PH107 (Autumn 2021): Tutorial solutions

Roshni Singh
Yuktee Gupta
Harshda Saxena
Vaishnav Rao
Mithil Vakde
Shashwat Chakraborty

Contents

Chapter 1

Tutorial 1

1.1 Photoelectric Effect

1.1.1 Question 1

Energy levels of Hydrogen atom are given by

$$E_n = -\frac{13.6}{n^2} \text{ eV} \tag{1.1}$$

The light emitted from the transitions of the hydrogen atom acts as the source of photons, each of energy $h\nu$ where ν is the frequency of the transition. We find the energy of the photons of each transition:

$$E = 13.6 \left(\frac{1}{n_f^2} - \frac{1}{n_i^2} \right) \text{ eV} \tag{1.2}$$

In the photoelectric effect, we know that the photon is absorbed by the electron, part of its energy is used in overcoming the work function of the material (ϕ), and the remaining is kinetic energy. The stopping potential is a measure of the maximum kinetic energy of the electron (stopping potential of V_s corresponds to a maximum kinetic energy of eV_s. This gives the following equation:

$$h\nu = \phi + eV_s \tag{1.3}$$

We use this expression along with the stopping potential given for each transition to find the three values work function, and find their average to arrive at our final answer for the work function of the material.

a) For $n = 4 \to n = 2$,

$$\begin{aligned} E_{4\to 2} = h\nu_1 &= 13.6 \times \left(\frac{1}{4} - \frac{1}{16} \right) \text{ eV} = 2.55 \text{ eV} \\ \phi_1 &= h\nu_1 - eV_s \\ &= (2.55 - 0.43) \text{ eV} = 2.120 \text{ eV} \end{aligned} \tag{1.4}$$

Similarly for $n = 5 \to n = 2$,

$$\begin{aligned} E_{5\to 2} = h\nu_2 &= 13.6 \times \left(\frac{1}{4} - \frac{1}{25} \right) \text{ eV} = 2.856 \text{ eV} \\ \phi_2 &= h\nu_2 - eV_s \\ &= (2.856 - 0.75) \text{ eV} = 2.106 \text{ eV} \end{aligned} \tag{1.5}$$

And for $n = 6 \rightarrow n = 2$,

$$\begin{aligned} E_{6\rightarrow 2} = h\nu_3 &= 13.6 \times \left(\frac{1}{4} - \frac{1}{36}\right) \text{ eV} = 3.022 \text{ eV} \\ \phi_3 &= h\nu_3 - eV_s \\ &= (3.022 - 0.94) \text{ eV} = 2.082 \text{ eV} \end{aligned} \tag{1.6}$$

Using the values of ϕ_1, ϕ_2, ϕ_3 from above we get,

$$\phi_{avg} = \frac{1}{3}(\phi_1 + \phi_2 + \phi_3) = 2.103 \text{ eV} \tag{1.7}$$

b) Balmer line ($n_f = 2$) of shortest wavelength corresponds to max energy difference, so $n_i = \infty$

$$\begin{aligned} h\nu &= \frac{13.6}{4} \text{ eV} = 3.4 \text{ eV} \\ eV_s &= h\nu - \phi_{avg} \\ V_s &= 1.297 \text{ V} \end{aligned} \tag{1.8}$$

c) The highest energy transition of the Paschen series $n = \infty \rightarrow n = 3$, has energy $= 13.6/9$ eV $= 1.51$ eV. Since this is less than the workfunction of the metal, we get no photocurrent.

1.1.2 Question 2

Recall that the stopping potential is that potential difference which is just sufficient to halt the most energetic photoelectrons emitted, and thereby reduce the current measured to 0. Thus, for a stopping potential V_0, the photoelectrons have the maximum Kinetic Energy as given by -

$$KE_{max} = eV_0$$

We also know from Einstein's theory of Photoelectric effect :

$$KE_{max} = h(\nu - \nu_0)$$

where h is the Planck's constant, ν, ν_0 are the incident frequency and threshold frequency respectively. Thus, we solve the following linear equations :

$$\begin{aligned} 1.6 * 10^{-19} * 4.62 &= h\left(\frac{3 * 10^8}{1850 * 10^{-10}} - \nu_0\right) \\ 1.6 * 10^{-19} * 0.18 &= h\left(\frac{3 * 10^8}{5460 * 10^{-10}} - \nu_0\right) \end{aligned}$$

Dividing the two and solving for ν_0, we get $\nu_0 = 5.06 * 10^{14}$Hz.
Plugging this into either of the equations, we get $h = 6.63 * 10^{-34}$Js.
(Round off to 3 significant digits).

1.1.3 Question 3

Given: Intensity of incident light (I)= $1.0\mu W/cm^2$, area of metal surface (a)= $1cm^2$, Work function of metal $\phi = 4.5eV$, absorption efficiency of the metal (A)= 3%, conversion efficiency (η)= 100%, and saturation current (I_s)= 2.4 nA

a) Number of electrons emitted per second= I_s/e. As conversion efficiency is 100%, no. of photons absorbed per second = no. of electrons emitted per second. Thus, no. of photons incident per second = no. of photons absorbed per second/ absorption efficiency = $I_s/(A \times e) = 5 \times 10^{11}$

b) Incident power (P)= $I \times a = 10^{-6}W$. Now,

$$\text{Energy per photon} = \frac{\text{Incident power}}{\text{no. of photons incident per second}} = \frac{P \times A \times e}{I_s} J$$

Thus,

$$\text{Energy of incident photon } (eV) = \frac{P \times A}{I_s} eV = 12.5eV$$

c) Kinetic enegy of ejected electron = $12.5 - 4.5$ eV= 8 eV. Thus, stopping potential = $8V$

1.1.4 Question 4

a) Find the slopes of this graph (approximate values are fine). We get slope = 86.9 for 480nm and 202.9 for 613nm. Extend the lines to the point of no current (0nA). The potential difference here is the stopping potential.

$$86.9 = \frac{76.3 - 0}{-0.1 + V_s} \implies V_s \approx 0.98V$$

and

$$202.9 = \frac{64.7 - 0}{-0.1 + V_s} \implies V_s \approx 0.42V$$

Using the standard equations, you can get the work function and cutoff wavelength easily.
Work function = 1.6 eV, Cutoff wavelength ≈ 770nm

b) Max K.E is charge times stopping potential. Answer = 0.98eV
To find the required photon energy, add the work function to half the Max K.E. Convert this to wavelength using the standard relation. Answer ≈ 590 nm

c) Energy is proportional to frequency.
Frequency increases 1.2x $\implies$ Energy increases 1.2x
Hence work function of new material = $1.2 \times 1.6eV = 1.92eV$

1.1.5 Question 5

$$\frac{hc}{\lambda} = \phi + KE_{max}.$$

Given $\phi = 4.2eV$. So

$$\frac{12400}{2000} = 4.2 + KE_{max} \implies KE_{max} = 2.0eV.$$

Note that the value of KE_{max} is much less than the rest mass energy of electron which is $0.51MeV$ so our non-relativistic assumption is more or less justified.
Slowest moving electrons are those moving with zero velocity, hence zero kinetic energy.

$$\text{Stopping potential} = \frac{KE_{max}}{e} = 2V.$$

Let the cutoff wavelength be denoted by λ'. It is calculated using

$$\frac{hc}{\lambda'} = \phi \implies \lambda' = \frac{hc}{\phi} = \frac{12400}{4.2}\ \text{Å} = 2952.38\ \text{Å}.$$

1.2 Black Body Radiation

1.2.1 Question 1

Given the spectral energy density $u(\lambda)$ for a **fixed T**:

$$u(\lambda, T) = \frac{8\pi hc}{\lambda^5} \cdot \frac{1}{\exp\frac{hc}{K_bT\lambda} - 1}$$

For part a, to find the value of λ_{max} for which $u(\lambda)$ is maximised, we can now differentiate wrt. λ directly since **we have a fixed T**, and equate it to zero.

$$\frac{du}{d\lambda} = 0$$

$$-5\frac{8\pi hc}{\lambda^6} \cdot \frac{1}{\exp\frac{hc}{K_bT\lambda} - 1} + \frac{hc}{K_bT\lambda^2} \cdot \frac{8\pi hc}{\lambda^5} \cdot \frac{\exp\frac{hc}{K_bT\lambda}}{\exp\frac{hc}{K_bT\lambda} - 1^2} = 0$$

$$5\frac{K_bT\lambda}{hc} = \frac{\exp\frac{hc}{K_bT\lambda}}{\exp\frac{hc}{K_bT\lambda} - 1}$$

We can solve this graphically; replace $\frac{hc}{K_bT\lambda}$ as x and plot $\frac{5}{x}$ and $\frac{e^x}{e^x-1}$, their intersection is the solution for x. (here we ignore x=0,$-\infty$)
Now $\lambda_{max} = \frac{hc}{4.965K_bT}$.

For part b, replace $\lambda_{max} = \frac{\alpha}{T}$, then :

$$u_{max}(T) = \frac{8\pi hcT^5}{\alpha^5} \cdot \frac{1}{\exp\frac{hc}{K_b\alpha} - 1}$$

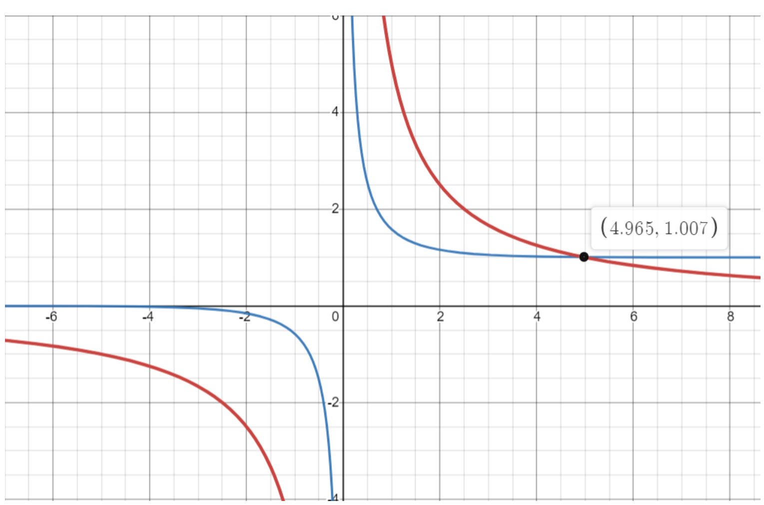


Figure 1.1: Source:Desmos, here seen the red curve $(5/x)$ and blue curve $(\frac{e^x}{e^x-1})$ intersect at 4.965 which is our solution for x

1.2.2 Question 2

Power radiated by a black body = σAT^4 (Stefan-Boltzmann law).

Therefore power radiated by the sun,P_s= $\sigma(4\pi R_s^2)T_s^4$.

Intensity of radiation from the sun at the earth = $\frac{P_s}{4\pi D^2}$, where D is the distance between the sun and the earth.

Therefore power absorbed by the earth from the sun's radiation = $\frac{P_s}{4\pi D^2} \times \pi R_e^2$.

Power radiated by the earth, = $\sigma(4\pi R_e^2)T_e^4$.

For equilibrium, Power radiated by the earth = power absorbed by the earth,

Therefore,

$$\begin{aligned} \sigma(4\pi R_e^2)T_e^4 &= \frac{\sigma(4\pi R_s^2)T_s^4}{4\pi D^2} \times \pi R_e^2 \\ T_e &= \left(\frac{R_s T_s^2}{2D}\right)^{\frac{1}{2}} = 424.26K \end{aligned} \tag{1.9}$$

1.2.3 Question 3

Since Rayleigh-Jeans is not covered explicitly in the lectures, lets have an overview first. Physicists were concerned with a theoretical formulation of the spectral energy density (energy per unit volume per unit frequency) of the radiation within a blackbody, written as $u(f,T)$.

Wiens exponential Law

A dude called Wien (hopefully he wasn't bullied a lot) "guessed" (yes, that happens a lot in physics) the form of this as :

$$u(f,T) = Af^3 e^{-\beta f/T}$$

with A and B as constants. This is called Wien's Exponential Law, however it failed to explain the curve in low energy regions (for higher λ).

Rayleigh Jeans Law

They had a nicer approach, and likened a standing EM wave inside the blackbody to a 1-D CLASSICAL oscillator and used some statistical mechanics (dont worry about this now) to finally come to the conclusion :

$$u(f,T)df = \frac{8\pi f^2}{c^3} k_B T df$$

However, this failed at the high energy regions (for shorter λ), and this is what is known as the ultraviolet catastrophe.

Planck's Law

Ma boi Planck considered discrete values of energy for the now QUANTUM oscillator description, again using some statistical mechanics and building upon the work by Rayleigh Jeans, came to the conclusion of the following law:

$$u(f,T)df = \frac{8\pi f^2}{c^3}\left(\frac{hf}{e^{hf/k_BT}-1}\right)df$$

All the three are compared in the following plot:

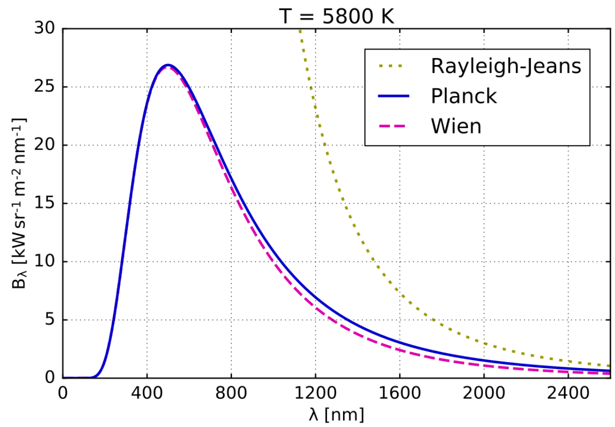


Figure 1.2: The comparison of the following descriptions, and we know that Planck's description explains experimentally found values perfectly

Finally, onto the question

a)Now that we know Rayleigh Jeans fails at short λ, we use the approximation of very high λ. We have :

$$u(\lambda,T) = \frac{8\pi hc}{\lambda^5}\frac{1}{e^{\frac{hc}{\lambda k_BT}}-1}$$

In the high λ limit, the exponential factor becomes negligible, we approximate the denominator as

$$exp\left(\frac{hc}{\lambda k_BT}-1\right) \approx \frac{hc}{\lambda k_BT}$$

using which, we finally get the Planckian limit as -

$$u(\lambda,T)d\lambda = \frac{8\pi}{\lambda^4}k_BTd\lambda$$

Now, we consider the RHS of the Rayleigh-Jeans as presented in the short description. A SUBTLETY here is that we need to find the corresponding relation for the energy density, which is the final integral from 0 to ∞ and hence "df is multiplied" both sides. While doing a change in variables, in general, the derivative of the variable might have a functional dependence, which we need to incorporate too. We retain df, and do the following calculation:

$$\begin{aligned} u(f,T)df &= \frac{8\pi f^2}{c^3}k_BTdf \\ &= \frac{8\pi c^2}{\lambda^2 c^3}k_BTd(\frac{c}{\lambda}) \\ &= \frac{8\pi}{\lambda^2}k_BT\frac{1}{\lambda^2}d\lambda \\ u(\lambda,T)d\lambda &= \frac{8\pi}{\lambda^4}k_BTd\lambda \end{aligned}$$

(The - sign is accounted for in the change of limits in the integration finally).
This is the same as the limit of the Planck's law, and hence Rayleigh Jeans formula is obtained given Planck's formula.
b) This basically means that for ν_0, the Rayleigh-Jeans formula gives a value 10 times that of Plancks formula, that is:

$$\frac{8\pi\nu_0^2}{c^3}k_BT = 10 * \frac{8\pi\nu_0^2}{c^3}\frac{h\nu_0}{e^{h\nu_0/kBT}-1}$$

Let $x = \frac{h\nu_0}{k_BT}$, thus the implicit equation becomes:

$$e^x - 1 = 10x$$

c) Draw the graph, and calculate the $h(x) = e^x - 1 - 10x$ for integer values of 1,2,3 and 4 of x. Using Intermediate Value theorem, note that the sign changes between $x = 3$ and $x = 4$. Thus the root lies between them. Do the same for 0.1 increments in this range, and you will find that the sign changes between 3.6 and 3.7. Similarly for the next decimal place to round off, you will finally find that $x = 3.6$ is the correct solution.

1.2.4 Question 4

We know that Planck's formula for the spectral energy density in terms of wavelength is given by

$$u(\lambda,T)d\lambda = \frac{8\pi hc}{\lambda^5(e^{hc/\lambda k_BT}-1)}d\lambda$$

To find the wavelength at which the function $u(\lambda,T)$ peaks, we differentiate the function with respect to λ and equate it to zero. Thus,

$$8\pi hc\left(\frac{-5}{\lambda^6(e^{hc/\lambda k_BT}-1)} + \frac{1}{\lambda^5(e^{hc/\lambda k_BT}-1)^2} \times \frac{hc}{\lambda^2 k_BT}\right) = 0$$

Writing $hc/\lambda k_BT$ as x, this simplifies to the transcendental equation

$$5(e^x - 1) = xe^x \implies (x-5)e^x + 5 = 0$$

Using Desmos, this can be graphed to get an exact solution ($x = 4.965$). However, if we make the approximation that $e^x \approx e^x - 1$, we get $x \approx 5$ (which agrees with our approximation). Thus,

$$\frac{hc}{\lambda_{max}k_BT} \approx 5 \implies \lambda_{max}T \approx 2.88 \times 10^{-3}$$

which agrees very well with the Wein's constant of 2.89×10^{-3}

1.3 Compton Effect

1.3.1 Question 1

This is a simple question requiring:

- The wavelength formula to calculate incident frequency ν_0
- Conservation of momentum to calculate recoil angle ϕ

Incident frequency:

$$\lambda' = \lambda_0 + \lambda_c(1 - \cos\theta)$$
$$2\lambda_0 = \lambda_0 + \lambda_c(1 - \cos\frac{\pi}{2})$$
$$\lambda_0 = \lambda_c$$
$$\frac{c}{\nu_0} = \lambda_c$$
$$\implies \boxed{\nu_0 = \frac{m_e c^2}{h}}$$

Recoil Angle:
(Draw the momentum diagram yourself to verify!)
Let the final momentum of electron be p_e. You get 2 equations:

$$\text{Parallel conservation: } \frac{h}{\lambda_0} = p_e \cos\phi$$

$$\text{Perpendicular conservation: } \frac{h}{2\lambda_0} = p_e \sin\phi$$

$$\implies \boxed{\phi = \arctan(\frac{1}{2})}$$

1.3.2 Question 2

We can approximate $\sqrt{1 + \frac{E_0^2}{E^2}}$ by checking that $\frac{1}{8}(\frac{1}{2.5})^2 << 1$. So we can use the non-relativistic method to a good extent.

$$\lambda' = \lambda_0 + \lambda_c(1 - \cos\theta).$$

Maximum kinetic energy of electron corresponds to maximum λ' *i.e.* wavelength of scattered photon, hence to $\theta = \pi$. So

$$\lambda'_{max} = \lambda_0 + 2\lambda_c.$$

From energy conservation we have

$$\frac{hc}{\lambda_0} = \frac{hc}{\lambda'_{max}} + \frac{m_e c^2}{2.5}.$$

Substituting the first expression for λ'_{max} (in terms of λ_0) in the second expression we get the solution for λ_0 as

$$\lambda_0 = (\sqrt{6} - 1)\lambda_c.$$

$$E_{X-ray} = \frac{hc}{\lambda_0} = \frac{m_e c^2}{\sqrt{6} - 1} = 0.69 m_e c^2$$

1.3.3 Question 3

Let us first show photoelectric effect is not possible with a free electron. Initially, we have a free electron, and a photon with some wavelength λ. Without a loss of generality, we can assume initial momentum of the electron is 0 (if not, shift to a frame where it is zero). After the electron absorbs the photon, let it have some momentum p. Now conserving momentum:

$$\frac{h}{\lambda} + 0 = p$$

And conserving energy(accounting for rest-mass of the electron as well since non negligible here):

$$\frac{hc}{\lambda} + \sqrt{(m_e c^2)^2 + (0.c)^2} = \sqrt{(m_e c^2)^2 + (p.c)^2}$$

using p from the momentum:

$$\rightarrow 2\frac{hc^3 m_e}{\lambda} = 0$$

Which implies either $m_e = 0$, which is not possible or initial momentum of the photon, $\frac{h}{\lambda} = 0$ which implies no collision took place. Thus photoelectric effect is not possible for a free electron.
On the other hand, Let us see Compton effect. Again, we assume initial momentum of the electron to be zero, and a photon of wavelength λ striking it. The electron say, finally is propelled with a momentum $\vec{p}$ making angle θ with the initial direction of photon, and the photon is scattered with wavelength λ' making an angle ϕ in the opposite direction.
Conserving momentum:

$$\frac{h}{\lambda} + 0 = pcos(\theta) + \frac{h}{\lambda'}cos(\phi)$$

$$psin(\theta) = \frac{h}{\lambda'}sin(\phi)$$

Conserving energy:

$$\frac{hc}{\lambda} + \sqrt{(m_e c^2)^2 + (0.c)^2} = \sqrt{(m_e c^2)^2 + (p.c)^2} + \frac{hc}{\lambda'}$$

Solving these equations, doesn't give any contradiction, and non zero values of p can be found, hence Compton effect for a free electron is possible, since photon absorption and re-emission is taking place.

1.3.4 Question 4

Recall the change in wavelength due to Compton scattering as derived in the lectures :

$$\lambda' - \lambda = \frac{h}{m_0 c}(1 - \cos\theta)$$

Where $\lambda_c = \frac{h}{m_0 c}$ is the Compton wavelength and m_0 is the mass of the scatterer. We assume that both the experiments were performed on the same target material.
a) For the first experiment, $\Delta\lambda = 7 \times 10^{-14}$m and $\theta = 45°$

$$7 \times 10^{-14} = \lambda_c(1 - \frac{1}{\sqrt{2}})$$

$$\lambda_c = 2.4 \times 10^{-13} m \quad \text{(Compton Wavelength)}$$

$$m_0 = 0.92 \times 10^{-29} Kg \quad \text{(Mass of scatterer)}$$

b) For the second experiment, $\lambda' = 9.9 \times 10^{-12}$m and $\theta = 60°$, and let λ_2 be the incident wavelength

$$9.9 \times 10^{-12} - \lambda_2 = 2.4 \times 10^{-13}(1 - \frac{1}{2})$$
$$\lambda_2 = 9.8 \times 10^{-12} m$$
$$\lambda_1 = 4.9 \times 10^{-12} m$$

since $E_2 = E_1/2 \implies \lambda_2 = 2 \times \lambda_1$.

