PH 107 : Quantum Physics
Solution Booklet

Rwitaban Goswami

Contents

1 Black Body Radiation

1.1. Rayleigh-Jean's law gives the radiant energy density (energy per unit volume) as

$$u_\nu(\nu)\,d\nu = \frac{8\pi\nu^2}{c^3}kT\,d\nu$$

Show that in terms of wavelength interval, Rayleigh-Jean's law can be expressed as

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

Solution:
Using physical intuition:
Rayleigh-Jean's law physically means that there is $\frac{8\pi\nu^2}{c^3}kT\,d\nu$ amount of energy density between frequencies ν and $\nu+d\nu$. Since $\nu = \frac{c}{\lambda}$, this means that there is $\frac{8\pi c^2}{c^3\lambda^2}kT\,d\nu = \frac{8\pi}{c\lambda^2}kT\,d\nu$ worth of energy density between frequencies ν and $\nu + d\nu$.

But we want the amount of energy density between λ and $\lambda + d\lambda$. To find that we need the relation between $d\lambda$ and $d\nu$. We know that

$$\nu = \frac{c}{\lambda} \tag{1.1.1}$$

$$\implies d\nu = -\frac{c}{\lambda^2}d\lambda \tag{1.1.2}$$

So the amount of energy density between ν and $\nu + d\nu$ should be scaled by $\frac{c}{\lambda^2}$ to get the amount between λ and $\lambda + d\lambda$ (ignore the sign, it simply means that as λ decreases ν increases, so it's actually the energy density between λ and $\lambda - d\lambda$, which makes no difference really)

So the amount becomes $\frac{c}{\lambda^2}\frac{8\pi}{c\lambda^2}kT\,d\lambda = \frac{8\pi}{\lambda^4}kT\,d\lambda$
Therefore

$$u_\lambda(\lambda)\,d\lambda = \frac{8\pi}{\lambda^4}kT\,d\lambda \tag{1.1.3}$$

A more mathematically rigorous method:
Let $\nu_1\lambda_1 = \nu_2\lambda_2 = c$, where WLOG $\nu_1 < \nu_2$, $\lambda_2 < \lambda_1$
Since the range of frequencies (ν_1, ν_2) corresponds to the same modes as (λ_2, λ_1), they should contain they same amount of total energy

$$\implies \int_{\nu_1}^{\nu_2} u_\nu(\nu)\,d\nu = \int_{\lambda_2}^{\lambda_1} u_\lambda(\lambda)\,d\lambda \tag{1.1.4}$$

$$\tag{1.1.5}$$

Notice the opposite limits for u_λ and u_ν, this is because λ and ν are inversely related

$$\text{Subsitute } \nu = \frac{c}{\lambda} \text{ in } u_\nu$$

$$\implies -\int_{\lambda_1}^{\lambda_2} u_\nu(\frac{c}{\lambda})\frac{c}{\lambda^2}\,d\lambda = \int_{\lambda_2}^{\lambda_1} u_\lambda(\lambda)\,d\lambda \tag{1.1.6}$$

$$\implies \int_{\lambda_2}^{\lambda_1} u_\nu(\frac{c}{\lambda})\frac{c}{\lambda^2}\,d\lambda = \int_{\lambda_2}^{\lambda_1} u_\lambda(\lambda)\,d\lambda \tag{1.1.7}$$

Since the integrals are equal for all values of λ_1 and λ_2, this must mean the integrands must also be equal

$$\implies u_\lambda(\lambda) = \frac{c}{\lambda^2}u_\nu(\frac{c}{\lambda}) \tag{1.1.8}$$

This is exactly the same result as before, we scale by $\frac{c}{\lambda^2}$, and replace all ν by $\frac{c}{\lambda}$. Notice that no negative sign appears here.

