition

$$\frac{N^2}{4\pi} \int_{r_0}^{\infty} 4\pi r^2 dr \frac{e^{-2\alpha(r-r_0)}}{r^2} = 1$$

So that

$$N^2 = 2\alpha$$

The matrix element involves

$$\begin{aligned} & \frac{N}{\sqrt{4\pi}} \frac{4\pi}{k} \int_{r_0}^{\infty} r dr \sin kr \frac{e^{-\alpha(r-r_0)}}{r} = \\ & = \frac{N\sqrt{4\pi}}{k} \int_0^{\infty} dx \sin k(x+r_0) e^{-\alpha x} \\ & = \frac{N\sqrt{4\pi}}{k} \int_0^{\infty} dx (\sin kr_0 \operatorname{Re}(e^{-x(\alpha-ik)}) + \cos kr_0 \operatorname{Im}(e^{-x(\alpha-ik)})) \\ & = \frac{N\sqrt{4\pi}}{k} \left(\frac{\alpha}{\alpha^2 + k^2} \sin kr_0 + \frac{k}{\alpha^2 + k^2} \cos kr_0 \right) \end{aligned}$$

The square of this is

$$\frac{4\pi N^2}{k^2} r_0^2 \left(\frac{\alpha r_0}{\alpha^2 r_0^2 + k^2 r_0^2} \sin kr_0 + \frac{k r_0}{\alpha^2 r_0^2 + k^2 r_0^2} \cos kr_0 \right)^2$$

It follows that

$$\frac{d\sigma}{d\Omega} = 2 \left(\frac{e^2}{4\pi\epsilon_0 \hbar c} \right) \frac{p r_0}{M\omega} (\alpha r_0) \left[\frac{\alpha r_0}{\alpha^2 r_0^2 + k^2 r_0^2} \sin kr_0 + \frac{k r_0}{\alpha^2 r_0^2 + k^2 r_0^2} \cos kr_0 \right]^2$$

We can easily check that this has the correct dimensions of an area.

For numerical work we note that $\alpha r_0 = 0.52$; $k r_0 = 0.26 \sqrt{E_{MeV}}$ and $\hbar\omega = E_B + \frac{p^2}{M}$.

9. The change in the calculation consists of replacing the hydrogen wave function

$$\frac{1}{\sqrt{4\pi}} 2 \left(\frac{Z}{a_0} \right)^{3/2} e^{-Zr/a_0}$$

by

$$\begin{aligned} \psi(r) &= \frac{N}{\sqrt{4\pi}} \frac{\sin qr}{r} & r < r_0 \\ &= \frac{N}{\sqrt{4\pi}} \frac{e^{-\kappa r}}{r} & r > r_0 \end{aligned}$$

where the binding energy characteristic of the ground state of the electron determines κ as follows

$$\kappa^2 = 2m_e |E_B| / \hbar^2 = (m_e c \alpha / \hbar)^2$$

with $\alpha = 1/137$. The eigenvalue condition relates q to κ as follows:

$$qr_0 \cot qr_0 = -\kappa r_0$$

where

$$q^2 = \left(\frac{2m_e V_0}{\hbar^2} - \kappa^2 \right)$$

and V_0 is the depth of the square well potential. The expression for the differential cross section is obtained from Eq. (19-116) by dividing by $4(Z/a_0)^2$ and replacing the wave function in the matrix element by the one written out above,

$$\frac{d\sigma}{d\Omega} = \frac{2\pi}{\hbar} \frac{m_e p_e}{(2\pi\hbar)^3} \frac{1}{c} \left(\frac{e}{m_e} \right)^2 \frac{\hbar}{2\varepsilon_0 \omega} \frac{p_e^2}{4\pi} (\hat{\varepsilon} \cdot \hat{\mathbf{p}})^2 \left| \int d^3 r e^{i(\mathbf{k} - \mathbf{p}_e/\hbar) \cdot \mathbf{r}} \psi(r) \right|^2$$

We are interested in the energy-dependence of the cross section, under the assumptions that the photon energy is much larger than the electron binding energy and that the potential has a very short range. The energy conservation law states that under these assumptions $\hbar\omega = p_e^2 / 2m_e$. The factor in front varies as $p_e^3 / \omega \propto p_e \propto \sqrt{E_\gamma}$, and thus we need to analyze the energy dependence of $\left| \int d^3 r e^{i(\mathbf{k} - \mathbf{p}_e/\hbar) \cdot \mathbf{r}} \psi(r) \right|^2$. The integral has the form

$$\int d^3 r e^{i\mathbf{Q} \cdot \mathbf{r}} \psi(r) = \frac{4\pi}{Q} \int_0^\infty r dr \sin Qr \psi(r)$$

where $\mathbf{Q} = \mathbf{k} - \mathbf{p}_e / \hbar$ so that $Q^2 = k^2 + \frac{p_e^2}{\hbar^2} - 2 \frac{k p_e}{\hbar} (\hat{\mathbf{k}} \cdot \hat{\mathbf{p}})$.