1.3.5 Question 5

Let the minimum possible energy of the photon for 50% energy transfer be E ($= E_i$) and thus, $E_f = E/2$. For the Compton effect, the equation is:

$$\begin{aligned}
\Delta\lambda &= \frac{h}{m_e c}(1 - \cos\theta) \\
\implies hc\left(\frac{1}{E_f} - \frac{1}{E_i}\right) &= \frac{h}{m_e c}(1 - \cos\theta) \\
\implies \frac{1}{E} &= \frac{1}{m_e c^2}(1 - \cos\theta) \\
\implies E &= \frac{m_e c^2}{(1 - \cos\theta)}
\end{aligned} \tag{1.10}$$

For minimum possible energy, take $\cos\theta = -1$, m

$$E = \frac{1}{2} m_e c^2 = 0.255 MeV$$

1.3.6 Question 6

Consider the expression for wavelength shift for Compton scattering as derived in class:

$$\lambda' - \lambda_0 = \frac{h}{m_e c}(1 - \cos\theta)$$

Note that this was derived **without** any approximations. Since it is given in the question that we are detecting back-scattered radiation, $\theta = 180°$. Plugging this in, we get the answer to part a. Now, the wavelength of the scattered radiation is

$$\lambda' = \frac{2h}{m_e c} + \lambda_0$$

Dividing both sides by hc, we get the energy of scattered radiation to be

$$\frac{1}{E'} = \frac{2}{m_e c^2} + \frac{1}{E}$$

But, we are given that $E >> m_e c^2$. Hence, we can safely neglect the second term on the RHS with respect to the first and get the energy of scattered radiation to be

$$E' = \frac{m_e c^2}{2}$$

This answers part b. Now, by energy conservation, we have

$$E + m_e c^2 = E' + E_e \implies E_e - m_e c^2 = E - E' = E - \frac{m_e c^2}{2}$$

Which is just the recoil kinetic energy of the electron. Plugging in the values for part c and taking the rest mass energy of an electron to be 0.5110 MeV, we get the recoil kinetic energy of the electron to be 149.7445 MeV.

1.3.7 Question 7

This question isn't correct. Here are some correct concepts related to what the question is trying to say:

Let us take $k = \frac{E}{m_0 c^2}$ and $k' = \frac{E'}{m_0 c^2}$ (Hence we are re-scaling the photon energy in terms of the rest mass energy of the electron)

$$E' = \frac{hc}{\lambda'}$$

$$E' = \frac{hc}{\lambda + \lambda_c(1 - \cos\theta)}$$

$$E' = \frac{hc}{\frac{hc}{E} + \frac{hc}{m_0 c^2}(1 - \cos\theta)}$$

$$E' = \frac{1}{\frac{1}{E} + \frac{1}{m_0 c^2}(1 - \cos\theta)}$$

$$\frac{E'}{m_0 c^2} = \frac{1}{\frac{m_0 c^2}{E} + (1 - \cos\theta)}$$

$$k' = \frac{1}{\frac{1}{k} + (1 - \cos\theta)} \tag{1.11}$$

Now we can treat k and k' as energy terms. (In fact, they are energy terms, but in different scales. You can make sense of this as dividing all the SI units in physics by $m_0 c^2$. Hence we are doing the same physics, but in different units.)

Equation (11) relates the energy of the scattered photon k' to the energy of the incoming photon k when the photon scattering angle θ is given. It is easy to see that for any fixed angle, increasing the incoming energy increases the scattered photon energy. (Put the equation in a graphing calculator yourself and mess around!). From the figure below, you can see that energy peaks at 0 and is minimum at 180 degrees.

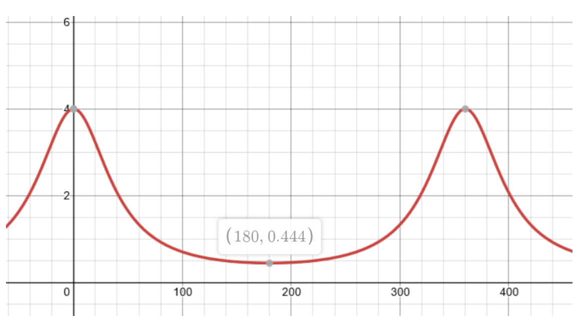


Figure 1.3: Value of outgoing photon energy k' vs scattering angle (in degrees) for k = 4

Now taking the limit of the incoming photon energy tending to infinity ($k \to \infty$), we get: (Plotted below)

$$k' = \frac{1}{1 - \cos\theta}$$

Obviously, any value of k' must lie below this line. Hence ***for every scattering angle, there is a maximum*** for the energy of scattered photon, but ***overall there is no maximum*** as we can get arbitrarily large values of energy for scattering angles close to 0 degrees. (For example, at 180 degrees, the max energy is $0.5m_0c^2$)

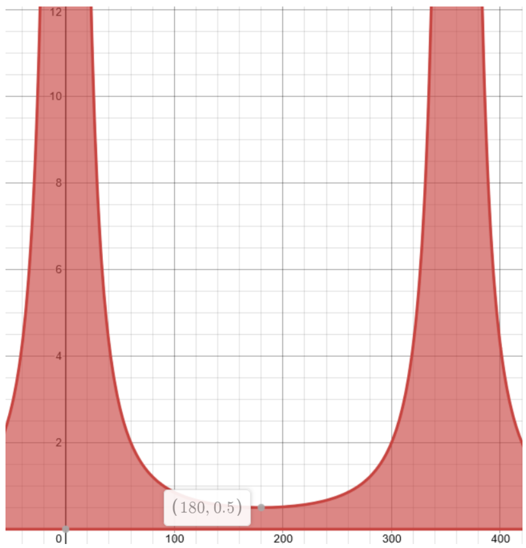


Figure 1.4: Limit of k' vs scattering angle (in degrees) for infinite k

1.3.8 Question 8

$$\lambda_2 = \lambda_1 + \lambda_c(1 - \cos\theta),$$
$$\lambda_3 = \lambda_2 + \lambda_c(1 - \cos\frac{\pi}{2} - \theta).$$

(a) Adding the two equations and doing some manipulations we get

$$\sin 2\theta = (2 - \frac{\Delta\lambda}{\lambda_c})^2 - 1 = 0.867 = \sin\frac{\pi}{3} = \sin\frac{2\pi}{3} = ...$$

But clearly the angle θ shown in figure lies between $\frac{\pi}{4}$ and $\frac{\pi}{2}$. So $\theta = \frac{\pi}{3}$ is the solution.
(b)

$$\lambda_1 = \lambda_2 - \frac{h}{mc}(1 - \cos\theta) = 0.068 - 0.00243(1 - \cos\frac{\pi}{3}) = 0.066785nm$$

From momentum conservation, we have

$$p_e \sin\phi = \frac{h}{\lambda_2}\sin\theta,$$
$$p_e \cos\phi = \frac{h}{\lambda_1} - \frac{h}{\lambda_2}\cos\theta.$$

Dividing the two equations we get

$$\tan\phi = \frac{\frac{\sin\theta}{\lambda_2}}{\frac{1}{\lambda_1} - \frac{\cos\theta}{\lambda_2}} = 1.67 \implies \phi = 59.1°.$$

Chapter 2

Tutorial 2

2.1 de Broglie Wavelength

2.1.1 Question 1

This is a fairly straightforward question to get you used to order of magnitude estimates.

$$\lambda = \frac{h}{p} \tag{2.1}$$

Note that we need to use the relativistic expression for momentum wherever applicable (i.e. $p = \gamma m_0 v$).

For a car of mass 2000 kg, and v = 100 km/h = 27.78 m/s, it is sufficient to consider the non-relativistic momentum since $v << c$.

$$\begin{aligned}\lambda &= \frac{6.626 \times 10^{-34}}{2000 \times 27.78} \text{ m} \\ &= 1.19258 \times 10^{-38} \text{ m}\end{aligned} \tag{2.2}$$

This is obviously very small compared to the actual dimensions of a macroscopic car (4-5 m), and hence it is not possible to observe the wave nature and too small to measure with any reasonable apparatus.

For the cricket ball also, it is sufficient to use the nonrelativistic value of momentum.

$$\begin{aligned}\lambda &= \frac{6.626 \times 10^{-34}}{0.28 \times 40} \text{ m} \\ &= 5.916 \times 10^{-35} \text{ m}\end{aligned} \tag{2.3}$$

While this is a few orders of magnitude higher than the de Broglie wavelength of the car, it is still not possible to observe the wave nature since it is negligible compared to the dimension of the cricket ball (around 10 cm), and too small to measure with any reasonable apparatus.

For the electron, we may consider the relativistic momentum.

$$\begin{aligned}p &= \frac{mv}{\sqrt{(1 - v^2/c^2)}} \\ &= 9.315 \times 10^{-24}\end{aligned} \tag{2.4}$$

$$\lambda = \frac{6.626 \times 10^{-34}}{0.28 \times 40} \text{ m}$$
$$= 7.11 \times 10^{-11} \text{ m} \tag{2.5}$$

This can be measured, and is comparable to the size of an atom (few Å) within which the electron can be considered to be localised. The wave nature can thus be observed.

2.1.2 Question 2

We will use the wave nature of the electron to make sense of the Bohr's quantization condition, which was a purely observational result. The de Broglie wavelength of an electron $\lambda_{dB} = h/p_e$. If we somehow manage to show that the allowed orbits are precisely the ones that can be exactly spanned by an integer multiple of the de Broglie wavelength, then we can infer that the electron forms standing waves along the orbital circumference. Just have a look at the following figure. Things will make more sense.

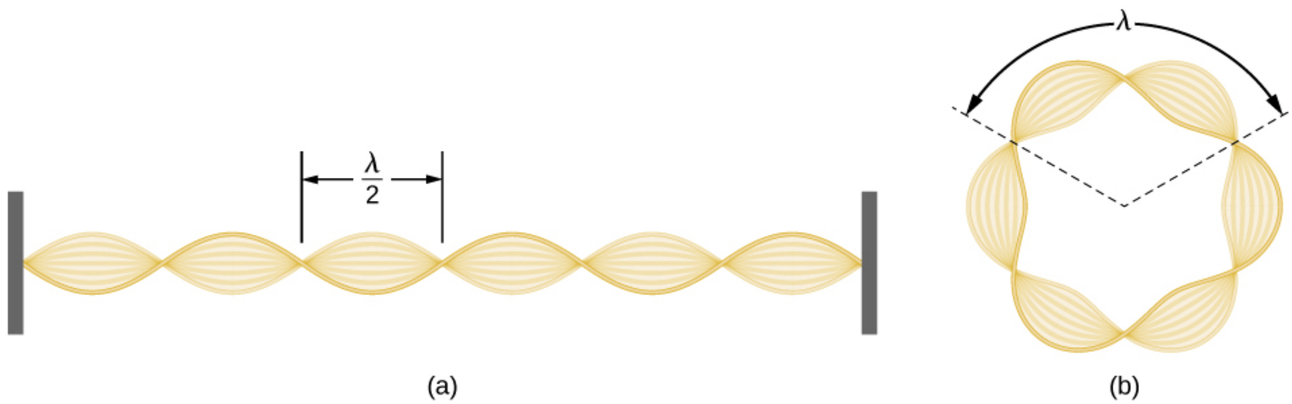


Figure 2.1: Standing waves on (a) a string tied between two rigid supports; (b) the orbital circumference

You may be wondering why the circumference has to be $n\lambda$ and not $n\lambda/2$. The problem with the odd multiples of $\lambda/2$ is that it causes "*destructive interference*". For stability, the "*wave function*" of the electron must match itself after completing a 2π cycle. Don't worry if you are unable to understand the above statement right now because you will learn stuff like this in detail in your quantum chemistry course!

Recall the Bohr's quantization condition: "*The angular momentum of the electron is an integer multiple of $h/2\pi$.*"

$$L = r_n p_e = n\frac{h}{2\pi} \tag{2.6}$$

$$2\pi r_n = n\frac{h}{p_e} \tag{2.7}$$

$$2\pi r_n = n\lambda_{dB} \tag{2.8}$$

Hence, the orbital circumference is the an integer multiple of the electron's de Broglie wavelength. This is what we wanted to show!

2.1.3 Question 3

a) We know that the wavelength of a photon is given by

$$\lambda = \frac{hc}{E} = \frac{6.625 \times 10^{-34} \times 3 \times 10^{8}}{5 \times 10^{3} \times 1.6 \times 10^{-19}} = 0.248 \text{ nm}$$

b) The de-Broglie wavelength of a matter particle is given by (non-relativistically)

$$\lambda = \frac{h}{p} = \frac{h}{\sqrt{2m(KE)}}$$

For an electron,

$$\lambda_e = \frac{h}{\sqrt{2 \times 500 \times 5}} \times \frac{c}{keV} = 0.0176 \text{ nm}$$

c) For a neutron,

$$\lambda_n = \frac{h}{\sqrt{2 \times 1000 \times 5}} \times \frac{c}{\text{keV}} = 0.0124 \text{ nm}$$

2.1.4 Question 4

A case of sequential logic:

1. Temperature is related to the thermal kinetic energy.
2. Thermal kinetic energy is related to momentum
3. Momentum is related to the de Broglie wavelength

$$\text{Kinetic Energy } = K_B T = \frac{p^2}{2m_p}$$

$$\implies T = \frac{p^2}{2m_p K_B}$$

$$T = \frac{(\frac{h}{\lambda})^2}{2m_p K_B}$$

$$T = \frac{(\frac{h}{2r_1})^2}{2m_p K_B}$$

$$T = \frac{h^2}{8r_1^2 m_p K_B}$$

$$T \approx 847K$$

2.2 Interference, Diffraction, YDSE, Davison-Germer experiment

2.2.1 Question 1

A single molecule of Buckminster Fullerene C_60 has rest mass $m_0 = 60 \times 12 \times 1.67262 * 10^{-27}$ kg $=$ $1204.2864 * 10^{-27}$ kg. Notice that

$$p = \gamma m_0 v = \frac{m_0 v}{\sqrt{1 - \frac{v^2}{c^2}}} \approx m_0 v (1 + \frac{1}{2}\frac{v^2}{c^2}) \approx m_0 v$$

since $\frac{m_0 v^3}{2c^2} <<< 1$.
(a) de Broglie Wavelength

$$\lambda = \frac{h}{p} = \frac{h}{m_0 v} = \frac{6.626 * 10^{-34}}{1204.2864 * 10^{-27} \times 100} m = 0.0055 * 10^{-9} \text{ m} = 0.0055 \text{ nm}$$

(b) Frindge width

$$\beta = \frac{\lambda D}{d} = \frac{0.0055}{150} \times 1.25\text{m} = 45.85\ \mu\text{m}.$$

(c) Distance between consecutive frindges is approximately 45850 times more than the diameter of buckballs. Visibility of interference frindges gets disrupted if size of buckballs become comparable to frindge width as we cannot treat the molecules as point particles then. Basically we want to find the initial velocity v such that

$$10\ \text{Å} = \frac{\lambda D}{d} = \frac{\frac{h}{m_e v} D}{d}.$$

This gives us $v = 4.598 \times 10^6$ m/s.

2.2.2 Question 2

We have both the $\vec{k}$ vectors given, hence can write the equations of two waves, w_1 and w_2, with amplitudes A_1 and A_2 as :

$$w_1 = A_1 \cdot e^{i(\frac{2\pi}{\lambda}(x+y+z) - \sqrt{3}wt)}$$
$$w_2 = A_2 \cdot e^{i(\frac{2\pi}{\lambda}(z) - wt)}$$

The resultant sum can then be written as:

$$w = w_1 + w_2$$
$$w = A_1 \cdot e^{i(\frac{2\pi}{\lambda}(x+y+z) - \sqrt{3}wt)} + A_2 \cdot e^{i(\frac{2\pi}{\lambda}(z) - wt)}$$
$$w = A_1 \cdot e^{i(\frac{2\pi}{\lambda}(x+y+z) - wt)} \cdot (e^{(1-\sqrt{3})wt} + \frac{A_2}{A_1} e^{-i(\frac{2\pi}{\lambda}(x+y))})$$

Though it isn't mentioned in the question, we can assume the amplitudes to be the same, i.e., $A_1 = A_2 =$ A. (if not we just have to simplify the previous expression)

$$w = A \cdot e^{i(\frac{2\pi}{\lambda}(z) - wt)} \cdot (1 + e^{i(\frac{2\pi}{\lambda}(x+y)) + (1-\sqrt{3})wt})$$

Now, Intensity is proportional to $|w|^2$ ie:

$$I = A^2 \cdot 2(1 + \cos(\frac{2\pi}{\lambda}(x+y) + (1-\sqrt{3})wt))$$

This, if plotted will show up as sinusoidal variations in intensity traveling along the $x = y$ line, and as constant intensity along lines with slope -1.

2.2.3 Question 3

Note that distance between slits (d) $= 0.8mm = 8\times10^{-4}m$ and distance between screen and plane of slits (D) $=$ $1.6m$. Since $d << D$, we consider the approximation $\sin\theta \approx \tan\theta = \frac{y}{D}$ is valid, for small enough y, which is the distance from the centre on the screen.

a) Roughly, the intensity pattern looks something like –

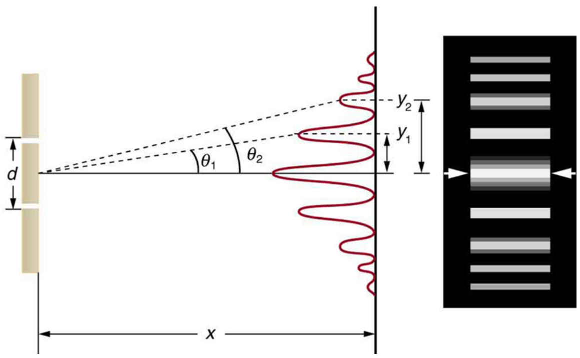


Figure 2.2: The intensity pattern at the screen

With the broad effect of diffraction visible at larger distances, and hence decreasing the amplitude (and hence Intensity) of the successive maxima formed by the interference through the two slits.

b) For a maxima, assuming the distance calculated is within the above approximation limit, we have

$$d\frac{\Delta y}{D} = \Delta n\lambda$$
$$\implies \lambda = 8 \times 5 \times 10^{-7}/1.6$$
$$\implies \lambda = 2500 \text{ nm}$$

c) Here, covering the slits with a thin film changes the effective distance travelled by light, and hence the interference pattern. The central maxima is usually at distance 0, or for equal path lengths from the two slits. Note that after the introduction of a slab with refractive index μ and thickness x, the net change in path length using the above approximation is $(\mu - 1)x$. Thus, we have the central maximum to now occur at:

$$(\mu - 1)x = \frac{yd}{D}$$
$$\text{Fringe width} = \frac{\lambda D}{d}$$
$$\implies (\mu - 1)x = \frac{2.2\lambda D/d \times d}{D}$$
$$\implies x = 2.2 \times 2500/0.4nm$$
$$\implies x = 0.014mm$$

d) Using the superposition principle, the net intensity on the screen would be the superposition of the individual interference patterns. According to the above question, for $\lambda_1 = 450nm$ and $\lambda_2 = 600nm$ we have the first case:

$$\begin{aligned} d\sin\theta &= n\lambda_1 \\ d\sin\theta &= (m+1/2)\lambda_2 \\ \implies 3n &= 4m+2 \end{aligned}$$

Which holds at the lowest order for $n = 2$ and $m = 1$, and for the second case :

$$\begin{aligned} d\sin\theta &= n\lambda_2 \\ d\sin\theta &= (m+1/2)\lambda_1 \\ \implies 4n &= 3m+1.5 \end{aligned}$$

Which will not hold for any integer values, and hence we disregard this case.
Thus, the 1st order minima of 600nm coincides with the 2nd order maxima of 450 nm.

2.2.4 Question 4

When the light source is used to determine which of the slits the electron passes through, the resultant intensity is just the sum of the individual intensities.

$$I_{tot} = \frac{|A_1|^2 + |A_2|^2}{1+y^2} \tag{2.9}$$

We can explicitly find the normalisation constants A_1, A_2 using $\int_{-\infty}^{\infty} dy \psi_i^* \psi_i = 1$. This yields,$A_1 = A_2 = \frac{1}{\sqrt{\pi}}$. This gives us:

$$I_{tot} = \frac{2}{(1+y^2)\pi} \tag{2.10}$$

When the light source is not used to determine the slit through which the electron passes, we have to first consider the total wavefunction $\psi = \psi_1 + \psi_2$, and then find the corresponding intensity $\psi^*\psi$.

$$\begin{aligned} \psi &= \frac{1}{\sqrt{\pi(1+y^2)}} \times (e^{-i(ky-\omega t)} + e^{-i(ky+\pi y-\omega t)}) \\ \psi &= \frac{1}{\sqrt{\pi(1+y^2)}} e^{-i(ky-\omega t)}(1+e^{-i\pi y}) \\ I_{tot} = \psi^*\psi &= \frac{1}{\pi(1+y^2)}|(1+e^{-i\pi y})|^2 \\ &= \frac{4}{\pi(1+y^2)}\cos^2(\frac{\pi y}{2}) \end{aligned} \tag{2.11}$$

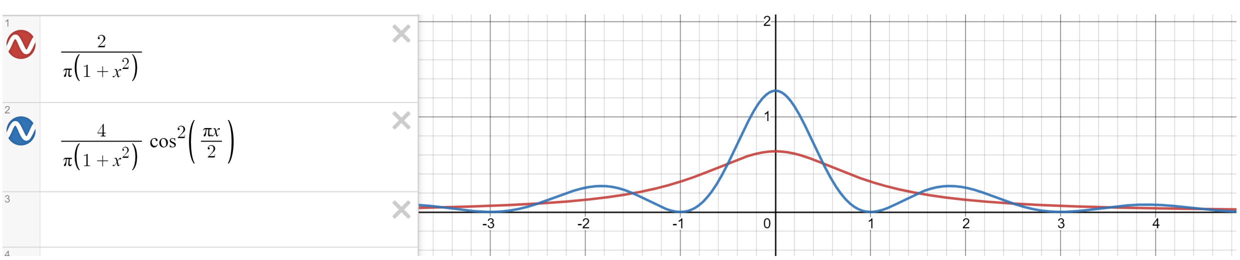


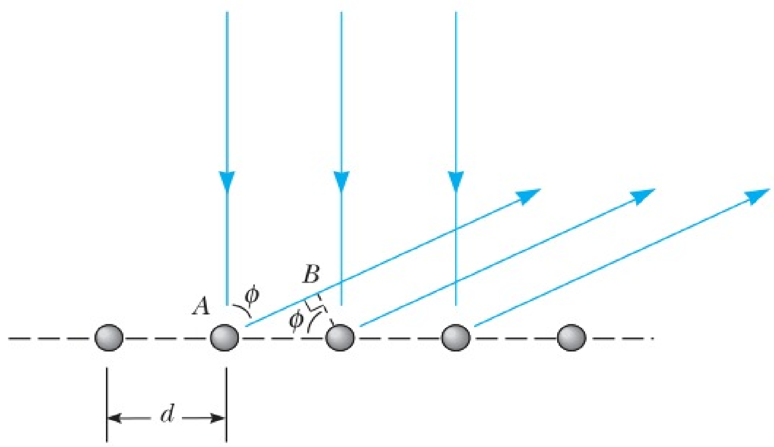
Figure 2.3: Red: Light source determines which slit the electron passes through, no interference, Blue: Light source does not determine which slit the electron passes through, interference maxima and minima observed

2.2.5 Question5

a) Our first step is to find out the de Broglie wavelength of the electrons being used ($\lambda_{dB} = h/p$).

$$\lambda_{dB} = \frac{h}{\sqrt{2mE}} \approx 1.69 \text{ Å} \tag{2.12}$$

First maxima occurs at $\theta = 35°$. Thus, $\lambda_{dB} = d \sin\theta \implies d = 1.69/\sin(35°)$ Å $= 2.94$ Å. At this point, you may be confused about the formula $\lambda_{dB} = d\sin\theta$. In the situation under consideration, the path difference is different from what we already have in mind.