1.2. Use Planck's equation and show that the expression for radiant intensity (in terms of λ) is given by

$$I(\lambda)\,d\lambda = \frac{2\pi hc^2}{\lambda^5}\frac{1}{e^{\frac{hc}{\lambda kT}}-1}\,d\lambda$$

Solution: Planck's equation states that

$$I(\nu,T)d\nu = \frac{c}{4}\frac{8\pi h\nu^3}{c^3}\frac{1}{e^{\frac{h\nu}{kT}}-1}\,d\nu \tag{1.2.1}$$

$$= \frac{2\pi h\nu^3}{c^2}\frac{1}{e^{\frac{h\nu}{kT}}-1}\,d\nu \tag{1.2.2}$$

$$\tag{1.2.3}$$

Where $I(\nu,T)$ is the radiant intensity in terms of ν
Using similar logic as above, we scale this by $\frac{c}{\lambda^2}$ to obtain

$$I(\lambda,T)\,d\lambda = \frac{2\pi hc^2}{\lambda^5}\frac{1}{e^{\frac{hc}{\lambda kT}}-1}\,d\lambda \tag{1.2.4}$$

1.3. According to Planck, the spectral energy density $u(\lambda)$ of a black body maintained at temperature T is given by

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

where λ denotes the wavelength of radiation emitted by the black body.

(a) Find an expression for $\lambda_{\max}$ at which $u(\lambda, T)$ attains its maximum value (at a fixed temperature T). $\lambda_{\max}$ should be in terms of T and fundamental constants h, c and k_B.

Solution: We simply differentiate $u(\lambda, T)$ by λ and set to zero

$$\left.\frac{\partial u(\lambda, T)}{\partial \lambda}\right|_{\lambda=\lambda_{\max}} = 0 \tag{1.3.1}$$

$$\implies -5\frac{8\pi hc}{\lambda_{\max}^6}\frac{1}{e^{\frac{hc}{\lambda_{\max}k_BT}}-1} + \frac{8\pi hc}{\lambda_{\max}^5}\frac{hce^{\frac{hc}{\lambda_{\max}k_BT}}}{\lambda_{\max}^2 k_BT(e^{\frac{hc}{\lambda_{\max}k_BT}}-1)^2} = 0 \tag{1.3.2}$$

$$\implies 5\lambda_{\max}T(e^{\frac{hc}{\lambda_{\max}k_BT}}-1) = \frac{hc}{k_B}e^{\frac{hc}{\lambda_{\max}k_BT}} \tag{1.3.3}$$

We can further see that if we put $x = \frac{hc}{\lambda_{\max}k_B}T$

$$\frac{xe^x}{e^x-1} - 5 = 0 \tag{1.3.4}$$

This equation can be solved numerically (you can use Desmos or Wolfram Alpha) to get $x = 4.9651$, so we get $\lambda_{\max}T = \frac{hc}{4.9651k_B} = 0.0029$ m K
This is the Wein's law that you studied in JEE!
Note that this constant is going to be different if you calculate the maximum of $u(\nu, T)$, because the function $u(\nu, T) \neq u(\lambda, T)$, they represent different things physically (one represents energy density between ν and $\nu + d\nu$, the other between λ and $\lambda + d\lambda$. Since $d\lambda$ and $d\nu$ aren't related proportionally, so the two functions are also different but have similar shape. Hence the constant will differ)

(b) Expressing $\lambda_{\max}$ as $\frac{\alpha}{T}$, obtain an expression for $u_{\max}(T)$ in terms of α, T and the fundamental constants

Solution: We know from above that $\alpha = 0.0029$ m K
We can simply put $\lambda_{\max} = \frac{\alpha}{T}$ in $u(\lambda, T)$ to get $u_{\max}(T)$

$$u_{\max}(T) = u(\lambda_{\max}, T) \tag{1.3.5}$$

$$= u\left(\frac{\alpha}{T}, T\right) \tag{1.3.6}$$

$$= \frac{8\pi hcT^5}{\alpha^5}\frac{1}{e^{\frac{hc}{\alpha k_B}}-1} \tag{1.3.7}$$

1.4. The earth rotates in a circular orbit about the sun. The radius of the orbit is 140×10^6 km. The radius of the earth is 6000 km, and the radius of the sun is 700,000 km. The surface temperature of the sun is 6000 K. Assuming that the sun and the earth are perfect black bodies, calculate the equilibrium temperature of the earth.