Now $\hbar^2 k^2 / p_e^2 = \hbar^2 \omega^2 / p_e^2 c^2 = \hbar \omega \frac{p_e^2 / 2m}{p_e^2 c^2} = \frac{\hbar \omega}{2m_e c^2}$. We are dealing with the nonrelativistic regime, so that this ratio is much smaller than 1. We will therefore neglect the k -dependence, and replace Q by p_e / \hbar . The integral thus becomes

$$\frac{4\pi}{Q} \frac{N}{\sqrt{4\pi}} \left[\int_0^{r_0} dr \sin Qr \sin qr + \int_{r_0}^{\infty} dr \sin Qr e^{-\kappa r} \right]$$

The first integral is

$$\begin{aligned} & \frac{1}{2} \int_0^{r_0} dr (\cos(Q-q)r - \cos(Q+q)r) = \\ & \frac{1}{2} \left(\frac{\sin(Q-q)r_0}{Q-q} - \frac{\sin(Q+q)r_0}{Q+q} \right) \approx -\frac{1}{Q} \cos Qr_0 \sin qr_0 \end{aligned}$$

where, in the last step we used $Q \gg q$. The second integral is

$$\text{Im} \int_{r_0}^{\infty} dr e^{-r(\kappa - iQ)} = \text{Im} \frac{e^{-r_0(\kappa - iQ)}}{\kappa - iQ} \approx \frac{\cos Qr_0}{Q} e^{-\kappa r_0}$$

The square of the matrix element is therefore

$$\frac{4\pi N^2}{Q^2} \frac{1}{Q^2} (\cos Qr_0 (e^{-\kappa r_0} - \sin qr_0))^2$$

The square of the cosine may be replaced by 1/2, since it is a rapidly oscillating factor, and thus the dominant dependence is $1/Q^4$, i.e. $1/E_\gamma^2$. Thus the total dependence on the photon energy is $1/E_\gamma^{3/2}$ or $1/p_e^3$, in contrast with the atomic $1/p_e^7$ dependence.

10. The differential *rate* for process I, $a + A \rightarrow b + B$ in the center of momentum frame is

$$\frac{dR_I}{d\Omega} = \frac{1}{(2j_a + 1)(2J_A + 1)} \frac{1}{(2\pi\hbar)^3} p_b^2 \frac{dp_b}{dE_b} \sum_{spins} |M_I|^2$$

The sum is over all initial and final spin states. Since we have to *average* (rather than sum) over the initial states, the first two factors are there to take that into account. The phase factor is the usual one, written without specification of how E_b depends on p_b . The rate for the inverse process II, $b + B \rightarrow a + A$ is, similarly

$$\frac{dR_{II}}{d\Omega} = \frac{1}{(2j_b + 1)(2J_B + 1)} \frac{1}{(2\pi\hbar)^3} p_a^2 \frac{dp_a}{dE_a} \sum_{spins} |M_{II}|^2$$

By the principle of detailed balance the sum over all spin states of the square of the matrix elements for the two reactions are the same provided that these are at the same center of momentum energies. Thus

$$\sum_{spins} |M_I|^2 = \sum_{spins} |M_{II}|^2$$

Use of this leads to the result that

$$\frac{(2j_a + 1)(2J_A + 1)}{p_b^2(dp_b/dE_b)} \frac{dR_I}{d\Omega} = \frac{(2j_b + 1)(2J_B + 1)}{p_a^2(dp_a/dE_a)} \frac{dR_{II}}{d\Omega}$$

Let us now apply this result to the calculation of the radiative capture cross section for the process $N + P \rightarrow D + \gamma$. We first need to convert from rate to cross section. This is accomplished by multiplying the rate R by the volume factor V , and dividing by the *relative velocity* of the particles in the initial state. For the process I, the photo-disintegration $\gamma + D \rightarrow N + P$, the relative velocity is c , the speed of light. For process II, the value is $p_b/m_{red} = 2p_b/M$. Thus

$$\frac{d\sigma_I}{d\Omega} = \frac{V}{c} \frac{dR_I}{d\Omega}, \quad \frac{d\sigma_{II}}{d\Omega} = \frac{MV}{2p_b} \frac{dR_{II}}{d\Omega}$$

Application of the result obtained above leads to

$$\begin{aligned} \frac{d\sigma_{II}}{d\Omega} &= \frac{MV}{2p_b} \frac{dR_{II}}{d\Omega} \\ &= \frac{MV}{2p_b} \frac{p_a^2(dp_a/dE_a)}{(2j_b + 1)(2J_B + 1)} \times \frac{(2j_a + 1)(2J_A + 1)}{p_b^2(dp_b/dE_b)} \frac{c}{V} \frac{d\sigma_I}{d\Omega} \end{aligned}$$

We can calculate all the relevant factors. We will neglect the binding energy of the deuteron in our calculation of the kinematics.

First

$$\frac{(2j_\gamma + 1)(2J_D + 1)}{(2j_p + 1)(2J_N + 1)} = \frac{2 \times 3}{2 \times 2} = \frac{3}{2}$$

Next, in the center of momentum frame, the center of mass energy is

$$W = p_a c + \frac{p_a^2}{2M_D} \approx p_a c + \frac{p_a^2}{4M}$$

so that $(dE_a / dp_a) = c + \frac{p_a}{2M}$. In reaction II,

$$W = 2 \times \frac{p_b^2}{2M} = \frac{p_b^2}{M}$$

so that $(dE_b / dp_b) = 2p_b / M$. There is a relation between p_a and p_b since the values of W are the same in both cases. This can be simplified. For photon energies up to say 50 MeV or so, the deuteron may be viewed as infinitely massive, so that there is no difference between the center of momentum. This means that it is a good approximation to write $W = E_\gamma = p_a c = p_b^2 / M$. We are thus finally led to the result that

$$\frac{d\sigma(NP \rightarrow D\gamma)}{d\Omega} = \frac{3}{2} \left(\frac{E_\gamma}{Mc^2} \right) \frac{d\sigma(\gamma D \rightarrow NP)}{d\Omega}$$