$AB = d\sin\phi = n\lambda$

Clearly from the above figure, the path difference Δx is $d\sin\phi$. In our case, $\phi = \theta$. Therefore, $n\lambda = d\sin\theta$! Once we have this formula in hand, rest of the parts become fairly straightforward.

For the second maxima, we shall simply put $n = 2$ in the formula we derived above.

$$2\lambda_{dB} = d\sin\theta_2$$
$$\sin\theta_2 = \frac{2\lambda_{dB}}{d} = \frac{2 \times 1.69}{2.94} > 1$$

Thus, no other angle exists for which a maxima occurs.

Now, suppose we triple the energy, then the momentum gets scaled up by $\sqrt{3} \implies \lambda'_{dB} = \lambda_{dB}/\sqrt{3}$. Using this we find the angle at which the first maxima occurs:

$$\lambda'_{dB} = d\sin\theta'_1$$
$$\sin\theta'_1 = \frac{1.69}{2.94 \times \sqrt{3}} = 0.332$$
$$\theta'_1 = 19.39°$$

Similarly, the angle at which the other peaks occurs can be found out as follows:

$$n\lambda'_{dB} = d\sin\theta'_n$$
$$\sin\theta'_1 = \frac{n \times 1.69}{2.94 \times \sqrt{3}} = \frac{n}{3.01}$$

For a valid θ'_n to exist, sine of that angle must be less than 1 $\implies n < 3.01$. Thus, for $n = 1, 2$ and 3, we can observe maxima. Although the maxima corresponding to $n = 3$ is very difficult to observe since $theta'_3$ is very close to $90°$.

2.2.6 Question 6

a) Easy substitution of formula

$$\lambda = d \sin\theta$$
$$\frac{h}{\sqrt{2mE}} = d \sin\theta$$
$$\frac{h}{\sin\theta\sqrt{2mE}} = d$$
$$\implies \boxed{d = 5.64 \text{ A}^\circ}$$

b)
Calculating Na: $6 \times \frac{1}{2}$ faces $+8 \times \frac{1}{8}$ corners $= 4$
Therefore, answer must be 4
(Re-check using Cl: $12 \times \frac{1}{4}$ edges $+1$ centre $= 4$)

c)

$$\text{Density} \;=\; \frac{\text{Mass of cube}}{\text{Volume of cube}}$$
$$\text{Density} \;=\; \frac{\text{No. of molecules in cube } \times \text{ Weight of 1 molecule}}{\text{Volume of cube}}$$
$$\text{Density} \;=\; \frac{\text{No. of molecules in cube } \times \text{ Weight of 1 mole of NaCl}}{\text{Volume of cube } \times \text{ Avogadro's number}}$$
$$\implies \text{Avogadro's number} \;=\; \frac{\text{No. of molecules in cube } \times \text{ Weight of 1 mole of NaCl}}{\text{Volume of cube } \times \text{ Density}}$$
$$\text{Avogadro's number} \;=\; \frac{4 \times 58.44\text{g}}{(5.64 \times 10^{-10})^3 \times \frac{2.17\text{g}}{10^{-6}}}$$
$$\boxed{\text{Avogadro's number } = 6 \times 10^{23}}$$

Chapter 3

Tutorial 3

3.1 Wave packets, Group and Phase Velocity

3.1.1 Question 1

We consider the following wave-functions:

$$\begin{aligned}\psi_1(y,t) &= 5y\cos(7t)\\ \psi_2(y,t) &= -5y\cos(9t)\end{aligned} \tag{3.1}$$

Their superposition gives us:

$$\begin{aligned}\psi &= \psi_1 + \psi_2\\ &= 5y(\cos(7t) - \cos(9t))\\ &= 10y\left(\sin(\frac{(7+9)t}{2}\sin\frac{(9-7)t}{2}\right)\\ &= 10y\sin(8t)\sin(t)\end{aligned} \tag{3.2}$$

The higher frequency wave $\sin(8t)$ will be modulated by the lower frequency wave $\sin(t)$. This lower frequency waved is the modulating wave. It forms the envelope within which higher frequency oscillations take place.

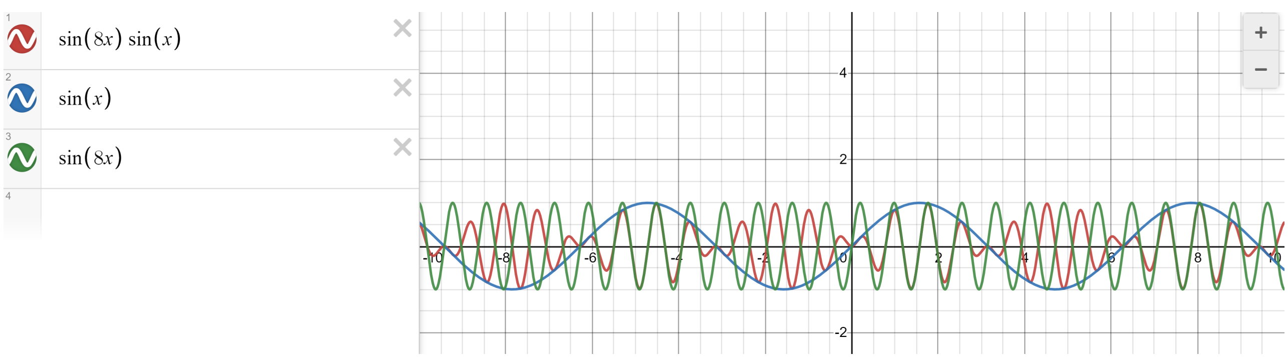


Figure 3.1: The sin(t) forms the envelope, which modulates the signal. Within the envelope, there are faster oscillations, which are due to the higher frequency wave, sin (8t) in green. The resultant modulated wave is shown in red.

3.1.2 Question 2

We are given two wave equations $y_1 = 0.002\cos(8.0x - 400t)$ and $y_2 = 0.002\cos(7.6x - 380t)$. Our first task is to find the resultant wave, which is simply the sum of the two:

$$y = y_1 + y_2 = 0.002\{\cos(8.0x - 400t) + \cos(7.6x - 380t)\} \tag{3.3}$$
$$= 0.004\{\cos(7.8x - 390t)\cos(0.2x - 10t)\} \tag{3.4}$$

The first cosine on the right hand side represents the fast oscillating wave part, and the second cosine represents the envelop. Thus, the phase velocity v_p can be obtained from the wave part, and the group velocity v_g from the envelop part.

$$v_p = \frac{\omega}{k} = \frac{390}{7.8} = 50 \text{ m/s} \tag{3.5}$$
$$v_g = \frac{\Delta\omega}{\Delta k} = \frac{10}{0.2} = 50 \text{ m/s} \tag{3.6}$$

In order to find out Δx, we just have to locate two adjacent zeroes of the envelop part.

$$0.2x_1 - 10t = \frac{\pi}{2} \tag{3.7}$$
$$0.2x_2 - 10t = \frac{\pi}{2} \tag{3.8}$$
$$0.2(x_2 - x_1) = \pi \tag{3.9}$$
$$\Delta x = 5\pi \tag{3.10}$$

Δk is the difference between the k's of the two given waves, i.e., 0.4 $\implies$

$$\Delta x \Delta k = 5\pi \times 0.4 = 2\pi \tag{3.11}$$

3.1.3 Question 3

We know that phase velocity and group velocity are given by

$$v_p = \frac{\omega}{k}, \qquad v_g = \frac{d\omega}{dk}$$

Thus,

$$v_p = \sqrt{\frac{g}{k} + \frac{Tk}{\rho}}, \qquad v_g = \frac{1}{2\sqrt{gk + Tk^3/\rho}} \times \left(g + \frac{3k^2T}{\rho}\right)$$

a) For large wavelengths or small k,

$$v_p = \sqrt{\frac{g}{k}}$$

$$v_g = \frac{1}{2\sqrt{gk}}\left(g + \frac{3k^2T}{\rho}\right)\left(1 + \frac{Tk^2}{g\rho}\right)^{-1/2} \approx \frac{1}{2\sqrt{gk}}\left(g + \frac{3k^2T}{\rho}\right)\left(1 - \frac{Tk^2}{2g\rho}\right)$$

Ignoring, higher order k terms,

$$v_g = \frac{1}{2}\sqrt{\frac{g}{k}}$$

b) For small wavelengths or large k,

$$v_p = \sqrt{\frac{Tk}{\rho}}$$

$$v_g = \frac{1}{2}\left(\frac{1}{g/k + Tk/\rho}\right)^{1/2}\left(\frac{g}{k} + \frac{3kT}{\rho}\right)$$

Ignoring $1/k$ terms,

$$v_g = \frac{3}{2}\sqrt{\frac{Tk}{\rho}}$$

3.1.4 Question 4

Consider a relativistic particle of mass m and travelling with a velocity v. The phase velocity is given by

$$v_p = \lambda\nu$$

Now,

$$h\nu = E = \gamma mc^2 \implies \nu = \frac{\gamma mc^2}{h}$$

Also,

$$p = \gamma mv = \frac{h}{\lambda} \implies \lambda = \frac{h}{\gamma mv}$$

Thus,

$$v_p = \left(\frac{h}{\gamma mv}\right)\left(\frac{\gamma mc^2}{h}\right) = \frac{c}{v} > c$$

We know the Einstein energy-momentum relation to be

$$E^2 = p^2c^2 + m^2c^4 \implies \hbar^2\omega^2 = \hbar^2k^2c^2 + m^2c^4$$

Dividing throughout by $\hbar^2$,

$$\omega^2 - k^2c^2 = \frac{m^2c^2}{\hbar^2}$$

which is the required relation between ω and k. Thus,

$$2\omega d\omega - 2kc^2dk = 0 \implies v_g = \frac{d\omega}{dk} = \frac{kc^2}{\omega} = \frac{c^2}{v_p} = \frac{c^2}{c^2/v} = v$$

3.1.5 Question 5

(a) $v_p = \frac{\omega}{k} = \frac{1}{\sqrt{\epsilon\mu}} = \frac{c}{\sqrt{\epsilon_r\mu_r}}$
(b) $\frac{\omega}{k} = \frac{c}{\sqrt{1-\frac{\omega_p^2}{\omega^2}}} \implies \omega(k) = \sqrt{k^2c^2 + \omega_p^2}$
(c) $v_p = \frac{\omega}{k} = \frac{3\sqrt{2}}{4}c = 1.06c$
$v_g = \frac{d\omega}{dk} = \frac{c^2k}{\omega} = \frac{c^2}{v_p} = \frac{2\sqrt{2}}{3}c = 0.94c$

3.1.6 Question 6

Here,

$$v_p = \frac{\omega}{k} = \frac{\omega_0 sin(ka/2)}{k}$$

and

$$v_g = \frac{d\omega}{dk} = \frac{\omega_0 acos(ka/2)}{2}$$

For the wave to be non-dispersing, for part a, we have to show the group and phase velocities are the same at large wavelengths, ie the limit λ goes to infinity. This means k in the limit goes to zero. Then:

$$v_p = \frac{\omega_0 sin(ka/2)}{ka0.5} \cdot \frac{a}{2} = \frac{\omega_0 a}{2}$$

$$v_g = \frac{\omega_0 a cos(0)}{2} = \frac{\omega_0 a}{2}$$

Here in the limit we see $v_p = v_g$ hence is non dispersing.
For part b, we simply have to evaluate v_p and v_g for the given k value, π/a which gives $\omega_0 a/\pi$ and 0 respectively.

3.1.7 Question 7

From the given dispersion relation of the large number of SHO (possibly a solid), we have :

$$w(\vec{k}) = \sqrt{\frac{2\beta_x(1-\cos(k_x a_x)) + 2\beta_y(1-\cos(k_y a_y))}{m}}$$

The generalization of the definition you have studied for the group velocities for higher dimensions is :

$$v_g = \nabla_{\vec{k}} \vec{w}$$

Which for our case becomes:

$$\begin{aligned} v_g &= \frac{\partial w}{\partial k_x}\vec{i} + \frac{\partial w}{\partial k_y}\vec{j} \\ &= \frac{\beta_x a_x}{mw}\sin(k_x a_x)\vec{i} + \frac{\beta_y a_y}{mw}\sin(k_y a_y)\vec{j} \\ \implies v_g &= \frac{\beta_x a_x}{mw}\sin(k_x a_x)\vec{i} + \frac{\beta_y a_y}{mw}\sin(k_y a_y)\vec{j} \end{aligned}$$

This is the group velocity, and the angle it makes with the x axis is simply :

$$\theta = \tan^{-1}\left(\frac{\beta_y a_y \sin(k_y a_y)}{\beta_x a_x \sin(k_x a_x)}\right)$$

Chapter 4

Tutorial 4

4.1 Fourier Transform

4.1.1 Question 1

We are given the following function in k-space

$$\phi(k) = \begin{cases} A(a - |k|) & \text{if} \quad |k| <= a \\ 0 & \text{otherwise} \end{cases} \tag{4.1}$$

First, we find the normalization factor.

$$\begin{aligned} \int_{-\infty}^{\infty} \phi^*(k)\phi(k)dk &= 1 \\ \int_{-a}^{a} |A|^2(a - |k|)^2 dk &= 1 \\ 2|A|^2 \int_{0}^{a} (a - k)^2 dk &= 1 \\ 2|A|^2 \frac{a^3}{3} &= 1 \\ |A| &= \sqrt{\frac{3}{2a^3}} \end{aligned} \tag{4.2}$$

We use the inverse Fourier transform of this function, to get the function in x-space.

$$
\begin{aligned}
f(x) &= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \phi(k) e^{ikx} dk \\
&= \frac{1}{\sqrt{2\pi}} \int_{-a}^{a} A(a-|k|) e^{ikx} dk \\
&= \frac{A}{\sqrt{2\pi}} \left[\left[a \left(\frac{e^{ikx}}{ix} \right) \right]_{-a}^{a} - \left[k \frac{e^{ikx}}{ix} \right]_{0}^{a} + \left[\frac{e^{ikx}}{(ix)^2} \right]_{0}^{a} - \left[-k \frac{e^{ikx}}{ix} \right]_{-a}^{0} + \left[-\frac{e^{ikx}}{(ix)^2} \right]_{-a}^{0} \right] \\
&= \frac{A}{\sqrt{2\pi}} \frac{(2 - e^{iax} - e^{-iax})}{x^2} \\
&= \frac{A}{\sqrt{2\pi}} \frac{(2 - 2\cos(ax))}{x^2} \\
&= \frac{4A}{\sqrt{2\pi}} \frac{(\sin^2(\frac{ax}{2}))}{x^2} \\
&= \frac{Aa^2}{\sqrt{2\pi}} \text{sinc}^2(\frac{ax}{2})
\end{aligned} \tag{4.3}
$$

An estimate for the uncertainty can be taken to be the distance between the centre to the first zero of the sinc functiont. Therefore, $\Delta x = \frac{2\pi}{a}$.

Similarly, an estimate for the uncertainty in momentum from the triangular graph gives, $\Delta k = a$.

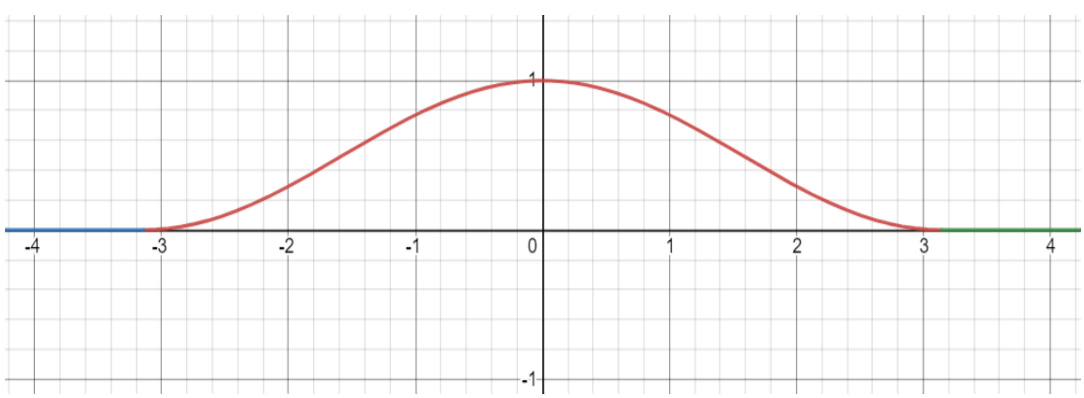
$$
\begin{aligned}
\Delta x \Delta k &= 2\pi \\
\Delta x \Delta p &= 2\pi\hbar >= \frac{\hbar}{2}
\end{aligned} \tag{4.4}
$$

Hence it is consistent with HUP.

4.1.2 Question 2

We are given a wave-packet of the form $f(x) = \cos^2(\frac{x}{2})$ for $x \in [-\pi, \pi]$ and 0 otherwise. It is a very easy to plot function which you may have sketched several times in your JEE days.

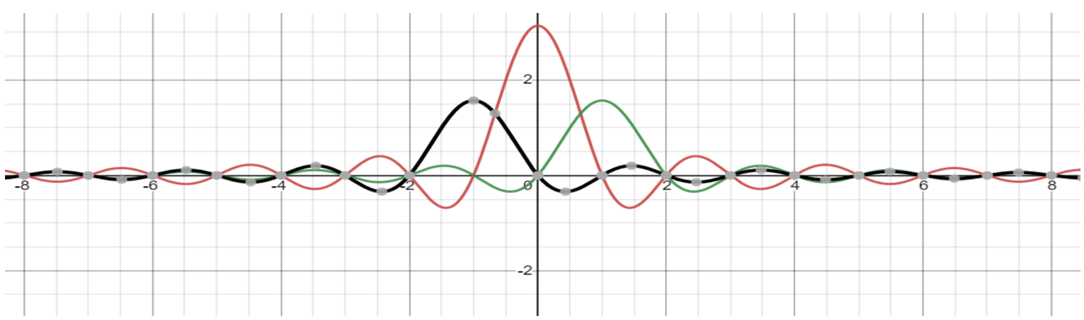
a) The plot of $f(x)$ vs x looks like:



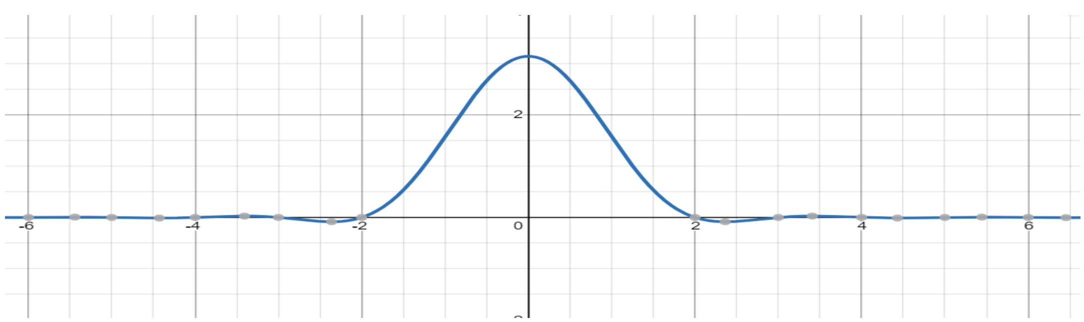
b) Next, we need to find out the Fourier transform of $f(x)$. We can re-write $\cos^2(x/2)$ as $(1 + \cos x)/2$.

$$\begin{aligned}
g(k) &= \int_{-\infty}^{\infty} f(x) e^{-ikx} dx && (4.5)\\
&= \frac{1}{2}\int_{-\pi}^{\pi} (1+\cos x) e^{-ikx} dx && (4.6)\\
&= \frac{1}{2}[\frac{e^{ik\pi} - e^{-ik\pi}}{ik}] + \frac{1}{4}\int_{-\pi}^{\pi} e^{-i(k-1)x} + e^{-i(k+1)x} dx && (4.7)\\
&= \frac{\sin k\pi}{k} + \frac{1}{2}[\frac{\sin(k-1)\pi}{k-1} + \frac{\sin(k+1)\pi}{k+1}] && (4.8)\\
&= -\frac{\sin k\pi}{k(k^2-1)} && (4.9)
\end{aligned}$$

c) In this part, we have to find out the maximum value of $|g(k)|$. It has removable discontinuities as $0, 1$ and -1 which can be filled in by assigning the limits to the function at those location. Let's try to find it out intuitively. Observe that the roots of the denominator are $-1, 0$ and 1. Clearly the limits of the function at these points are $\frac{\pi}{2}, \pi$ and $\frac{\pi}{2}$. At all other integers the function will be 0. I claim that the function is maximum at $k = 0$ because it renders the largest functional value among the zeroes of the denominator (poles). To understand this better, let's plot the three functions in equation (42).



$g(k)$ is the sum of these three curves which one can do qualitatively to obtain the following:



Therefore, the maximum value of $g(k)$ is π.

d) The first zeroes of $g(k)$ occur at $k = -2$ and 2 which can be easily inferred from the above graph.

e) First zeroes of $f(x)$ are $x = -\pi$ and π. I will follow the half width convention according to which $\Delta x = \pi$ and $\Delta k = 2$. Therefore, the product of the two uncertainties is $\Delta x.\Delta k = 2\pi$.

4.1.3 Question 3

Given: $\psi(x) = \sqrt{2/L}\sin(\pi x/L)$ for $0 \leq x \leq L$ and $\psi(x) = 0$ otherwise

a)

$$\psi(x) = \int_{-\infty}^{\infty} a(k)e^{ikx}dk \implies a(k) = \frac{1}{2\pi}\int_{-\infty}^{\infty}\psi(x)e^{-ikx}dx$$

$$a(k) = \frac{1}{2\pi}\int_0^L \sqrt{\frac{2}{L}}\sin(\pi x/L)e^{-ikx}dx$$

Writing π/L as k', we have

$$\begin{aligned}
a(k) &= \frac{1}{2\pi}\sqrt{\frac{2}{L}}\int_0^L \frac{e^{ik'x} - e^{-ik'x}}{2i}e^{-ikx}dx \\
&= \frac{1}{4\pi i}\sqrt{\frac{2}{L}}\int_0^L e^{i(k'-k)x} - e^{-i(k'+k)x}dx \\
&= \frac{1}{4\pi i}\sqrt{\frac{2}{L}}\left[\frac{e^{i(k'-k)L} - 1}{i(k'-k)} + \frac{e^{-i(k'+k)L} - 1}{i(k'+k)}\right] \\
&= \frac{1}{4\pi}\sqrt{\frac{2}{L}}\left[\frac{e^{-ikl} + 1}{k'-k} + \frac{e^{-ikL} + 1}{k'+k}\right] \\
&= \frac{1}{4\pi(k'^2 - k^2)}\sqrt{\frac{2}{L}}[e^{-ikL} + 1]2k' \\
&= \frac{k'}{2\pi(k'^2 - k^2)}\sqrt{\frac{2}{L}}[e^{-ikL} + 1]
\end{aligned}$$

b) For wavelength L, $k = 2\pi/L$. Thus,

$$\begin{aligned}
a(2\pi/L) &= -\frac{1}{2\pi}\sqrt{\frac{2}{L}}\frac{L}{3\pi}[e^{-2\pi i} + 1] \\
&= -\frac{\sqrt{2L}}{3\pi^2}
\end{aligned}$$

which is the required amplitude of the plane wave of wavelength L.