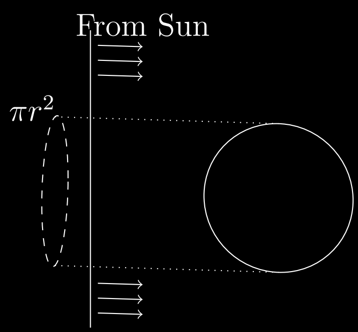
Solution: At equilibrium, energy absorbed by Earth (due to sun's blackbody emission) should equal the energy emitted by Earth (due to its own blackbody emission)

Now,

$$E_{\text{absorbed}} = E_{\text{emitted\_by\_sun}} \frac{\pi r^2}{4\pi R^2} \tag{1.4.1}$$

Where r = radius of Earth, R = radius of Earth's orbit
Now why do we divide by $4\pi R^2$? Because not all of Sun's emission falls on Earth, so we want to find the intensity of Sun's emission falling on Earth, or Energy per unit area. The total energy is spread out over a sphere surface of area $4\pi R^2$, so we divide by it to get intensity.

Why do we multiply by πr^2? We need to multiply the intensity by the area seen by the sun. Note that this is πr^2 (the area the disk of Earth that the Sun sees), not $2\pi r^2$ (the curved area of earth that receives the sunlight). This is made clear from the following diagram (notice that the sphere surface over which the energy is spread out is almost a plane at the Earth's scale)



Now, $E_{\text{emitted\_by\_sun}} = \sigma 4\pi r_{\text{sun}}^2 T_{\text{sun}}^4$
$\implies E_{\text{absorbed}} = \sigma\pi r_{\text{sun}}^2 T_{\text{sun}}^4 \frac{r^2}{R^2}$
Now, $E_{\text{emitted}} = \sigma 4\pi r^2 T^4$
But $E_{\text{absorbed}} = E_{\text{emitted}}$, so $\sigma 4\pi r^2 T^4 = \sigma\pi r_{\text{sun}}^2 T_{\text{sun}}^4 \frac{r^2}{R^2}$
$\implies T^4 = T_{\text{sun}}^4 \frac{r_{\text{sun}}^2}{4R^2}$
Putting in values for T_{sun}, r_{sun}, R
$T^4 = 6000^4 \frac{7^2\times 10^{10}}{4\times 140^2\times 10^{12}}$
$\implies T = 300K = 27\ °\text{C}$, which does check out with the actual surface temperature

1.5. (a) Given Planck's formula for the energy density, obtain an expression for the Rayleigh-Jean's formula for $U(\nu, T)$

Solution: Planck's formula for energy density tells us that

$$U_{\text{Planck}}(\nu, T) = \frac{8\pi h\nu^3}{c^3} \frac{1}{e^{\frac{h\nu}{k_B T}} - 1} \tag{1.5.1}$$

We know that $\lim_{\nu\to 0} U_{\text{Planck}}(\nu, T) = U_{\text{Rayleigh-Jean}}(\nu, T)$

$$\begin{aligned} U_{\text{Rayleigh-Jean}}(\nu, T) &= \lim_{\nu\to 0} U_{\text{Planck}}(\nu, T) && (1.5.2) \\ &= \frac{8\pi k_B T \nu^2}{c^3} \lim_{\nu\to 0}\left(\frac{\frac{h\nu}{k_B T}}{e^{\frac{h\nu}{k_B T}} - 1}\right) && (1.5.3) \\ &= \frac{8\pi k_B T \nu^2}{c^3} \lim_{x\to 0}\left(\frac{x}{e^x - 1}\right) && (1.5.4) \\ &= \frac{8\pi\nu^2}{c^3} k_B T && (1.5.5) \end{aligned}$$

(b) For a black body at temperature T, $U(\nu, T)$ was measured at $\nu = \nu_0$. This value is found to be one tenth of the value estimated using Rayleigh Jeans formula. Obtain an implicit equation in terms of $\frac{h\nu_0}{k_B T}$

Solution:

$$\begin{aligned} U_{\text{Rayleigh-Jean}}(\nu_0, T) &= 10 U_{\text{Planck}}(\nu_0, T) && (1.5.6) \\ \implies \frac{8\pi\nu_0^2}{c^3} k_B T &= 10 \frac{8\pi h\nu_0^3}{c^3} \frac{1}{e^{\frac{h\nu_0}{k_B T}} - 1} && (1.5.7) \\ \implies 10\frac{h\nu_0}{k_B T} &= e^{\frac{h\nu_0}{k_B T}} - 1 && (1.5.8) \\ \implies 10x &= e^x - 1 && (1.5.9) \end{aligned}$$

where $x = \frac{h\nu_0}{k_B T}$

(c) Solve the above equation to obtain the value of $\frac{h\nu}{k_B T}$, up to the first decimal place.