4.1.4 Question 4

a)

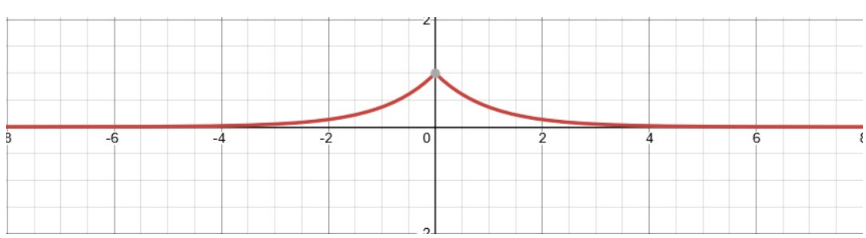


Figure 4.1:

b)

$$|e^{-\alpha|x|}| = 0.5$$

$$e^{-\alpha|x|} = 0.5$$
$$-\alpha|x| = ln(0.5) = -0.693$$
$$|x| = \frac{0.693}{\alpha}$$
$$x = \pm\frac{0.693}{\alpha}$$

Therefore full width at half maxima is:

$$\Delta x = 2 \times \frac{0.693}{\alpha} = \frac{1.386}{\alpha}$$

c)

$$g(k) = \int_{-\infty}^{\infty} f(x)e^{ikx}dx$$
$$g(k) = \int_{-\infty}^{\infty} e^{-\alpha|x|}e^{ik_ox}e^{ikx}dx$$
$$g(k) = \int_{-\infty}^{\infty} e^{i(k+k_o)x-\alpha|x|}dx$$
$$g(k) = \int_{-\infty}^{0} e^{(\alpha+i(k+k_o))x}dx + \int_{0}^{\infty} e^{(-\alpha+i(k+k_o))x}dx$$
$$g(k) = \left(\frac{e^{(-\alpha+i(k+k_o))x}}{-\alpha+i(k+k_o)} - \frac{e^{-(\alpha+i(k+k_o))x}}{\alpha+i(k+k_o)}\right)\Bigg|_{x=0}^{\infty}$$
$$g(k) = \left(\frac{1}{\alpha-i(k+k_o)} + \frac{1}{\alpha+i(k+k_o)}\right)$$
$$g(k) = \frac{2\alpha}{\alpha^2+(k+k_o)^2}$$

d)

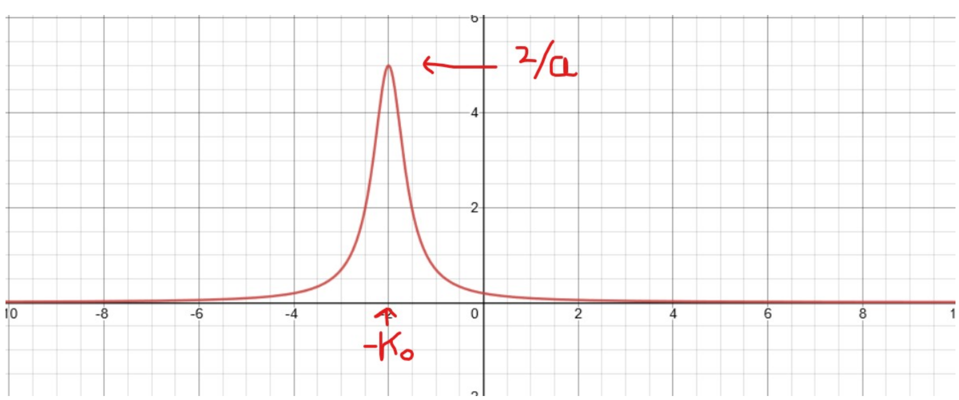


Figure 4.2:

e) The max height occurs when $k + k_o = 0$. The value of this is $2/\alpha$. Hence, half of max value is $1/\alpha$

$$\frac{2\alpha}{\alpha^2+(k+k_o)^2} = \frac{1}{\alpha}$$

$$2\alpha^2 = \alpha^2 + (k + k_o)^2$$
$$\alpha^2 = (k + k_o)^2$$
$$(k + k_o) = \pm\alpha$$
$$k = -k_o \pm \alpha$$

Since uncertainty is full width at half maxima, we get:

$$\Delta k = 2\alpha$$

Now,

$$\Delta x \Delta k = \frac{1.386}{\alpha} \times 2\alpha$$
$$\Delta x \Delta k = 2.773$$

4.2 Heisenberg Uncertainty Principle

4.2.1 Question 1

First calculate de Broglie wavelength $\lambda = \frac{h}{p} = \frac{h}{\gamma m_0 v}$. Since it's a free particle in both cases (i.e. zero potential), we can take uncertainity in position to be equal to standard deviation i.e.

$$\Delta x = \sigma = \frac{\lambda}{2}$$

(a) λ turns out to be $\frac{0.01}{\gamma}$nm ≈ 0.01nm. Thus $\Delta x = 0.005$nm.
(b) λ turns out to be $\frac{6.626\times10^{-36}}{\gamma}$m $\approx 6.626 \times 10^{-36}$m. Thus $\Delta x = 3.313 \times 10^{-36}$m.

4.2.2 Question 2

We have that the proton is bound in the nucleus, of radius $7 \cdot 10^{-15}$, and hence can take Δx as the radius. From the uncertainty relation given: $\Delta x \Delta p \geq \hbar/2$ we have to estimate the **root mean square** of the velocity, or $\sqrt{< v^2 >}$.
One thing to keep in mind is that since the proton is effectively bound in a sphere, it will have equal negative and positive velocities, hence $< p >= 0$. This implies:

$$\Delta p^2 =< p^2 > - < p >^2$$
$$\Delta p^2 =< p^2 >$$
$$\sqrt{< p^2 >} = \Delta p = \frac{\hbar}{2\Delta x}$$
$$\sqrt{< p^2 >} = \Delta p = \frac{\hbar}{2 \cdot 7 \cdot 10^{-15}}$$
$$\sqrt{< p^2 >} = 3.7663278 \cdot 10^{-21}$$

For the root mean square of the velocity now, we divide by the proton's mass.

$$\sqrt{< v^2 >} = 2 \cdot 3.7663278 \cdot 10^{-21}/m_p$$
$$\sqrt{< v^2 >} = 4.503502 \cdot 10^6$$

4.2.3 Question 3

Given, $\Delta x \Delta p_x \geq \frac{\hbar}{2}$, and that we are considering a non-relativistic electron.

a) Since the electron is localized within a region of size a, this means that from the mean (approximately the center to a good approximation), the uncertainty in position $\Delta x = \frac{a}{2}$. From Heisenberg, this leads to $\Delta p_x \geq \frac{\hbar}{a}$, from the mean momentum. Some people also use the uncertainity as a, which is just a different convention. Thus, minimum Kinetic Energy for this non relativistic electron is

$$K.E._{min} = \frac{\Delta p_x^2}{2m} = \frac{\hbar^2}{2ma^2}$$

b) We are given that $\Delta x = \lambda = \frac{h}{p}$, and thus

$$\Delta p_x \geq \frac{\hbar p}{2h} = \frac{p}{4\pi} \approx p_x$$

Here, since the electron is non relativistic, $\Delta v_x \approx v_x$. This is what we call an order analysis, that is, the error in the velocity is of the same order as that of the velocity itself.

c)Let us use the exact version here, specifically

$$\Delta v_x = \frac{v_x}{4\pi} = \sqrt{\frac{2E}{m}}\frac{1}{4\pi} = 6.7 \times 10^5 m/s$$

d) Let the motion of the electron be along the x direction, and passing through the hole leads to an uncertainty along the y direction (also the x direction, but it is insignificant compared to v_x). The Energy as measured is before passing through, and hence gives us the velocity in the x direction as

$$v_x = \sqrt{\frac{2E}{m}}$$

Using Heisenberg relation for uncertainty along the y direction, we get $\Delta y \Delta p_y \geq \frac{\hbar}{2}$, and thus

$$\Delta v_y \approx v_y = \frac{\hbar}{2ma}$$

where a is the hole radius. Thus, using $\tan\theta \approx \theta$, we get

$$\Delta\theta = \frac{v_y}{v_x} = \frac{\hbar}{2ma}\sqrt{\frac{m}{2E}} = 4.3 \times 10^{-5} \text{ rad}$$

4.2.4 Question 4

Classically, for such a potential ($V(x) = \alpha|x|$), we expect the ground state to be at x=0 and p=0 - corresponding to being at rest at the minimum of potential energy position. However, quantum mechanically, we cannot have x=0 and p=0 simultaneously. Therefore, consider an uncertainty Δx in position about $x = 0$, and an uncertainty in momentum about $p = 0$ as Δp.

$$KE = \frac{(\Delta p)^2}{2m}$$

$$PE = \alpha \Delta x$$

Therefore, the total energy is:

$$E = KE + PE = \frac{(\Delta p)^2}{2m} + \alpha \Delta x \tag{4.10}$$

Here we use HUP, and assume $\Delta x \Delta p = \hbar$ (Note: we aren't using $\hbar/2$ which is the minimum possible uncertainty. $\hbar$ is a good estimation for the general case and to get correct order of magnitude approximations.)

$$E = \frac{\hbar^2}{2m(\Delta x)^2} + \alpha \Delta x \tag{4.11}$$

We minimize this energy to get the minimum total energy of a particle of mass m.

$$\begin{aligned} \frac{\partial E}{\partial \Delta x} &= -2\frac{\hbar^2}{2m(\Delta x)^3} + \alpha = 0 \\ \Delta x &= \left(\frac{\hbar^2}{m\alpha}\right)^{\frac{1}{3}} \end{aligned} \tag{4.12}$$

Substituting this in the expression for energy, we get the minimum energy is:

$$\begin{aligned} E &= \frac{\hbar^2}{2m}\left(\frac{m\alpha}{\hbar^2}\right)^{\frac{2}{3}} + \alpha\left(\frac{\hbar^2}{m\alpha}\right)^{\frac{1}{3}} \\ &= \frac{3}{2}\left(\frac{\hbar^2\alpha^2}{m}\right)^{\frac{1}{3}} \end{aligned} \tag{4.13}$$

Therefore A = 1.5, B = $\left(\frac{\hbar^2\alpha^2}{m}\right)^{\frac{1}{3}}$

Chapter 5

Tutorial 5

5.1 Operators and Wave-functions

5.1.1 Question 1

Let us start with the concept of linearity. What is a linear operator?

Very simply, a linear operator is one which satisfies the following properties:

$$\begin{aligned}\hat{A}(f+g) &= \hat{A}f + \hat{A}g \\ \hat{A}(cf) &= c\hat{A}f\end{aligned} \tag{5.1}$$

where the operator $\hat{A}$ acts on the functions f, g and c is a scalar value.

We can condense both the above properties into the single definition given below:

$$\hat{A}(af+bg) = a\hat{A}f + b\hat{A}g \tag{5.2}$$

To check if an operator A is Hermitian, take it's conjugate transpose $A^\dagger$ and check whether $A = A^\dagger$. If the operators are not in matrix form, then remember the following facts while taking conjugate transpose:

$$\begin{aligned}x^\dagger &= x, \\ (\frac{d}{dx})^\dagger &= -\frac{d}{dx}, \\ i^\dagger &= -\imath\end{aligned}$$

Therefore, in general, we can always use the following definition of a hermitian operator:

$$\int dx v^*(x)\hat{A}u(x) = \int dx(\hat{A}v(x))^* u(x) \tag{5.3}$$

The above should hold for any two functions $v(x), u(x)$ that you choose. This can help you prove something isn't hermitian by giving an example of simple functions (constants, f(x) = x etc) if you have difficulty proving it isn't hermitian otherwise. For proving it's Hermitian, you need to show it holds for any choice of two functions. We work out the (b) as an example:

$$\begin{aligned}\int_{-\infty}^{\infty} dxv^*(x)\hat{A}u(x) &= \int_{-\infty}^{\infty} dxv^*(x)\frac{\partial}{\partial x}u(x) \\ &= v^*(x)\int_{-\infty}^{\infty} dx\frac{\partial}{\partial x}u(x) - \int_{-\infty}^{\infty} dx(\frac{\partial}{\partial x}v^*(x))u(x) \\ &= -\int_{-\infty}^{\infty} dx(\frac{\partial}{\partial x}v(x))^*u(x)\end{aligned} \tag{5.4}$$

Here in the first step, we used integration by parts, in the second line we used the fact that the functions are given to be well-behaving and vanish at $x = \pm\infty$. In the last line, we get the negative of the expression $\int dx(\hat{A}v(x))^* u(x)$, so this operator is called 'anti-Hermitian'. Note that the momentum operator is Hermitian, because when the conjugate of the operator is taken $i \to (-i)$, and this will cancel with the negative sign appearing in the last step of this calculation.

(a) Not linear, not Hermitian

(b) Linear, not Hermitian (note: if multiplied by i it becomes Hermitian, but as it is, it is anti-Hermitian)

(c) Linear, not Hermitian

(d) Not linear, not Hermitian

(e) Linear, not Hermitian

(f) Not linear, not Hermitian

(g) Linear, Hermitian (integrate by parts twice)

5.1.2 Question 2

a) We are given two Hermitian operators $\hat{A}$ and $\hat{B}$ which satisfy the commutation relation $[\hat{A}, \hat{B}] = i\hat{C}$. An operator is said to be Hermitian if it's ***Hermitian conjugate*** is same as the operator itself. To understand Hermitian conjugate, we can think of operators as square matrices and the functions they act on as column vectors (the reason why this can be done is beyond the scope right now). The Hermitian conjugate $A^\dagger$ of a matrix A can be found in the following way:

- Take the complex conjugate of the matrix first, i.e., $P \to P^*$
- Then take the transpose, i.e., $P^* \to (P^*)^T$

For example, the Hermitian conjugate of the matrix

$$P = \begin{bmatrix} 1 & 2i & 2 \\ 3+4i & 2 & 5 \\ 1-\sqrt{2}i & 4 & 3 \end{bmatrix}$$

is given by

$$P^\dagger = \begin{bmatrix} 1 & 3-4i & 1+\sqrt{2}i \\ -2i & 2 & 4 \\ 2 & 5 & 3 \end{bmatrix}$$

Since a transpose is involved in the process of finding the Hermitian conjugate, it satisfies the properties of transpose! For example, $(PQ)^T = Q^T P^T \implies (PQ)^\dagger = Q^\dagger P^\dagger$. In the language of quantum mechanics, Hermitian conjugate is defined as the following:

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

If for operators $\hat{A}$ and $\hat{B}$ the following expression holds true for all ψ, ϕ, then $\hat{B}$ is the Hermitian conjugate of the operator $\hat{A}$.

To show that the operator $\hat{C}$ is Hermitian, we just have to show that its Hermitian conjugate is the same as itself.

Let's take the Hermitian conjugate on both sides of the given commutation relation.

$$\begin{aligned}
(i\hat{C})^\dagger = -i\hat{C}^\dagger &= [\hat{A}, \hat{B}]^\dagger \\
&= (\hat{A}\hat{B} - \hat{B}\hat{A})^\dagger \\
&= (\hat{A}\hat{B})^\dagger - (\hat{B}\hat{A})^\dagger \\
&= \hat{B}^\dagger \hat{A}^\dagger - \hat{A}^\dagger \hat{B}^\dagger \\
&= \hat{B}\hat{A} - \hat{A}\hat{B} = -i\hat{C}
\end{aligned}$$

We exploited the fact that $\hat{A}$ and $\hat{B}$ are both Hermitian in the last step. Therefore, we have $\hat{C}^\dagger = \hat{C}$.

Hence Proved!!!

b) In the above discussion, we also showed that $(\hat{A}\hat{B} - \hat{B}\hat{A})^\dagger = \hat{B}\hat{A} - \hat{A}\hat{B} \implies [\hat{A}, \hat{B}]^\dagger = -[\hat{A}, \hat{B}]$. Hence, $[\hat{A}, \hat{B}]$ is anti-Hermitian!

5.1.3 Question 3

Functions of operators are defined by their power series expansion. Given an operator $\hat{Q}$, we have

$$\begin{aligned}
e^{\hat{Q}} &\equiv 1 + \hat{Q} + \frac{1}{2}\hat{Q}^2 + \frac{1}{3!}\hat{Q}^3 + ... \\
\frac{1}{1-\hat{Q}} &\equiv 1 + \hat{Q} + \hat{Q}^2 + \hat{Q}^3 + ... \\
\ln(1+\hat{Q}) &\equiv \hat{Q} - \frac{1}{2}\hat{Q}^2 + \frac{1}{3}\hat{Q}^3 - \frac{1}{4}\hat{Q}^4 + ...
\end{aligned}$$

Now, we have $\hat{K}$ to be a Hermitian operator, which means $\hat{K}^\dagger = \hat{K}$ and

$$\begin{aligned}
e^{i\hat{K}} &= 1 + i\hat{K} - \frac{1}{2}\hat{K}^2 - \frac{i}{3!}\hat{K}^3 + ... \\
\implies (e^{i\hat{K}})^\dagger &= 1 - i\hat{K}^\dagger - \frac{1}{2}(\hat{K}^\dagger)^2 + \frac{i}{3!}(\hat{K}^\dagger)^3 + ... \\
\implies (e^{i\hat{K}})^\dagger &= e^{-i\hat{K}^\dagger} = e^{-i\hat{K}}
\end{aligned}$$

Note that

$$\begin{aligned}
e^{\hat{A}}e^{\hat{B}} &\neq e^{\hat{A}+\hat{B}} \\
&= e^{\hat{A}+\hat{B}}e^{[\hat{A},\hat{B}]/2}
\end{aligned}$$

(This is called the **Baker-Campbell-Hausdorff formula**)
But in our case, $[\hat{K}, \hat{K}] = 0$. Thus, we have

$$(e^{i\hat{K}})^{\dagger} e^{i\hat{K}} = e^{-i\hat{K}} e^{i\hat{K}} = e^{i(-\hat{K}+\hat{K})} = \mathbb{I}$$

Thus, $e^{i\hat{K}}$ is unitary if $\hat{K}$ is Hermitian.

For the converse, we take a result which follows from the **Spectral Theorem** of Linear Algebra. This says that for any unitary operator (matrix) $\hat{U}$, we have another unitary operator(matrix) $\hat{V}$ such that

$$\hat{U} = \hat{V}\hat{D}\hat{V}^{\dagger}$$

where D is a diagonal matrix comprising of the eigenvalues of $\hat{U}$. Now, a unitary operator (matrix) has eigenvalues of unit modulus. To see this,

$$\begin{aligned}
\phi(x) &= \hat{U}\psi(x) = \lambda\psi(x) \\
\phi^*(x) &= \hat{U}^{\dagger}\psi^*(x) = \lambda^*\psi^*(x) \\
1 = \int_{\infty}^{\infty} \phi^*(x)\phi(x)dx &= \int_{\infty}^{\infty} |\lambda|^2\psi^*(x)\psi(x)dx = |\lambda|^2
\end{aligned}$$

Thus, $D = \text{diag}(e^{i\theta_1}, e^{i\theta_2}, e^{i\theta_3}, ...)$. We now claim that

$$\hat{K} = \frac{1}{i}\ln\hat{U}$$

is the required Hermitian operator (matrix). To see this,

$$\begin{aligned}
\hat{K} = \frac{1}{i}\ln\hat{U} &= \frac{1}{i}\ln(\hat{V}\hat{D}\hat{V}^{\dagger}) \\
&= \frac{1}{i}\hat{V}\ln(\hat{D})\hat{V}^{\dagger} \qquad \text{(expand as power series and use } \hat{V}\hat{V}^{\dagger} = \mathbb{I}) \\
&= \hat{V}\text{diag}(\theta_1, \theta_2, \theta_3, ...)\hat{V}^{\dagger}
\end{aligned}$$

It isn't hard to check that $\hat{U} = e^{i\hat{K}}$. The Hermitian property of $\hat{K}$ immediately follows from the fact that θ_i are real. Thus, for any unitary operator (matrix), we have found a Hermitian operator that follows the property. Is this operator unique?

5.1.4 Question 4

For the sake of clarity, I have written '$f(x)$' as just 'f', '$g(x)$' as just 'g', and removed the 'dx' term, but ideally these should be written properly.

Recalling the definition of the ***hermitian adjoint*** of an operator:

$$\begin{aligned}
\int f^*\hat{O}^{\dagger}g &= \int (\hat{O}f)^*g \\
&= \int g(\hat{O}f)^* \\
&= \int (g^*\hat{O}f)^* \\
&= \left(\int g^*\hat{O}f\right)^*
\end{aligned}$$

$$\boxed{\int f^* \hat{O}^\dagger g = \left(\int g^* \hat{O} f\right)^*}$$

a) Substituting $\hat{O}$ with $\hat{A}^\dagger$:

$$\begin{aligned}
\int f^* (\hat{A}^\dagger)^\dagger g &= \left(\int g^* \hat{A}^\dagger f\right)^* \\
&= \left(\left(\int f^* \hat{A} g\right)^*\right)^* \\
&= \int f^* \hat{A} g
\end{aligned}$$

$$\boxed{\int f^* (\hat{A}^\dagger)^\dagger g = \int f^* \hat{A} g}$$

b) Substituting $\hat{O}$ with $\hat{A}\hat{B}$ in the original definition:

$$\int f^* (\hat{A}\hat{B})^\dagger g = \int (\hat{A}\hat{B} f)^* g$$

Now let $\hat{B} f = h$

$$\begin{aligned}
\int (\hat{A}\hat{B} f)^* g &= \int (\hat{A} h)^* g \\
&= \int h^* \hat{A}^\dagger g
\end{aligned}$$

Now let $\hat{A}^\dagger g = k$

$$\begin{aligned}
\int h^* \hat{A}^\dagger g &= \int h^* k \\
&= \int (\hat{B} f)^* k \\
&= \int f^* \hat{B}^\dagger k \\
&= \int f^* \hat{B}^\dagger \hat{A}^\dagger g
\end{aligned}$$

$$\boxed{\implies \int f^* (\hat{A}\hat{B})^\dagger g = \int f^* \hat{B}^\dagger \hat{A}^\dagger g}$$

c) Substituting $\hat{O}$ with $\left(\hat{A}+\hat{A}^\dagger\right)^\dagger$ in the original equation:

$$\begin{aligned}
LHS = \int f^*(\hat{A}+\hat{A}^\dagger)^\dagger g &= \int \left((\hat{A}+\hat{A}^\dagger)f\right)^* g \\
&= \int \left(\hat{A}f+\hat{A}^\dagger f\right)^* g \\
&= \int (\hat{A}f)^* g + \int (\hat{A}^\dagger f)^* g \\
&= \int f^*\hat{A}^\dagger g + \int f^*\hat{A}g \\
&= \int f^*\left(\hat{A}^\dagger g + \hat{A}g\right) \\
&= \int f^*(\hat{A}^\dagger + \hat{A})g \\
&= \int f^*(\hat{A} + \hat{A}^\dagger)g \\
\implies \int f^*(\hat{A}+\hat{A}^\dagger)^\dagger g &= \int f^*(\hat{A}+\hat{A}^\dagger)g
\end{aligned}$$

$$\boxed{\text{or } \left(\hat{A}+\hat{A}^\dagger\right)^\dagger = \left(\hat{A}+\hat{A}^\dagger\right)}$$

(This also proves the distributive property of the † operation.)