Solution: You can use Desmos or Wolfram Alpha to solve this numerically to get $x = 3.615$
$\implies \frac{\nu_o}{T} = \frac{k_B \times 3.615}{h} = 7.53 \times 10^{10}\ \text{s}^{-1}\text{K}^{-1}$

1.6. Using appropriate approximations, derive Wiens' displacement law from Planck's formula for energy density of black body radiation

Solution: Already solved in Q1.3(a)

1.7. Derive the Stefan-Boltzmann law from the expression from $I(\lambda)$ given in Q1.2

Solution:

$$I(\lambda,T)\,d\lambda = \frac{2\pi hc^2}{\lambda^5}\frac{1}{e^{\frac{hc}{\lambda kT}}-1}\,d\lambda \tag{1.7.1}$$

To obtain the total intensity of emission at a given temperature, we simply integrate this function out in terms of λ

$$I_{\text{total}}(T) = \int_{\lambda=0}^{\infty}\frac{2\pi hc^2}{\lambda^5}\frac{1}{e^{\frac{hc}{\lambda kT}}-1}\,d\lambda \tag{1.7.2}$$

$$= 2\pi hc^2\int_{\lambda=0}^{\infty}\frac{1}{\lambda^5 e^{\frac{hc}{\lambda kT}}-1}\,d\lambda \tag{1.7.3}$$

First subsitute $\lambda = \frac{c}{\nu}$

$$= \frac{2\pi h}{c^2}\int_{\nu=0}^{\infty}\frac{\nu^3}{e^{\frac{h\nu}{kT}}-1}\,d\nu \tag{1.7.4}$$

Now subsitute $x = \frac{h\nu}{kT}$

$$= \frac{2\pi k^4T^4}{h^3c^2}\int_{x=0}^{\infty}\frac{x^3}{e^x-1}\,dx \tag{1.7.5}$$

$$\int_{x=0}^{\infty}\frac{x^3}{e^x-1}\,dx \text{ is a well known result } = \frac{\pi^4}{15} \tag{1.7.6}$$

$$= \frac{2\pi k^4T^4}{h^3c^2}\frac{\pi^4}{15} \tag{1.7.7}$$

$$= \frac{2\pi^5k^4}{15h^3c^2}T^4 \tag{1.7.8}$$

$$= \sigma T^4 \tag{1.7.9}$$

$$\text{Where } \sigma = \tfrac{2\pi^5k^4}{15h^3c^2} = 5.65\times10^{-8}\ \tfrac{\mathrm{W}}{\mathrm{m^2K^4}} \tag{1.7.10}$$

Now $I(T)_{\text{total}} = \frac{P(T)}{A}$, where $P(T)$ = Power emitted by blackbody at temperature T, and A = Emission surface area of blackbody
$\implies P = \sigma AT^4$

2 Compton Scattering

2.1. A photon of energy $h\nu$ is scattered through 90° by an electron initially at rest. The scattered photon has a wavelength twice that of the incident photon. Find the frequency of the incident photon and the recoil angle of the electron.

Solution: First let us find the frequency of the incident photon

$$\lambda' - \lambda = \lambda_c(1 - \cos\theta) \tag{2.1.1}$$

Where $\lambda_c = \frac{h}{m_e c}$, or the compton wavelength of an electron

$$\implies \lambda' - \lambda = \lambda_c \left(1 - \cos\left(\frac{\pi}{2}\right)\right) \tag{2.1.2}$$

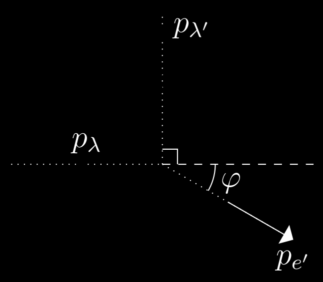
$$\implies 2\lambda - \lambda = \lambda_c \tag{2.1.3}$$

$$\implies \lambda = \lambda_c \tag{2.1.4}$$

$$\implies \frac{c}{\nu} = \frac{h}{m_e c} \tag{2.1.5}$$

$$\implies \nu = \frac{m_e c^2}{h} = 1.24 \times 10^{20} \text{ Hz} \tag{2.1.6}$$

Now to find the recoil angle φ of the electron



Through momentum conservation we have $\vec{p_{e'}} = \vec{p_\lambda} - \vec{p'_\lambda}$
Where $\vec{p_{e'}}$ is the electron momentum after scattering, $\vec{p_{\lambda'}}$ and $\vec{p_\lambda}$ are the photon momenta after and before scattering
Conserving components $||$ to incoming photon

$$p_\lambda = p_{e'} \cos\varphi \tag{2.1.7}$$

Conserving components $\perp$ to incoming photon

$$p'_\lambda = p_{e'} \sin\varphi \tag{2.1.8}$$

Divide (2.7.12) by (2.7.11) to get

$$\tan\varphi = \frac{p_{\lambda'}}{p_\lambda} \tag{2.1.9}$$

$$= \frac{\lambda}{\lambda'} = \frac{1}{2} \tag{2.1.10}$$

$$\implies \varphi = \tan^{-1}\left(\frac{1}{2}\right) = 26.56° \tag{2.1.11}$$

2.2. Find the energy of the incident x-ray if the maximum kinetic energy of the Compton electron is $\frac{m_e c^2}{2.5}$

Solution: By Energy conservation

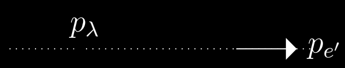
$$
\begin{aligned}
E_{e'} - E_e &= E_\lambda - E_{\lambda'} && (2.2.1)\\
\implies E_{e'} &= hc\left(\frac{1}{\lambda} - \frac{1}{\lambda'}\right) + m_e c^2 && (2.2.2)\\
&= hc\left(\frac{\lambda' - \lambda}{\lambda\lambda'}\right) + m_e c^2 && (2.2.3)\\
&= m_e c^2 \frac{\lambda_c^2}{\lambda^2}\left(\frac{1 - \cos\theta}{1 + \frac{\lambda_c}{\lambda}(1 - \cos\theta)}\right) + m_e c^2 && (2.2.4)\\
&= m_e c^2 \frac{\lambda_c^2}{\lambda^2}\left(\frac{1}{\frac{1}{1-\cos\theta} + \frac{\lambda_c}{\lambda}}\right) + m_e c^2 && (2.2.5)
\end{aligned}
$$

As we can easily see, for a given λ for the incident ray, the energy of the Compton electron is maximum at $\cos\theta = -1$, or $\theta = \pi$

$$
\begin{aligned}
\frac{m_e c^2}{2.5} = KE_{e'_{\max}} = E_{e'_{\max}} - m_e c^2 &= m_e c^2 \frac{\lambda_c^2}{\lambda(\frac{\lambda}{2} + \lambda_c)} && (2.2.6)\\
\implies \lambda^2 + 2\lambda_c\lambda - 5\lambda_c^2 &= 0 && (2.2.7)\\
\implies \lambda &= \frac{-2\lambda_c + \sqrt{24\lambda_c^2}}{2} && (2.2.8)\\
&= (\sqrt{6} - 1)\lambda_c && (2.2.9)\\
\implies E_\lambda = \frac{hc}{\lambda} &= \frac{1}{\sqrt{6} - 1} m_e c^2 = 0.69\ m_e c^2 && (2.2.10)
\end{aligned}
$$

2.3. Show that a free electron cannot absorb a photon so that a photoelectron requires bound electron. However, the electron can be free in Compton Effect. Why?