The other two are straightforward now that we have proved commutativity and distributivity over addition of the † and that its its own inverse:

$$\begin{aligned}
\left(i\left(\hat{A}-\hat{A}^\dagger\right)\right)^\dagger &= (i)^*\left(\hat{A}-\hat{A}^\dagger\right)^\dagger \\
&= -i\left(\hat{A}^\dagger-(\hat{A}^\dagger)^\dagger\right) \\
&= -i\left(\hat{A}^\dagger-\hat{A}\right) \\
&= i\left(\hat{A}-\hat{A}^\dagger\right)
\end{aligned}$$

$$\boxed{\left(i\left(\hat{A}-\hat{A}^\dagger\right)\right)^\dagger = i\left(\hat{A}-\hat{A}^\dagger\right)}$$

And lastly,

$$\boxed{\left(\hat{A}\hat{A}^\dagger\right)^\dagger = (\hat{A}^\dagger)^\dagger\hat{A}^\dagger = \hat{A}\hat{A}^\dagger}$$

5.1.5 Question 5

We are looking for $\phi(x)$ and a number λ such that

$$\hat{G}\phi(x) = \lambda\phi(x) \implies \imath\hbar\frac{\partial\phi}{\partial x} = (\lambda - Bx)\phi.$$

On rearranging and integrating this gives

$$\phi(x) = ke^{-\frac{\iota}{\hbar}(\lambda x - Bx^2/2)}$$

for an arbitrary constant k.
Putting the condition $\phi(a) = \phi(-a)$ in the above expression for ϕ we get

$$e^{-\iota\lambda a/\hbar} = e^{\iota\lambda a/\hbar} \implies e^{2\iota\lambda a/\hbar} = 1 = e^{\iota 2n\pi} \implies \lambda_n = \frac{n\pi\hbar}{a}.$$

For each λ_n we have $\phi_n(x)$.

5.1.6 Question 6

We have $\Psi_1(x)$ and $\Psi_2(x)$ given as two eigenfunctions of $\hat{P}$ with eigenvalues P_1 and P_2. Now for a wavefunction consisting of a combination of these two eigenfuntions, the probability of being in one state is the square of the normalised coefficient of that eigenfunction, i.e., here:

$$\text{Probability}(P_1) = \frac{(0.25)^2}{(0.25)^2 + (0.75)^2} = 0.1$$

Similarly Probability(P_2) can be found to be 0.9, which gives us the net probability of measuring P_1 or P_2 as 1, which makes sense, since our original wavefunction was a combination of $\Psi_1(x)$ and $\Psi_2(x)$ only.

5.1.7 Question 7

Firstly, this is what we mean by the probability of finding a particle in a specific state, or that the some value of an observable is measured as something with some probability. For a large enough number of experiments N, if the probability of finding a given value for an observable is z, the number of measurements in which z is found are z*N. Even though it does not matter for our final answer very much (think why!), let us normalize the given wavefunction anyway. Also, since the measurement is at the time $t = 0$, we do not need to add the time dependent part.

$$\Phi(x) = Aexp\left(\frac{-x^2}{b^2}\right)$$

$$\int_{-\infty}^{\infty} \Phi^*(x)\Phi(x)dx = 1$$

$$\implies A^2 \int_{-\infty}^{\infty} exp\left(\frac{-2x^2}{b^2}\right)dx = 1$$

$$\implies A = \left(\frac{2}{\pi b^2}\right)^{1/4}$$

Thus, the normalized wavefunction is

$$\Phi(x) = \left(\frac{2}{\pi b^2}\right)^{1/4} exp\left(\frac{-x^2}{b^2}\right)$$

We know that the probability of finding a particle between x and $x + dx$ is given by $P|_{\{x,x+dx\}} = |\Phi(x)|^2 dx$, and thus, if z is the number of measurements in which the particle would have been found in the infinitesimal interval of $x = b$ to $b + dx$:

$$\frac{100}{N} = |\Phi(2b)|^2 dx$$

$$\frac{z}{N} = |\Phi(b)|^2 dx$$

(Do you see now why A was unnecessary?).
Thus, we have:

$$\frac{100}{z} = \frac{exp(-8)}{exp(-2)}$$
$$\implies z = 100e^6$$

Thus, the number of of measurements in which the particle would have been found in the infinitesimal interval of $x = b$ to $b + dx$ is ≈ 40343 measurements.

5.1.8 Question 8

We are given that $\phi_1(x)$ and $\phi_2(x)$ are two normalised eigenfunctions of the operator $\hat{A}$ corresponding to the eigenvalues a_1 and a_2, respectively. Similarly, $u_1(x)$ and $u_2(x)$ are two normalised eigenfunctions of the operator $\hat{B}$ corresponding to the eigenvalues b_1 and b_2, respectively. The relationships between $\phi_1(x)$, $\phi_2(x)$ and $u_1(x)$, $u_2(x)$ are given to be:

$$\phi_1(x) = D(3u_1(x) + 4u_2(x))$$
$$\phi_2(x) = F(4u_1(x) - Pu_2(x))$$

We can easily find D using the fact that all the wavefunctions under discussion are normalised.

$$\int_{-\infty}^{\infty} \phi_1(x)^* \phi_1(x) dx = 1$$
$$|D|^2 \int_{-\infty}^{\infty} (3u_1^*(x) + 4u_2^*(x))(3u_1(x) + 4u_2(x)) dx = 1$$
$$|D|^2 \int_{-\infty}^{\infty} 9|u_1^2(x)| + 16|u_2(x)|^2 + 12(u_1(x)^* u_2(x) + u_2(x)^* u_1(x)) dx = 1$$

Now we will use the fact that the eigenstates of an operator corresponding to the different eigenvalues are orthogonal to each other. Thus, we have $\int_{-\infty}^{\infty} u_1(x)^* u_2(x) dx$ and $\int_{-\infty}^{\infty} u_2(x)^* u_1(x) dx$ both equal to zero!

So we get $|D|^2 \times 25 = 1 \implies |D| = \frac{1}{5}$. Now, since D can be complex, we can associate an arbitrary phase part to it, i.e., $D = \frac{1}{5} e^{i\theta_D}$.

We can find P using orthogonality of $\phi_1(x)$ and $\phi_2(x)$.

$$D \times F \times \int_{-\infty}^{\infty} (3u_1^*(x) + 4u_2^*(x))(4u_1(x) - Pu_2(x)) dx = 0$$
$$12 - 4P = 0$$
$$P = 3$$

Obtaining F is again fairly straightforward. We just have to use the normalisation condition.

$$\int_{-\infty}^{\infty} \phi_2^* \phi_2 dx = 1$$
$$|F|^2 \int_{-\infty}^{\infty} (4u_1(x)^* - 3u_2(x)^*)(4u_1(x) - 3u_2(x)) dx = 1$$
$$|F|^2 \int_{-\infty}^{\infty} 16|u_1(x)|^2 + 9|u_2(x)|^2 - 12(u_1(x)^* u_2(x) + u_2(X)^* u_1(x)) dx = 1$$
$$|F|^2 \times (25) = 1$$
$$F = \frac{1}{5} e^{i\theta_F}$$

The state of the particle at time $t = 0$ is given to be $\psi(x) = \frac{2}{3}\phi_1 + \frac{1}{3}\phi_2$. If we make a measurement of A on this system, the possible outcomes are only a_1 and a_2 because a quantum superposition collapses to one of the constituent eigenstates upon observation. Clearly the given wave function $\psi(x)$ is not normalised. So let's first normalise the wave function:

$$
\begin{aligned}
|N|^2 \int_{-\infty}^{\infty} \psi^*(x)\psi(x)dx &= 1 \\
|N|^2 \left(\frac{4}{9} + \frac{1}{9}\right) &= 1 \\
|N| &= \frac{3}{\sqrt{5}}
\end{aligned}
$$

Here we are free to choose any phase of N, because all we care about is its modulus squared, so let's choose 0 for simplicity, i.e., $N = \frac{3}{\sqrt{5}}$. The normalised wave function is $\frac{1}{\sqrt{5}} \times (2\phi_1(x) + \phi_2(x))$. The probability of obtaining a_1 is given by the mod square of the coefficient of the corresponding eigenfunction.

$$
\begin{aligned}
\text{Probability of } a_1 &= \frac{4}{5} \\
\text{Probability of } a_2 &= \frac{1}{5}
\end{aligned}
$$

After the measurement of A, if the value obtained is a_1, then it can be inferred that the system had collapsed to the eigenstate ϕ_1. Thus, measuring B in the system immediately after the previous measurement is equivalent to measuring B in a system described by ϕ_1. The only possible outcomes are, of course, b_1 and b_2.

$$
\begin{aligned}
\text{Probability of } b_1 &= \frac{9}{25} \\
\text{Probability of } b_2 &= \frac{16}{25}
\end{aligned}
$$

Now let's consider the case in which the measurement of B is performed initially at $t = 0$. The possible outcomes are b_1 and b_2. The state of the particle in terms of $u_1(x)$ and $u_2(x)$ is

$$
\begin{aligned}
\psi &= \frac{3}{\sqrt{5}} \times [\frac{2}{3}(\frac{3}{5}u_1 + \frac{4}{5}u_2)e^{i\theta_D} + \frac{1}{3}(\frac{4}{5}u_1 - \frac{3}{5}u_2)e^{i\theta_F}] \\
&= \frac{3}{\sqrt{5}} \times [(\frac{2}{5}e^{i\theta_D} + \frac{4}{15}e^{i\theta_F})u_1 + (\frac{8}{15}e^{i\theta_D} - \frac{1}{5}e^{i\theta_F})u_2]
\end{aligned}
$$

This implies

$$
\begin{aligned}
\text{Probability of } b_1 &= \frac{9}{5}|\frac{2}{5}e^{i\theta_D} + \frac{4}{15}e^{i\theta_F}|^2 = \frac{52}{125} + \frac{48}{175}\cos(\theta_D - \theta_F) \\
\text{Probability of } b_2 &= \frac{9}{5}|\frac{8}{15}e^{i\theta_D} - \frac{1}{5}e^{i\theta_F}|^2 = \frac{73}{125} - \frac{48}{175}\cos(\theta_D - \theta_F)
\end{aligned}
$$

If the outcome is b_2, then this implies that the state of particle collapsed to $u_2(x)$, i.e., $(\frac{4}{5}\phi_1 - \frac{3}{5}\phi_2)e^{i\theta_F}$. Thus, the probabilities of a_1 and a_2 are as follows:

$$
\begin{aligned}
\text{Probability of } a_1 &= \frac{16}{25} \\
\text{Probability of } a_2 &= \frac{9}{25}
\end{aligned}
$$

Chapter 6

Tutorial 6

6.1 Free particle

6.1.1 Question 1

$$\begin{aligned}
\psi(x) &= A\sin(kx) + B\cos(kx) \\
&= A\left(\frac{e^{ikx} - e^{-ikx}}{2i}\right) + B\left(\frac{e^{ikx} + e^{-ikx}}{2}\right) \\
&= \frac{1}{2}\left((B - iA)e^{ikx} + (B + iA)e^{-ikx}\right) \\
&= Ce^{ikx} + De^{-ikx}
\end{aligned} \tag{6.1}$$

where $C = \frac{1}{2}(B - iA)$ and $D = \frac{1}{2}(B + iA)$ Therefore, we have shown that $\sin(kx), \cos(kx)$ basis is equivalent to the e^{ikx}, e^{-ikx} basis.

6.1.2 Question 2

We need to show that the given wave-function ψ doesn't obey the time-dependent Schrodinger's equation for a free particle. The TDSE for a free particle is the following:

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

The given wave-function is $\psi = A\sin(kx - \omega t) + B\cos(kx - \omega t)$. Thus, we have

$$\begin{aligned}
\frac{\partial\psi}{\partial t} &= -\omega A\cos(kx - \omega t) + \omega B\cos(kx - \omega t) \\
\frac{\partial^2\psi}{\partial x^2} &= -k^2 A\sin(kx - \omega t) - k^2 B\cos(kx - \omega t)
\end{aligned}$$

Plugging these into TDSE for free particle gives

$$\begin{aligned}
&\frac{\hbar^2 k^2}{2m}A\sin(kx - \omega t) + \frac{\hbar^2 k^2}{2m}B\cos(kx - \omega t) = -i\hbar\omega A\cos(kx - \omega t) + i\hbar\omega B\sin(kx - \omega t) \\
&(\frac{\hbar^2 k^2}{2m}A - i\hbar\omega B)\sin(kx - \omega t) + (\frac{\hbar^2 k^2}{2m}B + i\hbar\omega A)\cos(kx - \omega t) = 0
\end{aligned}$$

For the above equation to hold for all t, we need the coefficients of the sine and cosine terms to be zero individually.

$$\frac{\hbar^2 k^2}{2m} A = i\hbar\omega B$$
$$\frac{\hbar^2 k^2}{2m} B = -i\hbar\omega A$$

The above two equations can hold simultaneously only if $A = \pm iB$, i.e. it is a solution only for special cases. Thus, the given wave-function is not a solution for all wave-functions of the given form.

6.1.3 Question 3

$$\phi(x) = Ae^{ikx} + Be^{-ikx} \implies \phi^*(x) = Ae^{-ikx} + Be^{ikx}$$
$$\phi^*(x)\phi(x) = A^2 + B^2 + AB(e^{2ikx} + e^{-2ikx}) = A^2 + B^2 + 2AB\cos(kx)$$

Now,

$$A^2 + B^2 + 2AB \geq A^2 + B^2 + 2AB\cos(kx) \geq A^2 + B^2 - 2AB$$
$$(A+B)^2 \geq \phi^*(x)\phi(x) \geq (A-B)^2 \geq 0$$

6.1.4 Question 4

Here, the value of A does not matter (can you think why?), so let us look at $e^{i(kx-\omega t)}$ term. We know that such terms are plane waves. We also know that these terms are momentum eigenstates. (Remember that delta functions are position eigenstates, and its fourier transform gives us e^{ikx}, which is a momentum eigenstate.)

Lastly, we know that measuring the observable of a corresponding eigenstate of an operator gives us the eigenvalue. Hence, the eigenvalue of e^{ikx} with respect to the momentum operator will give us the momentum of a particle in this state. There are 2 ways to do this: (note: here, $k = 5.02\times10^{11}$, and $\omega = 8.00\times10^{15}$)

a) $p = \frac{hk}{2\pi} = \boxed{5.29 \times 10^{-23}\text{kg.m.}s^{-1}}$ (We already know this is true for free particles. Derivation in (b))

b) Apply the momentum operator $-i\frac{h}{2\pi}\frac{\partial}{\partial x}$ to the wavefunction to find the eigenvalue.

$$-i\frac{h}{2\pi}\frac{\partial Ae^{i(kx-\omega t)}}{\partial x} = \left(-i\frac{h}{2\pi}\right)(ik)(Ae^{i(kx-\omega t)}) = \left(\frac{hk}{2\pi}\right)(Ae^{i(kx-\omega t)})$$

$$\implies \text{the eigenvalue } = \frac{hk}{2\pi} = \boxed{5.29 \times 10^{-23}\text{kg.m.}s^{-1}}$$

Now to derive Energy,

$$\text{a) } E = \frac{h\omega}{2\pi} = 1.342 \times 10^{-19} J$$

We can also do this by applying the Hamiltonian to the wave equation (we would need to find the mass of the particle from the value of k and ω given, hence this is needless additional work)

6.1.5 Question 5

(a) It is clear that the given function is continuous, differentiable once at $x = \pm a$, vanishes as $x = \pm\infty$ thus it qualifies as a wavefunction.
(b)

$$\int_{-a}^{+a} |A|^2 (1 + \cos\left(\frac{\pi x}{a}\right))^2 dx = 1 \implies 3a|A|^2 = 1 \implies |A| = \frac{1}{\sqrt{3a}}$$

(c)

$$\Delta x = \sqrt{\langle x^2 \rangle - \langle x \rangle^2}$$

$$\Delta p = \sqrt{\langle p^2 \rangle - \langle p \rangle^2}$$

We shall use $\langle \hat{O} \rangle = \int \psi^* \hat{O} \psi$ and $\hat{p} = -\iota\hbar\frac{\partial}{\partial x}$ to claim that $\langle x \rangle = 0$ (also noting that $\psi(x)$ is symmetric about $x = 0$) and that $\langle p \rangle = 0$ (noting that $\sin(\frac{\pi x}{a})$ is antisymmetric about the origin). Remaining non-zero terms

$$\langle x^2 \rangle = \int_{-a}^{a} \psi^* x^2 \psi = |A|^2 \frac{(2\pi^2 - 15)a^3}{2\pi^2} = \frac{(2\pi^2 - 15)a^2}{6\pi^2}$$

$$\langle p^2 \rangle = \int_{-a}^{a} \psi^* p^2 \psi = -\int_{-a}^{a} \psi^* \hbar^2 \frac{\partial^2}{\partial x^2} \psi = |A|^2 \hbar^2 a \frac{\pi^2}{a^2} = \frac{\hbar^2 \pi^2}{3a^2}.$$

The expressions for Δx and Δp are given by $\sqrt{\frac{(2\pi^2-15)a^2}{6\pi^2}}$ and $\sqrt{\frac{\hbar^2\pi^2}{3a^2}}$ respectively. Now you can verify that $(\Delta x \Delta p)^2 \approx 1.053157\frac{\hbar^2}{4}$. Thus, $\Delta x \Delta p > \frac{\hbar}{2}$.
(d) Classically allowed region is the one where $E - V > 0$ i.e. $E > V$. Putting this condition in the TISE, we get the bounds for the classically allowed region.

6.1.6 Question 6

We are given $\psi(x) = A(\frac{x}{x_0})^n \cdot e^{-x/x_0}$ and have to find V(x) such that $\psi(x)$ is a stationary state, and its given that V(x)=0 at extremal x values (plus/minus infinity). This means:

$$\hat{H}\psi(x) = E\psi(x)$$

Where E is the energy of the stationary state.

$$\hat{H}\psi(x) = \left(\frac{-\hbar^2}{2m}\frac{d^2}{dx^2} + \hat{V}(x)\right)\psi(x) = E\psi(x)$$

$$\left(\frac{-\hbar^2 n(n-1)}{2mx^2} + \frac{\hbar^2 n}{mxx_0} + \frac{-\hbar^2}{2mx_0^2} + \hat{V}(x)\right)\psi(x) = E\psi(x)$$

Since the first 3 terms on the LHS are not operators, we can take it to the RHS, and directly evaluate $\hat{V}(x)$. This gives us:

$$\hat{V}(x) = E + \frac{\hbar^2}{2mx_0^2} + \frac{\hbar^2 n(n-1)}{2mx^2} - \frac{\hbar^2 n}{mxx_0}$$

For the second part we use the fact that V(x) = 0 at ininity, giving E = $\frac{-\hbar^2}{2mx_0^2}$

Chapter 7

Tutorial 7

7.1 Particle in a box

7.1.1 Question 1

For a high energy particle in a particle in a box, we consider the nth eigenstate where $n >> 1$.

$$\psi(x) = \sqrt{(\frac{2}{L})}\sin(\frac{n\pi x}{L})$$

The probability of finding it between a and $b + a$ is given by:

$$\begin{aligned}
&\int_a^{b+a} |\psi(x)|^2 dx \\
&= \frac{2}{L}\int_a^{b+a} \sin^2(\frac{n\pi x}{L})dx \\
&= \frac{1}{L}\int_a^{b+a} \left(1 - \cos(\frac{2n\pi x}{L})\right) dx \\
&= \frac{b}{L} - \left(\frac{\sin(\frac{2n\pi(b+a)}{L}) - \sin(\frac{2n\pi a}{L})}{2n\pi/L}\right) \\
&\approx \frac{b}{L} \quad \lim n \to \infty
\end{aligned} \tag{7.1}$$

7.1.2 Question 2

Consider a particle confined to a 1D box of length L is in its ground state. We need the probability of finding it between $L/3$ and $2L/3$. The wave-function of the particle is as follows:

$$\psi_0 = \sqrt{\frac{2}{L}}\sin(\frac{\pi x}{L})$$

The probability of finding it in the space interval $(L/3, 2L/3)$ is given by:

$$
\begin{aligned}
P(\frac{L}{3} < x < \frac{2L}{3}) &= \frac{2}{L}\int_{\frac{L}{3}}^{\frac{2L}{3}} \sin^2(\frac{\pi x}{L})dx \\
&= \frac{2}{L}\int_{\frac{L}{3}}^{\frac{2L}{3}} \frac{1-\cos(\frac{2\pi x}{L})}{2}dx \\
&= \frac{2}{L}[\frac{x}{2} - \frac{L}{4\pi}\sin(\frac{2\pi x}{L})]_{\frac{L}{3}}^{\frac{2L}{3}} \\
&= \frac{2}{L}[\frac{L}{6} + \frac{L}{4\pi}(\sqrt{3})] \\
&= \frac{1}{3} + \frac{\sqrt{3}}{2\pi}
\end{aligned}
$$

7.1.3 Question 3

a) We know that the stationary state wavefunctions are given by

$$
\psi(x) = \sqrt{\frac{2}{a}}\sin\left(\frac{n\pi x}{a}\right), \quad 0 \le x \le a
$$

Now,

$$
\langle \hat{X} \rangle_n = \int_0^a \frac{2}{a} x \sin^2\left(\frac{n\pi x}{a}\right) dx = \frac{a}{2}
$$

This can be noticed just by observing the symmetry of $|\psi(x)|^2$ about $a/2$

$$
\langle \hat{X^2} \rangle_n = \int_0^a \frac{2}{a} x^2 \sin^2\left(\frac{n\pi x}{a}\right) dx = a^2\left(\frac{1}{3} - \frac{1}{2\pi^2 n^2}\right)
$$

$$
\begin{aligned}
\langle \hat{P} \rangle_n &= \int_0^a \frac{2}{a}\sin\left(\frac{n\pi x}{a}\right)\left[-i\hbar\frac{\partial}{\partial x}\left(\sin\left(\frac{n\pi x}{a}\right)\right)\right] dx \\
&= \frac{-2i\hbar n\pi}{a^2}\int_0^a \sin\left(\frac{n\pi x}{a}\right)\cos\left(\frac{n\pi x}{a}\right) dx = 0
\end{aligned}
$$

$$
\begin{aligned}
\langle \hat{P}^2 \rangle_n &= \int_0^a \frac{2}{a}\sin\left(\frac{n\pi x}{a}\right)\left[\hbar^2\frac{\partial^2}{\partial x^2}\left(\sin\left(\frac{n\pi x}{a}\right)\right)\right] dx \\
&= \frac{2\hbar^2}{a}\left(\frac{n\pi}{a}\right)^2\int_0^a \sin^2\left(\frac{n\pi x}{a}\right) dx \\
&= \frac{2\hbar^2 n^2\pi^2}{a^3}\frac{a}{2} = \frac{n^2\pi^2\hbar^2}{a^2}
\end{aligned}
$$

Classically, consider a particle continuously bouncing off of the walls of the container at $x = 0$ and $x = a$. Now, as it's travelling at a constant speed (potential does not vary within the box and hence force is zero), it is equally likely to find the particle in any interval dx (let it be Pdx). From the symmetry of the potential around $x = a/2$, we can conclude that the classical expectation value of the particle is $a/2$. Now, as the particle is travelling at a constant speed, it is travelling to the right for an equal amount of time as it is travelling to the left. Hence, we can conclude that the mean value of the classical momentum is 0. These match with the quantum mechanical expectation values.