Solution: Let us draw the scattering diagram for a free electron absorbing a photon



Apply Energy conservation

$$
\begin{aligned}
E_\lambda + E_e &= E_{e'} && (2.3.1)\\
p_\lambda c + m_e c^2 &= \sqrt{p_{e'}^2 c^2 + m_e^2 c^4} && (2.3.2)\\
\implies p_\lambda^2 + m_e^2 c^2 + 2 m_e c p_\lambda &= p_{e'}^2 + m_e^2 c^2 && (2.3.3)
\end{aligned}
$$

But according to momentum conservation $p_\lambda = p_{e'}$

$$
\begin{aligned}
\implies 2 m_e c p_\lambda &= 0 && (2.3.4)\\
\implies p_\lambda &= 0 && (2.3.5)\\
\implies \nu &= 0 && (2.3.6)
\end{aligned}
$$

Which is not really possible. $\therefore$ a free electron cannot absorb a photon.
OTOH, drawing the scattering diagram and applying momentum and energy conservation for Compton scattering yields a valid solution $\Delta\lambda = \lambda_c(1 - \cos\theta)$, $\therefore$ Compton scattering can and does in fact involve a free electron

2.4. Two Compton scattering experiments were performed using x-rays (incident energies E_1 and $E_2 = \frac{E_1}{2}$). In the first experiment, the increase in wavelength of the scattered x-ray, when measured at an angle $\theta = 45°$ is 7×10^{-14} m. In the second experiment, the wavelength of the scattered x-ray, when measured at an angle $\theta = 60°$ is 9.9×10^{-12} m.

(a) Calculate the Compton wavelength and the mass (m) of the scatterer

Solution:

$$\Delta\lambda_1 = \lambda_c(1 - \cos\theta_1) \tag{2.4.1}$$
$$\implies \lambda_c = \frac{\Delta\lambda_1}{1 - \cos\theta_1} \tag{2.4.2}$$
$$= \frac{7 \times 10^{-14}}{1 - \cos\left(\frac{\pi}{4}\right)} \tag{2.4.3}$$
$$= \frac{7\sqrt{2}}{\sqrt{2} - 1} \times 10^{-14} \text{ m} \tag{2.4.4}$$
$$= 2.39 \times 10^{-13} \text{ m} \tag{2.4.5}$$
$$\text{But } \frac{h}{mc} = \lambda_c \tag{2.4.6}$$
$$\implies m = \frac{h}{\lambda_c c} = 9.24 \times 10^{-30} \text{ kg} \tag{2.4.7}$$

(b) Find the wavelengths of the incident x-rays in the two experiments.

Solution:

$$\lambda_2' - \lambda_2 = \lambda_c(1 - \cos\theta_2) \tag{2.4.8}$$
$$\implies \lambda_2 = \lambda_2' - \lambda_c(1 - \cos\theta_2) \tag{2.4.9}$$
$$= 9.9 \times 10^{-12} - 2.39 \times 10^{-13}\left(1 - \cos\left(\frac{\pi}{3}\right)\right) \tag{2.4.10}$$
$$= 9.9 \times 10^{-12} - 0.119 \times 10^{-12} \tag{2.4.11}$$
$$= 9.781 \times 10^{-12} \text{ m} \tag{2.4.12}$$
$$\text{Now, } E_1 = 2E_2 \tag{2.4.13}$$
$$\implies \lambda_1 = \frac{\lambda_2}{2} = 4.89 \times 10^{-12} \text{ m} \tag{2.4.14}$$

2.5. Find the smallest energy that a photon can have and still transfer 50% of its energy to an electron initially at rest.

Solution:

By Energy conservation,

$$E_{e'} - E_e = E_\lambda - E_{\lambda'} \tag{2.5.1}$$
$$\implies 0.5E_\lambda = E_\lambda - E_{\lambda'} \tag{2.5.2}$$
$$\implies E_{\lambda'} = 0.5E_\lambda \tag{2.5.3}$$
$$\implies \lambda' = 2\lambda \tag{2.5.4}$$
$$\text{Now, } \lambda' - \lambda = \lambda_c(1-\cos\theta) \tag{2.5.5}$$
$$\implies \lambda = \lambda_c(1-\cos\theta) \tag{2.5.6}$$
$$\implies E_\lambda = \frac{hc}{\lambda} = \frac{hc}{\lambda_c(1-\cos\theta)} \tag{2.5.7}$$
$$= \frac{m_e c^2}{1-\cos\theta} \tag{2.5.8}$$

As we can see, E_λ is smallest for $\cos\theta = -1$, or $\theta = \pi$

$$\implies E_{\lambda_{\min}} = \frac{m_e c^2}{2} = \frac{0.511 \text{ MeV}}{2} = 0.256 \text{ MeV} \tag{2.5.9}$$

2.6. In Compton Scattering, Show that if the angle of scattering θ increases beyond a certain value θ_0, the scattered photon will never have energy larger than $2m_0c^2$, irrespective of the energy of the incident photon. Find the value of θ_0

Solution:

$$\lambda' - \lambda = \lambda_c(1-\cos\theta) \tag{2.6.1}$$
$$\lambda' = \lambda + \lambda_c(1-\cos\theta) \tag{2.6.2}$$
$$\implies E_{\lambda'} = \frac{hc}{\lambda + \lambda_c(1-\cos\theta)} \tag{2.6.3}$$
$$= \frac{m_0c^2}{\frac{\lambda m_0 c}{h} + 1 - \cos\theta} \tag{2.6.4}$$
$$= \frac{m_0c^2}{\frac{m_o c^2}{E_\lambda} + 1 - \cos\theta} \tag{2.6.5}$$

We want $E_{\lambda'} < 2m_0c^2 \ \forall \lambda > 0, \ \theta > \theta_0$

We know that

$$E_{\lambda'}\big|_{\theta>\theta_0} = \frac{m_0c^2}{\frac{m_oc^2}{E_\lambda} + 1 - \cos\theta} \tag{2.6.6}$$

$$< \frac{m_0c^2}{\frac{m_oc^2}{E_\lambda} + 1 - \cos\theta_0} \tag{2.6.7}$$

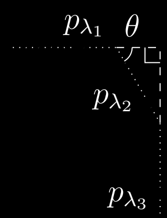
$$< \frac{m_0c^2}{1 - \cos\theta_0} \tag{2.6.8}$$

Thus $\frac{m_0c^2}{1-\cos\theta_0} = 2m_0c^2$

$$\implies \cos\theta_0 = 0.5 \tag{2.6.9}$$

$$\implies \theta_0 = 60^\circ \tag{2.6.10}$$

2.7. In a Compton scattering experiment (see figure), X-rays scattered off a free electron initially at rest at an angle $\theta > \frac{\pi}{4}$, gets re-scattered by another free electron, also initially at rest.



(a) If $\lambda_3 - \lambda_1 = 1.538 \times 10^{-12}$ m, find the value of θ

Solution:

$$\lambda_2 - \lambda_1 = \lambda_c(1 - \cos\theta) \tag{2.7.1}$$

$$\lambda_3 - \lambda_2 = \lambda_c\left(1 - \cos\left(\frac{\pi}{2} - \theta\right)\right) = \lambda_c(1 - \sin\theta) \tag{2.7.2}$$

Adding (2.7.1) and (2.7.2),

$$\implies \lambda_3 - \lambda_1 = \lambda_c(2 - \sin\theta - \cos\theta) \tag{2.7.3}$$

$$\implies \sin\theta + \cos\theta = 2 - \frac{\Delta\lambda}{\lambda_c} \tag{2.7.4}$$

$$\implies 1 + \sin(2\theta) = \left(2 - \frac{\Delta\lambda}{\lambda_c}\right)^2 \tag{2.7.5}$$

$$\implies \sin(2\theta) = \left(2 - \frac{\Delta\lambda}{\lambda_c}\right)^2 - 1 \tag{2.7.6}$$

$$= 0.867 \tag{2.7.7}$$

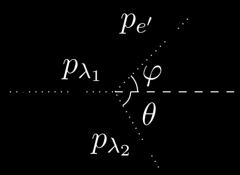
$$\implies \sin^{-1}(\sin(2\theta)) = \sin^{-1}(0.867) \approx \frac{\pi}{3} \tag{2.7.8}$$

$$\tag{2.7.9}$$

The solutions to this are $2\theta = \cdots \frac{-5\pi}{3}, \frac{\pi}{3}, \frac{7\pi}{3} \cdots$ and $2\theta = \cdots \frac{-4\pi}{3}, \frac{2\pi}{3}, \frac{8\pi}{3} \cdots$
But we only care about $\frac{\pi}{4} < \theta < \frac{\pi}{2}, \implies \frac{\pi}{2} < 2\theta < \pi$
$\implies 2\theta = \frac{2\pi}{3}, \implies \theta = \frac{\pi}{3} = 60°$

(b) If $\lambda_2 = 68 \times 10^{-12}$ m, find the angle at which the first electron recoils due to the collision.