Since the probability to find the particle in an interval dx is Pdx, where P is a constant,

$$\langle \hat{X}^2 \rangle = \frac{\int_0^a Px^2 dx}{\int_0^a Pdx} = \frac{\int_0^a x^2 dx}{\int_0^a dx} = \frac{a^2}{3}$$

This agrees with the quantum mechanical expectation value as $n \to \infty$. Now, if we know that the energy of the particle is $E_n = n^2\pi^2\hbar^2/2ma^2$ (the stationary state energy eigenvalues), classically we expect $p^2/2m$ to be equal to the kinetic energy. Thus, for the classical momentum p,

$$p^2 = 2mE_n = \frac{n^2\pi^2\hbar^2}{a^2}$$

which agrees with the quantum mechanical expectation value.

7.1.4 Question 4

The "goody-two-shoes" way to solve this problem is to find the n = 3 wavefunction for an infinite potential well. Then find the spatial probability using the square of the modulus of the wavefunction and integrate it between $x = 0$ and $x = L/6$

Here's a more fun method. We use 3 conditions:

a) It is a known fact that the ground state of any 1D bound system has 0 nodes and that the **mth excited state has m nodes**.

$$\boxed{\text{n = 3 corresponds to the 2nd excited state, hence there must be 2 nodes in this wavefunction}}$$

b) Since the eigenfunctions of the infinite well are sine or cos functions, and that we have 4 zeroes for this function (2 nodes and 2 at the edges of the well used as boundary conditions), we can say that the probabilities will be equal in each of the three sine quadrants of the wavefunction.
c) Now sine and cos functions are symmetric about their peak, hence each quadrant can be divided into 2 more zones where the total probability will be the same.

Hence the well is divided into 6 equal probability zones. Answer = $\boxed{1/6}$

P.S.
There is another way to solve it without requiring to know that the wave function will be a sine or cosine function. This involves changing the potential to an infinite number of periodic delta barriers, with consecutive barriers situated at a distance L from each other. (Which should give us the same answer as the infinite well, repeated each time between two consecutive barriers)

Using just symmetry arguments and the fact that the answer must have 2 nodes, we will easily be able to see that the function must have 6 equal probability zones. This method is often used while solving classical waves problems

7.1.5 Question 5

(a) Let us apply the TDSE in the region $0 \le x \le a$ and take the normalisation factor to be A:

$$\iota\hbar\frac{\partial\psi}{\partial t} = \hat{H}\psi \implies A\omega\sin(\pi x/a)e^{-\iota\omega t} = -\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2} + V(x)\psi$$

$$\implies A\omega\sin(\pi x/a)e^{-\iota\omega t} = A(\pi/a)^2\sin(\pi x/a)e^{-\iota\omega t} + V(x)A\sin(\pi x/a)e^{-\iota\omega t} \implies \omega = (\pi/a)^2 + V(x)$$

This implies that $V(x) = \omega - (\pi/a)^2 =$ constant in the region $0 \le x \le a$ and it is zero outside this region since wavefunction vanishes there (since it's a potential well).
(b) Normalization constant is $\sqrt{2/a}$. The required probability is

$$\int_{a/4}^{3a/4} |\psi(x,t)|^2 dx = \int_{a/4}^{3a/4} \sin^2(\pi x/a)\frac{2/a}{d}x = \frac{1}{2}\left(\frac{a}{2}\right)\frac{2}{a} = \frac{1}{2}$$

7.1.6 Question 6

Given, initially the box has a length a, and the particle is in the ground state, ie we can take the wave function of the particle to be:

$$\psi(x) = \sqrt{\frac{2}{a}}sin(\frac{\pi x}{a}) \text{ from x = 0 to a}$$

$$\text{and } \psi(x) = 0 \text{ otherwise}$$

When the box size is suddenly increased, till x=4a:

$$\psi_{new}(x) = \sqrt{\frac{2}{a}}sin(\frac{\pi x}{a}) \text{ from x = 0 to a}$$

$$\text{and } \psi_{new}(x) = 0 \text{ otherwise}$$

And the eigenstates of the box now are $\phi_n(x) = \sqrt{\frac{2}{4a}}sin(\frac{n\pi x}{4a})$
Now our $\psi(x)$ can be written as a sum of the eigenstates of the new box, ie

$$\psi(x) = \sum_{i=1}^{\infty} c_i\phi_i(x)$$

Now the probability of measuring $\psi(x)$ in the i^{th} state is equal to $c_i^* c_i$. To get c_j we can multiply $\phi_j(x)^\dagger$ and integrate (here from 0 to 4a since wavefunction 0 everywhere else).

$$\int_0^{4a} \phi_j(x)^\dagger\psi(x) = \sum_{i=0}^{\infty}\int_0^{4a} c_i\phi_j(x)^\dagger\phi_i(x)$$

$$\int_0^{4a} \phi_j(x)^\dagger\psi(x) = \sum_{i=0}^{\infty} c_i\delta_{i,j} = c_j$$

For part a, we have to find c_1:

$$c_1 = \int_0^{4a} \phi_1(x)^\dagger\psi(x) = \int_0^{a} \phi_1(x)^\dagger\sqrt{\frac{2}{a}}sin(\frac{\pi x}{a}) + \int_a^{4a} \phi_1(x)^\dagger \cdot 0$$

$$c_1 = \int_0^a \sqrt{\frac{2}{4a}} sin(\frac{1\pi x}{4a})^\dagger \sqrt{\frac{2}{a}} sin(\frac{\pi x}{a})$$

$$c_1 = \frac{8\sqrt{2}}{\pi 15}$$

Then probability of being in ground state is $\frac{128}{225\pi^2}$ or 0.05764.
Similarly for part b:

$$c_2 = \int_0^{4a} \phi_2(x)^\dagger \psi(x) = \int_0^a \phi_2(x)^\dagger \sqrt{\frac{2}{a}} sin(\frac{\pi x}{a}) + \int_a^{4a} \phi_2(x)^\dagger \cdot 0$$

$$c_2 = \int_0^a \sqrt{\frac{2}{4a}} sin(\frac{2\pi x}{4a})^\dagger \sqrt{\frac{2}{a}} sin(\frac{\pi x}{a})$$

$$c_2 = \frac{4}{3\pi}$$

Then probability of being in ground state is $\frac{16}{9\pi^2}$ or 0.1801265.

7.1.7 Question 7

Pretty general, you've seen this before. The region is from $-L/2 < x < L/2$ where V is 0, rest everywhere its infinity. For this region, the TDSE simply becomes

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

Which clearly has the general solution (for positive energy):

$$\psi(x) = A\sin(kx) + B\cos(kx)$$

, with $k = \sqrt{\frac{2mE}{\hbar^2}}$. Since the wavefunction in the region with infinite potential is 0, and the wavefunction is continuous, we have:

$$\psi(-L/2) = \psi(L/2) = 0$$
$$A\sin(kL/2) + B\cos(kL/2) = 0 = -A\sin(kL/2) + B\cos(kL/2)$$

Thus, $A = 0$ and $\cos(kL/2) = 0$ or $\sin(kL/2) = 0$ and $B = 0$. In the first case, $kL/2 = (2n+1)\pi/2$, and thus $E_n = \frac{(2n+1)^2\hbar^2}{2mL^2}$. In the second, $kL/2 = n\pi$, and thus $E_n = \frac{(2n)^2\hbar^2}{2mL^2}$. Thus, joining them together, we note that sin and cos functions alternate for the wavefunction, and the energy levels are the same as the case with $0 < x < L$, as expected.

7.1.8 Question 8

a)

$$\int_0^L |\psi(x)|^2 dx = 1$$

$$
\begin{aligned}
\int_0^L |\psi(x)|^2 dx &= |A|^2 \int_0^L \left(\sin^2(\frac{n\pi x}{L} + \sin^2(\frac{2n\pi x}{L}) + 2\sin(\frac{n\pi x}{L})\sin(\frac{2n\pi x}{L}) \right) dx \\
&= |A|^2 \left(\frac{L}{2} + \frac{L}{2} + 0 \right) \\
&= |A|^2 L
\end{aligned} \tag{7.2}
$$

This means $|A| = \frac{1}{\sqrt{L}}$

b)

$$
\begin{aligned}
\langle x \rangle &= \int_0^L \psi^*(x) x \psi(x) dx \\
&= \frac{1}{L}\int_0^L x \left(\sin^2(\frac{n\pi x}{L}) + \sin^2(\frac{2n\pi x}{L}) + 2\sin(\frac{n\pi x}{L})\sin(\frac{2n\pi x}{L}) \right) \\
&= \frac{1}{L}\int_0^L x \left(\frac{1-\cos(\frac{2n\pi x}{L})}{2} + \frac{1-\cos(\frac{2n\pi x}{L})}{2} + \cos(\frac{n\pi x}{L}) - \cos(\frac{3n\pi x}{L}) \right) \\
&= \frac{1}{L}\frac{L^2}{2} = \frac{L}{2}
\end{aligned} \tag{7.3}
$$

$$
\begin{aligned}
\langle x^2 \rangle &= \int_0^L \psi^*(x) x^2 \psi(x) dx \\
&= \frac{1}{L}\int_0^L x^2 \left(\sin^2(\frac{n\pi x}{L}) + \sin^2(\frac{2n\pi x}{L}) + 2\sin(\frac{n\pi x}{L})\sin(\frac{2n\pi x}{L}) \right) \\
&= \frac{1}{L}\int_0^L x^2 \left(\frac{1-\cos(\frac{2n\pi x}{L})}{2} + \frac{1-\cos(\frac{2n\pi x}{L})}{2} + \cos(\frac{n\pi x}{L}) - \cos(\frac{3n\pi x}{L}) \right) \\
&= \frac{1}{L}\frac{L^3}{3} = \frac{L^2}{3}
\end{aligned} \tag{7.4}
$$

Therefore, $(\Delta x)^2 = \langle x^2 \rangle - \langle x \rangle^2 = \frac{L^2}{12}$

$$\Delta x = L\sqrt{\frac{1}{12}}$$

c)

$$
\begin{aligned}
\langle p \rangle &= \int_0^L \psi^*(x) \left(-i\hbar \frac{\partial}{\partial x} \right) \psi(x) dx \\
&= \frac{-i\hbar}{L}\int_0^L \left(\sin(\frac{n\pi x}{L})\cos(\frac{n\pi x}{L}) + \sin(\frac{2n\pi x}{L})\cos(\frac{2n\pi x}{L}) + \sin(\frac{n\pi x}{L})\cos(\frac{2n\pi x}{L}) + \cos(\frac{n\pi x}{L})\sin(\frac{2n\pi x}{L}) \right) \\
&= 0
\end{aligned} \tag{7.5}
$$

$$
\begin{aligned}
\langle p^2\rangle &= \int_0^L \psi^*(x)\left(-\hbar^2\frac{\partial^2}{\partial x^2}\right)\psi(x)dx \\
&= -\hbar^2\int_0^L \psi^*(x)\left(\frac{\partial^2}{\partial x^2}\right)\psi(x)dx \\
&= \frac{\hbar^2}{L}\int_0^L \left(\frac{n^2\pi^2}{L^2}\sin^2(\frac{n\pi x}{L}) + \frac{4n^2\pi^2}{L^2}\sin^2(\frac{2n\pi x}{L}) + \frac{5n^2\pi^2}{L^2}\sin(\frac{n\pi x}{L})\sin(\frac{2n\pi x}{L})\right)dx \\
&= \frac{\hbar^2}{L}\frac{5n^2\pi^2}{2L} \\
&= \frac{5n^2\pi^2\hbar^2}{2L^2}
\end{aligned}
\tag{7.6}
$$

Therefore $\Delta p = \sqrt{\frac{5}{2}}\frac{n\pi\hbar}{L}$

d) The given wavefunction is an equal superposition of 2 energy eigenstates. Therefore, probability of measuring it in the first excited state ($n = 2$), is $\frac{1}{2}$.

7.1.9 Question 9

a) In all the boxes, the particles are in ground state. The ground state wave-function of a particle in a box ($[0, L]$) is

$$\phi_0 = \sqrt{\frac{2}{L}}\sin(\frac{\pi x}{L})$$

The probability of finding the particle in the region $[0, L/4]$ is

$$
\begin{aligned}
P(0 \le x \le \frac{L}{4}) &= \frac{2}{L}\int_0^{\frac{L}{4}}\sin^2(\frac{\pi x}{L})dx \\
&= \frac{1}{4} - \frac{1}{2\pi} \approx 0.0908
\end{aligned}
$$

Thus, we expect to find about 908 boxes (out of the 10,000 boxes) in which the particle is in the region $[0, L/4]$.

b) If we make a measurement right after the first measurement on the same box, the wave-function cannot collapse to a position eigenvector because they are non-normalisable. Thus, the wavefunction collapses to an eigenfunction having an eigenvalue close to the measurement, i.e., we can think of the resultant state to be a Gaussian with a mean close to the measured value and a small spread. Thus, after the first measurement, the spread will be small. Hence on making a second measurement would give a value which will lie in the interval $[0, L/4]$ as the spread won't grow to a value larger than $L/4$ because the second measurement is made immediately after the first.

7.1.10 Question 10

$$
\begin{aligned}
\psi(x, 0) &= \frac{2}{\sqrt{L}}\sin\left(\frac{3\pi x}{2L}\right)\cos\left(\frac{\pi x}{2L}\right) \\
&= \frac{1}{\sqrt{L}}\left[\sin\left(\frac{\pi x}{L}\right) + \sin\left(\frac{2\pi x}{L}\right)\right] \\
&= \frac{1}{\sqrt{2}}\left[\sqrt{\frac{2}{L}}\sin\left(\frac{\pi x}{L}\right) + \sqrt{\frac{2}{L}}\sin\left(\frac{2\pi x}{L}\right)\right]
\end{aligned}
$$

We know that the general solution to the Schrodinger equation for a particle in a box is given as a linear combination of

$$\psi_n(x,t) = \sqrt{\frac{2}{L}}\sin\left(\frac{n\pi x}{L}\right)e^{-iE_nt/\hbar}$$

where

$$E_n = \frac{n^2\pi^2\hbar^2}{2mL^2}$$

Now, we have just found that $\psi(x,0)$ is a combination of the $n=1$ and $n=2$ energy eigenstates. Thus, we can immediately write

$$\begin{aligned}\psi(x,t) &= \frac{1}{\sqrt{2}}\left[\sqrt{\frac{2}{L}}\sin\left(\frac{\pi x}{L}\right)e^{-iE_1t/\hbar} + \sqrt{\frac{2}{L}}\sin\left(\frac{2\pi x}{L}\right)e^{-iE_2t/\hbar}\right] \\ &= \frac{1}{\sqrt{2}}\left[\psi_1(x,t)+\psi_2(x,t)\right]\end{aligned}$$

Now, the probability of finding the electron between $L/4$ and $L/2$ is

$$\begin{aligned}P(t) &= \int_{L/4}^{L/2}\psi^*(x,t)\psi(x,t)dx \\ &= \frac{1}{L}\int_{L/4}^{L/2}\left[\sin^2\left(\frac{\pi x}{L}\right)+\sin^2\left(\frac{2\pi x}{L}\right)+\sin\left(\frac{\pi x}{L}\right)\sin\left(\frac{2\pi x}{L}\right)\left(e^{-i(E_1-E_2)t/\hbar}+e^{-i(E_2-E_1)t/\hbar}\right)\right]dx \\ &= \frac{1}{L}\int_{L/4}^{L/2}\left[\sin^2\left(\frac{\pi x}{L}\right)+\sin^2\left(\frac{2\pi x}{L}\right)+2\sin\left(\frac{\pi x}{L}\right)\sin\left(\frac{2\pi x}{L}\right)\cos\left(\frac{3\pi^2\hbar t}{2mL^2}\right)\right]dx \\ &= \frac{1}{L}\left[\frac{L}{8}+\frac{L}{4\pi}+\frac{L}{8}+\frac{(4-\sqrt{2})L}{3\pi}\cos\left(\frac{3\pi^2\hbar t}{2mL^2}\right)\right] \\ &= \frac{1}{4}+\frac{1}{4\pi}+\frac{(4-\sqrt{2})}{3\pi}\cos\left(\frac{3\pi^2\hbar t}{2mL^2}\right)\end{aligned}$$

Note that probability is not independent of time as the wavefunction is a superposition of two energy eigenstates.

7.1.11 Question 12

(a) We will use here what is commonly called the WKB approximation. We know that

$$V(x) = \begin{cases}\infty & x<0 \\ \frac{x}{L}V_0 & 0\le x\le L \\ \infty & x>L\end{cases}$$

We want the energy eigenfunction with energy eigenvalue $E_1 < V_0$. Let us say that $V(x_0)=E_1$. Therefore, for $0\le x\le x_0$, $V(x)<E_1$, and for $x_0<x\le L$, $V(x)>E_1$. Therefore we have the TISE as

$$\frac{1}{\psi(x)}\frac{d^2\psi}{dx^2} = \begin{cases}-k(x)^2 & 0<x<x_0 \\ \kappa(x)^2 & x_0\le x<L\end{cases}$$

where

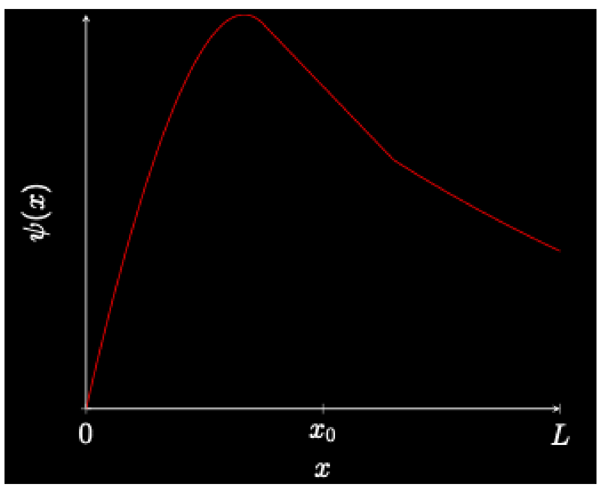
$$k(x) = \sqrt{\frac{2m(E_1 - V(x))}{\hbar^2}},$$

$$\kappa(x) = \sqrt{\frac{2m(V(x) - E_1)}{\hbar^2}}.$$

Thus, when $0 < x < x_0$ and x is not too close to x_0, then $k(x)$ is gradually varying in its neighborhood, and we can treat it as such while solving TISE. Similarly when $x_0 \leq x < L$, and x is not too close to x_0, then $\kappa(x)$ is gradually varying in its neighborhood, and we can treat it as such while solving TISE.

$$\implies \psi(x) \approx \begin{cases} A\sin(k(x)x) & 0 < x < x_0 - \epsilon \\ ?? & x_0 - \epsilon \leq x \leq x_0 + \epsilon \\ Be^{-\kappa(x)x} & x_0 + \epsilon < x < L. \end{cases}$$

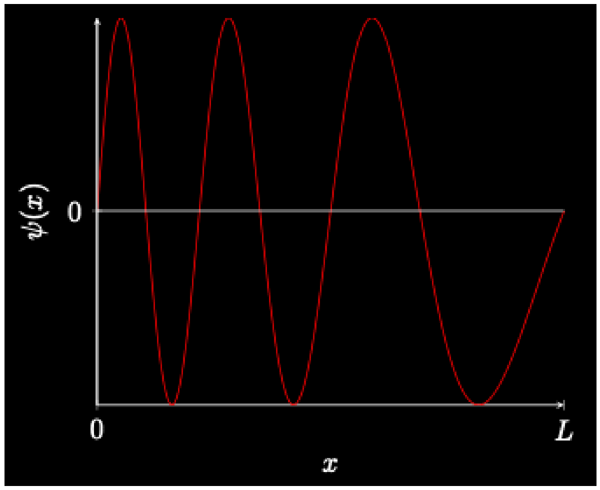
Note that when x is close x_0 we really cannot use these approximations, hence we cannot write the wavefunction so simply in a neighborhood of ε around x_0. Thus the main takeaway (and what you need to write in the examination, you really don't need the above explanation in that detail to be written in the exam), is that the wavefunction is approximately sinusoidal for $0 < x < x_0$, and approximately exponentially decaying in $x_0 < x < L$, with these solutions being patched together using appropriate boundary conditions. The graph thus will be approximately



(b) Using similar logic as above, we have

$$\sin(x) = Asin(k(x)x)$$

Since $V(x)$ is increasing as we increase x, therefore the wavelength 2π will also increase as we increase x. The graph is thus approximately



Chapter 8

Tutorial 8

8.1 Particle in a finite box

8.1.1 Question 1

Label the regions from left to right as 1,2,3. In these regions, Schrodinger equation takes the form

$$\frac{d^2\psi}{dx^2} = \alpha_1^2\psi, \quad x < 0$$

$$\frac{d^2\psi}{dx^2} + k^2\psi = 0, \quad 0 < x < L$$

$$\frac{d^2\psi}{dx^2} = \alpha_2^2\psi, \quad L < x$$

$$k = \sqrt{\frac{2mE}{\hbar^2}} \qquad \alpha_1 = \sqrt{\frac{2m(V_1 - E)}{\hbar^2}} \qquad \alpha_2 = \sqrt{\frac{2m(V_2 - E)}{\hbar^2}}$$

The solutions in the different regions are:

$$\psi = Ae^{\alpha_1 x}, \quad x < 0$$

$$\psi = B\cos kx + C\sin kx, \quad 0 < x < L$$

$$\psi = De^{-\alpha_2 x}, \quad L < x$$

We now demand continuity of the wavefunction and it's derivative at $x = 0$ and $x = L$. Thus,

$$A = B, \qquad De^{-\alpha_2 L} = B\cos kL + C\sin kL$$

Also,

$$A\alpha_1 = Ck, \qquad -D\alpha_2 e^{-\alpha_2 L} = -Bk\sin kL + Ck\cos kL$$

Divide the fourth equation by α_2, add it to the second equation and replace B and C with A to get

$$A\cos kL\left(1 + \frac{\alpha_1}{\alpha_2}\right) = A\sin kL\left(\frac{k}{\alpha_2} - \frac{\alpha_1}{k}\right)$$

Cancelling A and rearranging, we get the condition for quantization:

$$\tan kL = \frac{k(\alpha_1 + \alpha_2)}{k^2 - \alpha_1\alpha_2}$$

As $V_1 \to \infty$, $\alpha_1 \to \infty$. Thus, the condition become

$$\tan kL = -\frac{k}{\alpha_2}$$

Graph out the solutions to get allowed k values and hence allowed E values.

8.1.2 Question 2

A particle of mass m is confined in a finite potential well of length L and barrier potential height V_0. This case was discussed in the lecture in great detail. The wavefunction can be expressed in a piece-wise fashion as follows:

$$\psi(x) = \begin{cases} Ae^{\alpha x} & x < 0 \\ C\sin(kx) + D\cos(kx) & 0 < x < L \\ He^{-\alpha x} & x > L \end{cases}$$

with $\alpha = \sqrt{2m(V_0 - E))}/\hbar$ and $k = \sqrt{2mE}/\hbar$.

Boundary conditions:

1. $\psi(0^-) = \psi(0^+) \implies A = D$
2. $\psi'(0^-) = \psi'(0^+) \implies \alpha A = kC$
3. $\psi(L^+) = \psi(L^-) \implies C\sin(kL) + D\cos(kL) = He^{-\alpha L}$
4. $\psi'(L^-) = \psi'(L^+) \implies k(C\cos(kL) - D\sin(kL)) = -H\alpha e^{-\alpha x}$

From (1) and (2), we have $A = D$ and $C = \frac{\alpha}{k}C$. On making these substitutions in (3) and (4), we obtain:

$$\frac{\alpha}{k}A\sin(kL) + A\cos(kL) = He^{-\alpha L}$$
$$k(\frac{\alpha}{k}A\cos(kL) - A\sin(kL)) = -\alpha He^{-\alpha L}$$

Dividing the above two equations gives

$$\frac{\alpha\cos(kL) - k\sin(kL)}{\alpha\sin(kL) + k\cos(kL)} = -\frac{\alpha}{k}$$

After some simplification using trigonometric identities, the above equation can be re-written as the following:

$$\tan(kL) = \frac{2(\frac{\alpha}{k})}{1 + (\frac{\alpha}{k})^2}$$

The number of solutions of the above equation is equal to the total number of solutions of the following equations:

$$\tan(\frac{kL}{2}) = \frac{\alpha}{k}$$
$$-\cot(\frac{kL}{2}) = \frac{\alpha}{k}$$

Define $k_0 = \sqrt{2mV_0}/\hbar$. Using this, we can rewrite α/k as

$$\frac{\alpha}{k} = \sqrt{\frac{V_0}{E} - 1} = \sqrt{\frac{(k_0L/2)^2}{(kL/2)^2} - 1} = f(\frac{kL}{2})$$

So we need to find out the combined number of roots of the following equations in some variable u ($= kL/2$):

$$\tan(u) = f(u)$$
$$-\cot(u) = f(u)$$

We are given that $\sqrt{\frac{mV_0L^2}{2\hbar^2}} = 1 \implies kL/2 = 1$.

Clearly, the system has only one bound state!

8.1.3 Question 3

Label the regions from left to right as 1,2,3. In these regions, Schrodinger equation takes the form

$$\frac{d^2\psi}{dx^2} = \alpha^2\psi, \quad x < -L/2$$

$$\frac{d^2\psi}{dx^2} + k^2\psi = 0, \quad -L/2 < x < L/2$$

$$\frac{d^2\psi}{dx^2} = \alpha^2\psi, \quad L/2 < x$$

where

$$k = \sqrt{\frac{2mE}{\hbar^2}} \qquad \alpha = \sqrt{\frac{2m(V_0 - E)}{\hbar^2}}$$

The solutions in the different regions are:

$$\psi = Ae^{\alpha x}, \quad x < -L/2$$
$$\psi = Be^{ikx} + Ce^{-ikx}, \quad -L/2 < x < L/2$$
$$\psi = De^{-\alpha x}, \quad L/2 < x$$

We now demand continuity of the wavefunction and it's derivative at $x = -L/2$ and $x = +L/2$. Thus,

$$Ae^{-\alpha/2} = Be^{-ikL/2} + Ce^{ikL/2}$$
$$De^{\alpha/2} = Be^{ikL/2} + Ce^{-ikL/2}$$

Also,

$$A\alpha e^{-\alpha/2} = ik(Be^{-ikL/2} - Ce^{ikL/2})$$
$$-D\alpha e^{\alpha/2} = ik(Be^{ikL/2} - Ce^{-ikL/2})$$

Dividing the first two sets of equations and comparing it with the division of the second set of equations, we get the condition

$$B = \pm C$$

$B = +C$ corresponds to the symmetric state as $\psi \propto \cos kx$ in region 2 and $B = -C$ corresponds to the antisymmetric states as $\psi \propto \sin kx$ in region 2.

For the symmetric states
It immediately follows that $A = D$. Substituting this in the third boundary condition and comparing with the first boundary condition, we get

$$\alpha B(e^{-ikL/2} + e^{ikL/2}) = ikB(e^{-ikL/2} - e^{ikL/2})$$

from which we get the condition

$$\tan kL/2 = \frac{\alpha}{k}$$

For the antisymmetric states
It immediately follows that $A = -D$. Substituting this in the third boundary condition and comparing with the first boundary condition, we get

$$\alpha B(e^{-ikL/2} - e^{ikL/2}) = ikB(e^{-ikL/2} + e^{ikL/2})$$

from which we get the condition

$$\tan kL/2 = \frac{-k}{\alpha}$$

b)
The ground state is a symmetric wavefunction and hence the condition

$$\tan kL/2 = \frac{\alpha}{k}$$

applies. Now given $E_1 = 4.45eV$, we can get $k = \sqrt{2mE/\hbar^2}$. Thus, we get $kL/2 = 0.1718$. Now,

$$\tan kL/2 = \sqrt{\frac{V_0 - E}{E}}$$

Thus,

$$V_0 = E \tan kL/2^2 + E =$$

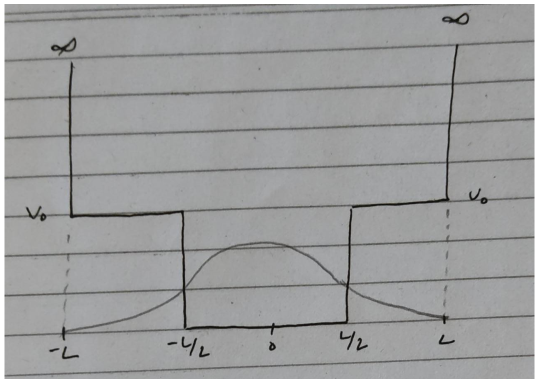


Figure 8.1: The potential is sketched in black, and the ground state in pencil

Question 4

Part a

for part a, we can see from the image that it looks very similar to the infinite well, and is symmetric, we can take hint from this and take the ground state to have
1) No nodes (ie probability will only be non zero is the potential is infinite and nowhere else, which means the wavefunction will not cross zero)
and
2) the maximum probability of finding the particle will be at the centre of the potential. These two assumptions give us a bell shaped wavefunction, that is zero for $|x| > L$, exponentially decaying for $L > |x| > \frac{L}{2}$ and sinusoidal for $\frac{L}{2} > |x|$

Part b

For a finite potential well, we know that the ground state eigenfunction must satisfy the following condition:

$$\sqrt{\frac{2\pi^2 mL^2V_0}{h^2} - \eta^2} = \eta \times tan(\eta) \text{ where } \eta = \frac{kL}{2}$$

$$\implies \sqrt{4.35 \times 10^{-12} - \eta^2} = \eta \times tan(\eta)$$

$$\text{but } tan(\eta) \approx \eta$$

$$\implies 4.35 \times 10^{-12} = \eta^2 + \eta^4$$

$$\eta = 2.1 \times 10^{-6}$$

$$\implies k = 4.2 \times 10^{-6} m^{-1}$$

$$\implies E = 1.1 \times 10^{-49} J$$

8.1.4 Question 5

(a) We can write the potential as

$$V(x) = \begin{cases} U & x < -L \\ 0 & -L \leq x \leq L \\ U & x > L \end{cases}$$

We are looking for a bound state, i.e. an energy eigenstate whose energy eigenvalue $E < V(\pm\infty) \implies V < U$. Let us first solve the TISE differential equation regionwise which we will patch together by imposing boundary conditions

$$\frac{1}{\psi(x)}\frac{d^2\psi}{dx^2} = \begin{cases} \alpha^2 & x < -L \\ -k^2 - L \leq x \leq L \\ \alpha^2 & x > L \end{cases}$$

$$\psi(x) = \begin{cases} Ae^{\alpha x} + Be^{-\alpha x} & x < -L \\ C\cos kx + D\sin kx & -L \leq x \leq L \\ Fe^{\alpha x} + Ge^{-\alpha x} & x > L \end{cases}$$

Again, $B = F = 0$ to prevent $\psi(x)$ from blowing up at $\pm\infty$. Since we are looking for symmetric solutions, we have $A = G$, $D = 0$. Imposing boundary conditions, we have
Continuity and differentiability at $x = L$.

$$Ae^{-\alpha L} = C\cos(kL)$$

$$A\alpha e^{-\alpha L} = kC\sin(kL).$$

Continuity and differentiability at $x = L$.

$$Ae^{-\alpha L} = C\cos(kL)$$

$$A\alpha e^{-\alpha L} = kC\sin(kL).$$

We have two redundant equations, so the assumption of symmetric solution was consistent. Let us write

$$\tan kL = \frac{\alpha}{k}.$$

This is the quantization condition we were looking for.
(b) As we know, the ground state is a symmetric one, hence the ground state energy is the lowest k and thus lowest E satisfying $\tan(kL) = \frac{\alpha}{k}$. Writing $k = \frac{\sqrt{2mU}}{\hbar}$, we have $\frac{\alpha}{k} = \sqrt{\frac{k_0^2L^2}{k^2L^2} - 1}$. We also have $k_0L = 2.298$. Thus we can now solve this equation numerically to get $kL = 1.081 = \implies E = \frac{\hbar^2k^2}{2mL^2} = 1.1\text{eV}$.
(c) As is clear from the picture, as we increase k_0, a new bound state is possible whenever the x intercept of $\sqrt{\frac{k_0L}{kL} - 1}$ crosses a multiple of π. Thus the number of bound states is ceiling($\frac{(k_0L)}{\pi}$) = ceiling($\frac{\sqrt{2mU}L}{\hbar\pi}$).

Question 6

We are given a potential well with a barrier in between of height $V_0 = E$ in the middle. We can divide the well into 5 regions;
1: from $-\infty$ to -2L where potential is ∞ and hence wavefunction is 0
2: from -2L to -L, where potential is 0
3: from -L to L where potential is a constant V_0 and given wavefunction is a constant C
4: from L to 2L, where potential is 0
5: from 2L to ∞ where potential is ∞ and hence wavefunction is 0

In region 4 where $\hat{V}(x) = 0$:

$$\hat{H}\psi(x) = E\psi(x)$$

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

Hence $\psi_{regn4}(x) = Ae^{ikx} + Be^{-ikx}$ for some constants A and B and $k = \hbar\sqrt{\frac{E}{2m}}$.
Similarly in region 2, $\psi_{regn2}(x) = Ee^{ikx} + Fe^{-ikx}$ for some constants E and F.
We need to now enforce the boundary conditions:

$$\psi_{regn2}(-2L) = \psi_{regn4}(2L) = 0$$

$$\psi_{regn2}(-L) = \psi_{regn4}(L) = C$$

$$\psi^{'}_{regn2}(-L) = \psi^{'}_{regn4}(L) = 0$$

This gives us A=F, B=E and

$$Ae^{ik2L} + Be^{-ik2L} = 0$$

$$B = -Ae^{ik4L}$$

and with the third condition:

$$ikAe^{ikL} - ikBe^{-ikL} = 0$$

$$B = Ae^{ik2L}$$

using this and the previous value of B we get $e^{ik2L} = -e^{ik4L}$ or $e^{ik2L} = -1 = e^{i\pi}$ which means $k = \frac{(2n+1)\pi}{2L}$
(where n is some integer)
so B = -A using this at x=L:

$$Ae^{ikL} - Ae^{-ikL} = C$$

$$A = \frac{-iC}{2sin(kL)} = \frac{-iC}{2}$$

$$|A|^2 = \frac{|C|^2}{4}$$

Lastly we should normalise $\psi(x)$ to find out C (we can assume C is real without loss of generality):

$$\int_{-2L}^{2L} \psi^{\dagger}(x)\psi(x) = \int_{-2L}^{-L} \psi^{\dagger}_{regn2}(x)\psi_{regn2}(x) + \int_{-L}^{L} C^{\dagger}C + \int_{L}^{2L} \psi^{\dagger}_{regn4}(x)\psi_{regn4}(x) = 1$$

It turns out the first and third term in the integral are equal, which gives us :

$$4L|A|^2 + \frac{|A|^2}{k}(1 - cos(2kL)) + 2L|C|^2 = 1$$

$$4L\frac{|C|^2}{4} + 2L\frac{|C|^2}{\pi 4}2 + 2L|C|^2 = 1$$

$$3L|C|^2 + L\frac{|C|^2}{\pi} = 1$$

$$|C|^2 = \frac{1}{L(3 + \pi^{-1})}$$

$$C = \pm\sqrt{\frac{1}{L(3 + \pi^{-1})}}$$

For part c, given L = 1 A and $m = m_e$. The two lowest k values are $\frac{\pi}{2L}$ and $\frac{3\pi}{2L}$ (ignore -ve since E is k squared). Also we have $k = \hbar\sqrt{\frac{E}{2m}}$ or $E = \frac{2k^2m}{\hbar^2}$. Which means:

$$E_{smallest} = \frac{\pi^2 m}{2\hbar^2 L^2} = 2.5228 \cdot 10^{77} eV$$

$$E_{2^{nd}smallest} = \frac{9\pi^2 m}{2\hbar^2 L^2} = 2.27058 \cdot 10^{78} eV$$

For part d, k=$\frac{\pi}{2L}$, and we have $psi(x)$ such that (for a known C, as above):
-2L to -L : $\psi_{regn2}(x) = \frac{iC}{2}e^{i0.5\pi x/L} + \frac{-iC}{2}e^{-i0.5\pi x/L} = -Csin(\frac{\pi x}{2L})$
-L to L : $\psi_{regn3}(x) = C$

L to 2L : $\psi_{regn4}(x) = \frac{-iC}{2}e^{i0.5\pi x/L} + \frac{iC}{2}e^{-i0.5\pi x/L} = Csin(\frac{\pi x}{2L})$
Then to calculate expectation values, use $\hat{x}\psi(x) = x\psi(x)$ and $\hat{p}\psi(x) = -i\hbar\frac{d}{dx}\psi(x)$:

$$< x >= \int \psi(x)^\dagger x\psi(x) = \int_{-2L}^{-L} \psi(x)^\dagger_{regn2} x\psi_{regn2}(x) + \int_{-L}^{L} \psi(x)^\dagger_{regn3} x\psi_{regn3}(x) + \int_{L}^{2L} \psi(x)^\dagger_{regn4} x\psi_{regn4}(x)$$

$$< x >= 0$$

$$< x^2 >= \int \psi(x)^\dagger x^2\psi(x) = \int_{-2L}^{-L} \psi(x)^\dagger_{regn2} x^2\psi_{regn2}(x) + \int_{-L}^{L} \psi(x)^\dagger_{regn3} x^2\psi_{regn3}(x) + \int_{L}^{2L} \psi(x)^\dagger_{regn4} x^2\psi_{regn4}(x)$$

$$< x^2 >= 2C^2L^3(1.5 - \frac{3}{\pi^2}) = \frac{2L^2}{(3+\pi^{-1})}(1.5 - \frac{3}{\pi^2})$$

$$< x^2 >\approx 0.72087L^2$$

$$< p >= -\int \psi(x)^\dagger i\hbar\frac{d}{dx}\psi(x)$$

$$= -\int_{-2L}^{-L} \psi(x)^\dagger_{regn2} i\hbar\frac{d}{dx}\psi_{regn2}(x) - \int_{-L}^{L} \psi(x)^\dagger_{regn3} i\hbar\frac{d}{dx}\psi_{regn3}(x) - \int_{L}^{2L} \psi(x)^\dagger_{regn4} i\hbar\frac{d}{dx}\psi_{regn4}(x)$$

$$< p >= 0$$

$$< p^2 >= -\int \psi(x)^\dagger \hbar^2\frac{d^2}{dx^2}\psi(x)$$

$$= -\int_{-2L}^{-L} \psi(x)^\dagger_{regn2} \hbar^2\frac{d^2}{dx^2}\psi_{regn2}(x) - \int_{-L}^{L} \psi(x)^\dagger_{regn3} \hbar^2\frac{d^2}{dx^2}\psi_{regn3}(x) - \int_{L}^{2L} \psi(x)^\dagger_{regn4} \hbar^2\frac{d^2}{dx^2}\psi_{regn4}(x)$$

$$< p^2 >= \frac{-\pi^2\hbar^2}{4L^2(3+\pi^{-1})} \approx \frac{-8.26942 \cdot 10^{-69}}{L^2}$$

From the calculated quantities, $\Delta x\Delta p \approx 7.7 \cdot 10^{-35}$ which is greater than $\frac{h}{4\pi} \approx 5.27286 \cdot 10^{-35}$ and hence satisfies the uncertainty principle.

Chapter 9

Tutorial 9

9.1 Scattering problems

9.1.1 Question 1

For $x > 0$ the Schrödinger equation is given by

$$\left(\frac{d^2}{dx^2} - k_2^2\right)\psi_2(x) = 0 \quad (x \geq 0)$$

where $k_2^2 = 2m\left(V_0 - E\right)/\hbar^2$. This equation's solution is

$$\psi_2(x) = Ce^{-k_2 x} + De^{k_2 x} \quad (x \geq 0).$$

Since the wave function must be finite everywhere, and since the term $e^{k_2 x}$ diverges when $x \to \infty$, the constant D has to be zero. Thus, the complete wave function is

$$\Psi(x,t) = \begin{cases} Ae^{i(k_1 x - \omega t)} + Be^{-i(k_1 x + \omega t)} & x < 0 \\ Ce^{-k_2 x}e^{-i\omega t} & x \geq 0 \end{cases}$$

Here,

$$k_1 = \sqrt{2mE/\hbar^2}$$

We know that probability density is $|\psi(x)|^2$. Therefore, the required condition is:

$$\frac{|\psi(x_0)|^2}{|\psi(0)|^2} = \frac{1}{e}$$

Which gives:

$$e^{-2k_2 x_0} = e^{-1}$$

Thus $x_0 = \frac{1}{2k_2}$

Taking $\Delta x = x_0$,

$$\Delta p \geq \frac{\hbar}{2x_0}$$

$$\Delta E \geq \frac{(\Delta p)^2}{2m}$$

The minimum value of this is:

$$\Delta E = \frac{(\frac{\hbar}{2x_0})^2}{2m} = \frac{\hbar^2 k_2^2}{2m} = (V_0 - E)$$

Therefore, we cannot be sure that the total energy is indeed less than V_0.

9.1.2 Question 2

9.1.3 Question 3

Label the regions from left to right as 1,2. Let the potential barrier be V_0 for $x > 0$. In the two regions, time independent Schrodinger equation takes the form

$$\frac{d^2\psi}{dx^2} + k^2\psi = 0, \quad x < 0$$

$$\frac{d^2\psi}{dx^2} = \alpha^2\psi, \quad 0 < x$$

$$k = \sqrt{\frac{2mE}{\hbar^2}} \qquad \alpha = \sqrt{\frac{2m(V_0 - E)}{\hbar^2}}$$

The solutions in the different regions are:

$$\psi = A\cos kx + B\sin kx, \quad x < 0$$

$$\psi = Ce^{-\alpha x}, \quad 0 < x$$

Probability of detecting the electron at $x = 0$ is $|C|^2$. Probability of detecting the electron at $x > 0$ is $|C|^2 e^{-2\alpha x}$. Thus,

$$\frac{|C|^2 e^{-2\alpha x}}{|C|^2} = e^{-2\alpha x} = \frac{1}{2}$$

Thus,

$$x = \frac{\hbar}{2\sqrt{2m(V_0 - E)}} \ln 2$$

Now, $E = 3eV$, $V_0 = 7eV$, $m = 9.1 \times 10^{-31}kg$. Substituting, we get

$$x = 2.127\mathring{A}$$

9.1.4 Question 4

The Schrödinger equation outside the barrier is given by

$$\left(\frac{d^2}{dx^2} + k^2\right)\psi(x) = 0$$

where $k^2 = 2mE/\hbar^2$.

The Schrödinger equation inside the barrier is given by

$$\frac{d^2}{dx^2}\psi(x) = 0$$

The latter equation is just the ODE for linear equations. The former we have dealt with in free particle questions. Setting the left edge of the barrier as the origin (choice of origin does not affect the answer), the solution is of the form:

$$\psi(x) = \begin{cases} Ae^{-ikx} + Be^{ikx} & x < 0 \\ Cx + D & 0 < x < L \\ Fe^{-ikx} + Ge^{ikx} & x > L \end{cases}$$

Constraints:

1. Particle moves from the left hand side $\implies F = 0$
2. Wavefunction is continuous at x = 0 $\implies A + B = D$
3. Wavefunction is continuous at x = L $\implies CL + D = Ge^{ikL}$
4. Wavefunction is differentiable at x = 0 $\implies (B - A)ik = C$
5. Wavefunction is differentiable at x = L $\implies C = Ge^{ikL}$

a)

Now transmission coefficient is defined as $|\frac{G}{B}|^2$ Solving the 5 simultaneous equations for G/B, we get:

$$\boxed{T = \frac{4}{4 + k^2L^2} = \frac{4\hbar^2}{4\hbar^2 + 2mEL^2}}$$

b)

$$T = \frac{1}{2}$$
$$\implies \frac{4}{4 + k^2L^2} = \frac{1}{2}$$
$$\implies 8 = 4 + k^2L^2$$
$$\implies 4 = k^2L^2 \implies kL = \pm 2$$
$$\implies 2\pi L = \pm 2\lambda$$
$$\boxed{\implies \lambda = \pm \pi L}$$

9.1.5 Question 5

First of all, supposing the given wavefunctions are correct, try to find a relation between the constants using boundary conditions. Continuity at $x = L$ yields

$$Ae^{-\iota k_1 L} = Be^{-\iota k_2 L}.$$

Differentiability at $x = L$ yields

$$Ak_1 e^{-\iota k_1 L} = Bk_2 e^{-\iota k_2 L}$$

Thus, it implies

$$k_1 = k_2 \implies V = 0$$

which is clearly not the case. Hence the claims are incorrect.

9.1.6 Question 6

a) Label the regions from left to right as 1,2,3. In these regions, Schrodinger equation takes the form

$$\frac{d^2\psi}{dx^2} + k_1^2\psi = 0, \quad x < 0$$

$$\frac{d^2\psi}{dx^2} + k_2^2\psi = 0, \quad 0 < x < d$$

$$\frac{d^2\psi}{dx^2} + k_3^2\psi = 0, \quad d < x$$

$$k_1 = \sqrt{\frac{2mE}{\hbar^2}} \qquad k_2 = \sqrt{\frac{2m(E-5V_0)}{\hbar^2}} \qquad k_3 = \sqrt{\frac{2m(E-nV_0)}{\hbar^2}}$$

The solutions in the different regions are:

$$\psi = Ae^{ik_1x} + Be^{-ik_1x}, \quad x < 0$$

$$\psi = Ce^{ik_2x} + De^{-ik_2x}, \quad 0 < x < d$$

$$\psi = Ee^{ik_3x}, \quad d < x$$

Since the transmission coefficient is 0.75,

$$\frac{k_3|E|^2}{k_1|A|^2} = 0.75$$

Given $E = 9V_0$, we can find $k_2d = \pi$. We now demand continuity of the wavefunction and it's derivative at $x = 0$ and $x = d$. Thus, at $x = 0$,

$$A + B = C + D, \qquad k_1(A - B) = k_2(C - D)$$

At $x = d$,

$$-(C + D) = Ee^{ik_3d}, \qquad -k_2(C - D) = Ek_3e^{ik_3d}$$

as $e^{i\pi} = e^{-i\pi} = -1$. For expressing A in terms of E,

$$(A + B) = -Ee^{ik_3d}, \qquad k_1(A - B) = -Ek_3e^{ik_3d}$$

Adding the two equations, we get

$$2A = -Ee^{ik_3d}\left(1 + \frac{k_3}{k_1}\right)$$

Taking the modulus squared on both sides,

$$4|A|^2 = |E|^2||e^{ik_3d}||1 + \frac{k_3}{k_1}|^2$$

If $n > 9$, then k_3 is purely imaginary. If we proceed in that direction, we will get that there is no such n that satisfies the relation (Check!). If $n < 9$, k_3 is real and moreover positive as we cannot have a left moving wave in region 3. Thus, using the relation between $|E|^2$ and $|A|^2$, we get

$$\left(1 + \frac{k_3}{k_1}\right)^2 = \frac{16k_3}{3k_1} \implies \frac{k_3}{k_1} = 3, \frac{1}{3}$$

Substituting the expressions for k_3 and k_1 and solving, we get

$$\sqrt{\frac{9-n}{9}} = 3 \implies \boxed{n = -72}, \qquad \sqrt{\frac{9-n}{9}} = \frac{1}{3} \implies \boxed{n = 8}$$

b) From the four boundary conditions, we have

$$\begin{aligned}
2A &= -Ee^{ik_3 d}\left(1 + \frac{k_3}{k_1}\right) \\
2C &= -Ee^{ik_3 d}\left(1 + \frac{k_3}{k_2}\right) \\
2D &= -Ee^{ik_3 d}\left(1 - \frac{k_3}{k_1}\right) \\
2B &= -Ee^{ik_3 d}\left(1 - \frac{k_3}{k_1}\right)
\end{aligned}$$

We thus get

$$\begin{aligned}
B &= \frac{A(k_1 - k_3)}{k_1 + k_3} \\
C &= \frac{Ak_1(k_2 + k_3)}{k_2(k_1 + k_3)} \\
D &= \frac{Ak_1(k_2 - k_3)}{k_2(k_1 + k_3)} \\
E &= -\frac{2Ak_1 e^{-ik_3 d}}{k_1 + k_3}
\end{aligned}$$

c) For the case $n = -72$, $k_3 = 3k_1$. Thus, B will have a phase factor of $e^{i\pi}$ with respect to A. For the case $n = 8$, $k_3 = k_1/3$. Thus, B will not have any phase compared to A. Since B is the amplitude for the reflected wave, the discussion above gives the relative phase between the incident and reflected waves.

Chapter 10

Tutorial 10

10.1 SHM and 2D/3D solutions

10.1.1 Question 3

We know that the energy levels of a quantum harmonic oscillator are:

$$E_n = \left(n + \frac{1}{2}\right)\hbar\omega, \qquad n = 0, 1, 2.3, ...$$

a) For the transition from $n = 3$ to $n = 2$, the wavelength of the photon emitted is

$$\lambda = \frac{hc}{\Delta E} = \frac{hc}{\hbar\omega} = \frac{2\pi c}{\omega} = 2\pi c\sqrt{\frac{m}{k}} = 128.8\mu m$$

b) The ground state energy is

$$E_0 = \frac{1}{2}\hbar\omega = \frac{\hbar}{2}\sqrt{\frac{k}{m}} = 7.7 \times 10^{-22} J$$

10.1.2 Question 4

a) Effective mass μ of a diatomic molecule is $\mu = m/2$

$$\implies \omega = \sqrt{\frac{k}{\mu}} = \sqrt{\frac{2k}{m}} = 1.16 \times 10^{15} Hz$$

b) From the energy formula $E = (n + 0.5)\hbar\omega$:
The energy between consecutive energy states is $\hbar\omega = 0.766eV$
The wavelength is calculated by $\lambda = \frac{2\pi c}{\omega} = 1.625 \times 10^{-6} m$

10.1.3 Question 5

(a) Use separation of variables

$$\psi(x, y) = \psi_x(x)\psi_y(y).$$

Put this in TISE

$$H\psi(x, y) = E\psi(x, y)$$

$$\implies -\frac{\hbar^2}{2m\psi_x(x)}\frac{\partial^2\psi_x(x)}{\partial x^2} + \frac{1}{2}kx^2 = -(-\frac{\hbar^2}{2m\psi_y(y)} + \frac{1}{2}ky^2 - E).$$

LHS is purely a fn of x and RHS of y, and the expression has to be true for all x, y. This is only possible if $LHS = RHS =$ some constant, which we can write as $E_x \leq E$

$$-\frac{\hbar^2}{2m\psi_x(x)}\frac{\partial^2\psi_x(x)}{\partial x^2} + \frac{1}{2}kx^2 = E_x,$$

$$-\frac{\hbar^2}{2m\psi_y(y)}\frac{\partial^2\psi_y(y)}{\partial y^2} + \frac{1}{2}ky^2 = E - E_x.$$

We already know the solutions to these 2 equations as

$$E_x = (n_x + \frac{1}{2})\hbar\omega,$$

$$E - E_x = (n_y + \frac{1}{2})\hbar\omega.$$

$$\implies E = (n_x + n_y + 1)\hbar\omega.$$

(b) The degeneracy of level $E = (n+1)\hbar\omega$ will be the number of solutions to $n_x + n_y = n$ which we can easily see will be $n + 1(n_x = 0, 1, 2, ..., n)$. Therefore the degeneracy of energy E will be $\frac{E}{\hbar\omega}$.

10.1.4 Question 6

(a) We follow the same procedure as above. Since the potentials are additive, that is $V(x, y) = V(x)+V(y)$, we can proceed with variable separation. Thus, we get:

$$\psi(q_1, q_2) = \psi_{q_1}(q_1)\psi_{q_2}(q_2).$$

Separating the LHS and RHS into constants as above, we obtain the following equations:

$$-\frac{\hbar^2}{2m\psi_{q_1}(q_1)}\frac{\partial^2\psi_{q_1}(q_1)}{\partial q_1^2} + \frac{1}{2}m\omega_1^2q_1^2 = E_{q_1}$$
$$-\frac{\hbar^2}{2m\psi_{q_2}(q_2)}\frac{\partial^2\psi_{q_2}(q_2)}{\partial q_2^2} + \frac{1}{2}m\omega_2^2q_2^2 = E_{q_2}$$

Lucky for us, we already have the exact solution to the above in terms of the Hermite polynomials:

$$\psi_{q_1}(q_1)^(n_1) = (\frac{m\omega_1}{\pi\hbar})^{1/4}\frac{1}{\sqrt{2^{n_1}(n_1)!}}H_{n_1}\left(\sqrt{\frac{m\omega_1}{\hbar}}q_1\right)e^{-\frac{m\omega_1q_1^2}{2\hbar}}$$
$$\psi_{q_2}(q_2)^(n_2) = (\frac{m\omega_2}{\pi\hbar})^{1/4}\frac{1}{\sqrt{2^{n_2}(n_2)!}}H_{n_2}\left(\sqrt{\frac{m\omega_2}{\hbar}}q_2\right)e^{-\frac{m\omega_2q_2^2}{2\hbar}}$$

with the eigenvalues:

$$E_{q_1} = \left(n_1 + \frac{1}{2}\right)\hbar\omega_1$$
$$E_{q_2} = \left(n_2 + \frac{1}{2}\right)\hbar\omega_2$$

Clearly, the (n_1, n_2) eigenstate is

$$\psi(q_1, q_2) = \psi_{q_1}(q_1)^{(n_1)}\psi_{q_2}(q_2)^{(n_2)}$$

, with the energy

$$E = (n_1\omega_1 + n_2\omega_2 + \frac{(\omega_1 + \omega_2)}{2})\hbar$$

, with the general E eigenstate being the superposition of these LI basis.

(b) When $\frac{\omega_1}{\omega_2} = \frac{3}{4}$, we need to find integer solutions to the equation:

$$3n_1 + 4n_2 = n$$

. The ground state is the one with $n_1 = 0, n_2 = 0$, and it is unique, with no degeneracy. The same happens for $(1,0)$ and $(0,1)$ states. The first time the degeneracy occurs is during the first solution of the above equation, for the 2 states of $(n_1, n_2) = (4,0)$ and $(n_1, n_2) = (0,3)$, with the total energy being $E = \frac{31}{8}\hbar\omega_2$

10.1.5 Question 7

We have been given a particle in a potential well $m\omega^2x^2/2$, and the expression of the wave-function in terms of β:

$$\psi(x) = (\frac{2\beta}{\sqrt{3}})(\frac{\beta}{\pi})^{1/4} x^2 \exp(-\beta x^2/2)$$

a) To find the dimension of β we can use the fact that the expression in the exponential must be dimensionless, ie $[\beta] = \dim(x^2)^{-2} = [L]^{-2}$.
Besides this note:
$\dim(\omega) = [T]^{-1}$
$\dim(\hbar\omega) = \dim(\mathrm{E}) = [M]\frac{[L]}{[T]}^2$
$\dim(\hbar) = [M]\frac{[L]^2}{[T]}$
dim(m) = [M]
With this information we can make a pretty educated guess as to how to express β in terms of m, ω and $\hbar$:

$$[\beta] = \frac{m\omega}{\hbar}$$

We could also have arrived at the same answer by comparing the given expression with the expression of eigenstates that we know, especially the exponential part.

b) We can do this part in two ways as well, either by finding the coefficients of the parts by multiplying by ψ_0^* or ψ_2^* and integrating , where:

$$a = \int \psi_0^*(x)\psi(x)$$

$$b = \int \psi_2^*(x)\psi(x)$$

or, the second way, by using the expression we have and knowledge or Hermite polynomials. We know (or one can google) $H_0(x) = 1$, $H_1(x) = x$ and $H_2(x) = x^2 - 1$. Hence $\beta x^2 = H_2(\sqrt{\beta}x) + H_0(\sqrt{\beta}x)$
also note the expressions of the eigenstate is as:

$$\psi_n(x) = \frac{1}{\sqrt{2^n n!}}(\frac{m\omega}{\pi\hbar})^{1/4}e^{-\frac{m\omega x^2}{2\hbar}}H_n(\sqrt{\frac{m\omega}{\hbar}}x)$$

where $H_n(x)$ is the Hermite polynomial.
and from part a, we can say $\beta = \frac{m\omega}{\hbar}$, ie :

$$\psi_n(x) = \frac{1}{\sqrt{2^n n!}}(\frac{\beta}{\pi})^{1/4} e^{-\frac{\beta x^2}{2}} H_n(\sqrt{\beta} x)$$

Using this, we can write out:

$$\psi(x) = (\frac{2}{\sqrt{3}}) \left(\frac{\beta}{\pi}^{1/4} \left((\sqrt{\beta} x)^2 - 1 \right) e^{-\beta x^2/2} + \frac{\beta}{\pi}^{1/4} e^{-\beta x^2/2} \right)$$

$$\psi(x) = (\frac{2}{\sqrt{3}}) \left(\sqrt{2^2 2!} \psi_2(x) + \sqrt{2^0 0!} \psi_0(x) \right)$$

$$\psi(x) = (\frac{4\sqrt{2}}{\sqrt{3}}) \psi_2(x) + (\frac{2}{\sqrt{3}}) \psi_0(x)$$

In the question, this expression isn't properly normalised hence after normalisation b = $\frac{4\sqrt{2}}{\sqrt{3}} \frac{1}{\sqrt{(\frac{4\sqrt{2}}{\sqrt{3}})^2 + (\frac{2}{\sqrt{3}})^2}}$ = $\frac{2\sqrt{2}}{3}$ and a = $\frac{1}{3}$. Also expectation value of energy $< E >= a^2 E_0 + b^2 E_2$ where $E_0 = \hbar\omega/2$ and $E_2 = 5\hbar\omega/2$, so

$$< E >= \frac{1}{9}\hbar\omega/2 + \frac{8}{9} 5\hbar\omega/2$$

$$< E >= \hbar\omega \left(\frac{41}{18} \right)$$

10.1.6 Question 9

a) The total potential experienced by the particle will be the harmonic oscillator potential plus the electromagnetic potential as measured from the $x = 0$ position. Thus

$$V(x) = \frac{1}{2} m\omega^2 x^2 - E_0 q x$$

b) To put the problem in a more familiar form, we complete the squares

$$V(x) = \frac{1}{2} \left(m\omega^2 x^2 - 2E_0 q x + \left(\frac{E_0 q}{\sqrt{m\omega^2}} \right)^2 \right) - \frac{1}{2} \left(\frac{E_0 q}{\sqrt{m\omega^2}} \right)^2$$

$$\implies V(x) = \frac{1}{2} \left(\sqrt{m\omega^2} x - \frac{E_0 q}{\sqrt{m\omega^2}} \right)^2 - \frac{E_0^2 q^2}{2m\omega^2}$$

$$\implies V(x) = \frac{1}{2} m\omega^2 \left(x - \frac{E_0 q}{m\omega^2} \right)^2 - \frac{E_0^2 q^2}{2m\omega^2}$$

This is nothing but the potential of a harmonic oscillator shifted in position by $E_0 q/m\omega^2$ and shifted in energy by $E_0^2 q^2/2m\omega^2$

d) Let $a = E_0 q/m\omega^2$ and $V_0 = E_0^2 q^2/2m\omega^2$. The Time-Independent Schrodinger equation is

$$-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} \psi(x) + \frac{1}{2} m\omega^2 \left(x - \frac{E_0 q}{m\omega^2} \right)^2 \psi(x) = (E + V_0)\psi(x)$$

Making the change of variable $x - a \to x'$, we have

$$-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x'^2}\phi(x') + \frac{1}{2}m\omega x'^2\phi(x') = (E + V_0)\phi(x')$$

where $\phi(x') = \psi(x' + a)$. We already know the solutions to this eigenvalue equation.

$$E + V_0 = \left(n + \frac{1}{2}\right)\hbar\omega, \qquad n = 0, 1, 2.3, ...$$

Thus, the stationary state energies are:

$$E_n = \left(n + \frac{1}{2}\right)\hbar\omega - \frac{E_0^2 q^2}{2m\omega^2}, \qquad n = 0, 1, 2.3, ...$$

The ground state energy is then just

$$\boxed{E_0 = \frac{\hbar\omega}{2} - \frac{E_0^2 q^2}{2m\omega^2}}$$

e) By the from of the Schrodinger equation, $\phi(x')$ is just the wavefunction of the usual quantum harmonic oscillator. We know that the square of these wavefunctions are symmetric about the origin $x' = 0$. Hence,

$$\langle \hat{X}' \rangle = \langle \hat{X} - a \rangle = 0$$

$$\boxed{\langle \hat{X} \rangle = \frac{E_0 q}{m\omega^2}}$$

Chapter 11

Tutorial 11

11.1 Statistical Mechanics

11.1.1 Question 1

No of ways to choose 5 balls out of 59 is ${}^{59}C_5$.

No of ways to choose 1 ball out of 35 is ${}^{35}C_1$

No of ways to choose 6 balls $= {}^{59}C_5 \times^{35} C1$

11.1.2 Question 2

We have 20 coins and we flip them all together.

(a) If all the coins are independent, then the outcome of each flip can either be "HEAD" or "TAIL" with equal probability. Thus, two possibilities corresponding to every coin. Thus, the total number of outcomes is 2^{20}.

(b) We need the number of ways for obtaining 12 heads and 8 tails. So we need to choose 12 (or 8) coins out of the 20 and assign them heads (or tails) and the rest automatically get tails (or heads). Thus, out answer is $\binom{20}{12}$.

(c) Here we need to find the number of probability of obtaining 12 heads and 8 tails regardless of the order. It will be simply $\frac{\binom{20}{8}}{2^{20}}$.

11.1.3 Question 3

Let the number of particles in the 3 energy levels be (n_0, n_E, n_{2E}). Given that the total available energy is $3E$, we have $n_E + 2n_{2E} = 3$. We also have $n_0 + n_E + n_{2E} = 3$. Subtracting the two equations we have $n_0 = n_{2E}$. From this we get that the only two distributions among the energy levels are $(0, 3, 0)$ and $(1, 1, 1)$. As these levels have degeneracy $2, 10, 20$

$$\textbf{No. of microstates of } (0, 3, 0) = \binom{10}{3} = 120$$

$$\textbf{No. of microstates of } (1,1,1) = \binom{2}{1}\binom{10}{1}\binom{20}{1} = 400$$

As each microstate is equally likely, the probability of the distributions are

$$\textbf{Prob. of } (0,3,0) = 0.23$$

$$\textbf{Prob. of } (1,1,1) = 0.77$$

11.1.4 Question 4

For a 3D anisotropic oscillator, We can split the hamiltonian:

$$H = H_x(\omega_x) + H_y(\omega_y) + H_z(\omega_z)$$

where

$$H_x(\omega_x) = \frac{-\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + \frac{1}{2}m\omega_x^2 x^2 \qquad \text{(and similarly for y and z)}$$

Now, we rewrite the potential given in the question to make it obvious that the question refers to a 3D anisotropic oscillator:

$$V(x,y,z) = \frac{1}{2}m\omega_x^2 x^2 + \frac{1}{2}m\omega_y^2 y^2 + \frac{1}{2}m\omega_z^2 z^2$$

with

$$\omega_x = \omega_y = \omega$$

$$\omega_z = 2\omega$$

This gives us an energy:

$$\begin{aligned}
E &= \left(n_x + \frac{1}{2}\right)\hbar\omega_x + \left(n_y + \frac{1}{2}\right)\hbar\omega_y + \left(n_z + \frac{1}{2}\right)\hbar\omega_z \\
&= \left(n_x + \frac{1}{2} + n_y + \frac{1}{2} + 2n_z + 1\right)\hbar\omega \\
&= \left(n_x + n_y + 2n_z + 2\right)\hbar\omega
\end{aligned}$$

where n_i is a non negative integer

a) Ground state is $2\hbar\omega$
b) Degeneracy of $7\hbar\omega$ equals the number of solutions to

$$7\hbar\omega = (n_x + n_y + 2n_z + 2)\hbar\omega$$

$$\implies 5 = (n_x + n_y + 2n_z)$$

$\boxed{\text{There are 12 solutions}}$

11.1.5 Question 5

(a) $n_E + 3n_{3E} + 5n_{5E} + 9n_{9E} = 9$ and $n_0 + n_E + n_{3E} + n_{5E} + n_{9E} = 4$. We thus have the possibilities

$$(n_0, n_E, n_{3E}, n_{5E}, n_{9E}) = (3,0,0,0,1) \text{ with probability proportional to } 1 \times \frac{4!}{3!} = 4$$

$$(n_0, n_E, n_{3E}, n_{5E}, n_{9E}) = (1,1,1,1,0) \text{ with probability proportional to } 1 \times 4! = 24$$

$$(n_0, n_E, n_{3E}, n_{5E}, n_{9E}) = (1,0,3,0,0) \text{ with probability proportional to } 1 \times \frac{4!}{3!} = 4.$$

Thus the probabilities for these cases are $\frac{4}{4+24+4} = 0.125$, $\frac{24}{4+24+4} = 0.75$, $\frac{4}{4+24+4} = 0.125$ repectively.
(b)

$$(n_0, n_E, n_{3E}, n_{5E}, n_{9E}) = (3,0,0,0,1) \text{ with probability proportional to } 1$$

$$(n_0, n_E, n_{3E}, n_{5E}, n_{9E}) = (1,1,1,1,0) \text{ with probability proportional to } 1$$

$$(n_0, n_E, n_{3E}, n_{5E}, n_{9E}) = (1,0,3,0,0) \text{ with probability proportional to } 1.$$

Thus the probabilities for each of these cases are $\frac{1}{1+1+1} = 1/3$.
(c)

$$(n_0, n_E, n_{3E}, n_{5E}, n_{9E}) = (3,0,0,0,1) \text{ with probability proportional to } 0$$

$$(n_0, n_E, n_{3E}, n_{5E}, n_{9E}) = (1,1,1,1,0) \text{ with probability proportional to } 1$$

$$(n_0, n_E, n_{3E}, n_{5E}, n_{9E}) = (1,0,3,0,0) \text{ with probability proportional to } 0.$$

Thus the probabilities for these cases are $0, 1, 0$ respectively.

11.1.6 Question 6

Given 3 electrons, and ten energy states (with spin degeneracy ie, each energy state can take 2 electrons only).
Two ways to fill up the electrons: 2 electrons in one energy state, and third in another(spin up or down), or all 3 electrons in different states.
Though this can be simply visualised by considering it to be a situation of selecting 3 seats from 20 available seats :
$C^3_{20} = 1140$
Where as the other case = $C^3_{10} * 3! = 720$
(C^3_{10} ways to select seats and 3! ways to arrange people in those seats)

11.1.7 Question 8

(a) *Classical particles:* all 5 can be accommodated in the $n = 0$ level. This is the lowest energy state and is the ground state having energy $\frac{5}{2}\hbar\omega$

Identical bosons: all 5 can be accommodated in the $n = 0$ level. This is the lowest energy state and is the ground state having energy $\frac{5}{2}\hbar\omega$

Identical fermions: Pauli's exclusion principle forbids all 5 from occupying the same energy level. A maximum of two fermions can be accommodated in any energy level. Therefore, we can have 2 in the $n = 0$ state, $n = 1$ state each and one in the $n = 2$ state. Therefore, it has energy $\frac{13}{2}\hbar\omega$. Considering spin, this ground state has a degeneracy of 2.

(b) *Classical particles:* Any one of the particles can be excited to the $n = 1$ level, and the remaining four can be accommodated in the $n = 0$ level. Since classical particles are distnguishable, we can choose the excited particle in 5 ways, leading to 5 distinct microstates unlike in the bosonic case.

Identical bosons: Any one of the bosons can be excited to a higher $n = 1$ level, and the remaining four can be accommodated in the $n = 0$ level. Since they are indistinguishable, there is only one microstate.

Identical fermions: There are two possible excitations. An electron in the $n = 1$ state can be excited to the $n = 2$ state or the electron in the $n = 2$ state can be excited to the $n = 3$ state. This results in 2 possible microstates. If we now consider that the unpaired electron has spin degeneracy, we get 4 possible microstates.

(c) At low temperatures, the lower energy states are more populated for bosons than classical particles. This can be inferred from the fact that there are more microstates for a given energy for classical particles in higher energy levels since they are distinguishable.