Solution:



We know,

$$\lambda_2 - \lambda_1 = \lambda_c(1 - \cos\theta) \tag{2.7.10}$$

We can use momentum conservation || and $\perp$ to $\vec{p_{\lambda_1}}$

$$p_{e'} \cos\varphi = p_{\lambda_1} - p_{\lambda_2} \cos\theta \tag{2.7.11}$$
$$p_{e'} \sin\varphi = p_{\lambda_2} \sin\theta \tag{2.7.12}$$

Dividing (2.7.12) by (2.7.11)

$$\tan\varphi = \frac{p_{\lambda_2} \sin\theta}{p_{\lambda_1} - p_{\lambda_2} \cos\theta} \tag{2.7.13}$$
$$= \frac{1}{p_{\lambda_1}} \frac{\sin\theta}{\frac{1}{p_{\lambda_2}} - \frac{1}{p_{\lambda_1}} \cos\theta} \tag{2.7.14}$$
$$= \frac{\lambda_1 \sin\theta}{\lambda_2 - \lambda_1 \cos\theta} \tag{2.7.15}$$
$$= \frac{\lambda_1 \sin\theta}{\lambda_2 - \lambda_1 + \lambda_1(1 - \cos\theta)} \tag{2.7.16}$$
$$= \frac{\sin\theta}{1 - \cos\theta} \frac{\lambda_1}{\lambda_c + \lambda_1} \tag{2.7.17}$$
$$= \frac{2\sin\left(\frac{\theta}{2}\right)\cos\left(\frac{\theta}{2}\right)}{2\sin^2\left(\frac{\theta}{2}\right)} \frac{\lambda_1}{\lambda_c + \lambda_1} \tag{2.7.18}$$
$$= \cot\left(\frac{\theta}{2}\right) \frac{1}{\frac{\lambda_c}{\lambda_1} + 1} \tag{2.7.19}$$

Thus we need λ_1 to find ϕ
Using (2.7.10)

$$\lambda_1 = \lambda_2 - \lambda_c(1 - \cos\theta) \tag{2.7.20}$$
$$\implies \frac{\lambda_c}{\lambda_1} = \frac{1}{\frac{\lambda_2}{\lambda_c} - (1 - \cos\theta)} = \frac{1}{\frac{68\times10^{-12}}{\lambda_c} - \left(1 - \cos\left(\frac{\pi}{3}\right)\right)} = 0.0364 \tag{2.7.21}$$

Putting in (2.7.19)

$$\tan\varphi = \frac{\cot\left(\frac{\pi}{6}\right)}{1.0364} = 1.67 \tag{2.7.22}$$
$$\implies \varphi = \tan^{-1} 1.67 = 59.1° \tag{2.7.23}$$

3 Specific Heat

3.1. Show that the Einstein's specific heat expression gives $C_v = 3R$ as $T \to \infty$ and $C_v = 0$ as $T \to 0$

Solution:

$$U = (3N)\left(\frac{h\nu}{e^{\frac{h\nu}{k_BT}} - 1}\right) \tag{3.1.1}$$

$$\implies C_v = \frac{\partial U}{\partial T} = \frac{3Nh\nu}{k_BT^2}\frac{h\nu e^{\frac{h\nu}{k_BT}}}{\left(e^{\frac{h\nu}{k_BT}} - 1\right)^2} \tag{3.1.2}$$

$$= 3Nk_B\left(\frac{h\nu}{k_BT}\right)^2\frac{e^{\frac{h\nu}{k_BT}}}{\left(e^{\frac{h\nu}{k_BT}} - 1\right)^2} \tag{3.1.3}$$

$$= 3R\left(\frac{h\nu}{k_BT}\right)^2\frac{e^{\frac{h\nu}{k_BT}}}{\left(e^{\frac{h\nu}{k_BT}} - 1\right)^2} \tag{3.1.4}$$

Now, we take limits

$$\lim_{T\to\infty} C_v = 3R\lim_{T\to\infty}\left(\frac{h\nu}{k_BT}\right)^2\frac{e^{\frac{h\nu}{k_BT}}}{\left(e^{\frac{h\nu}{k_BT}} - 1\right)^2} \tag{3.1.5}$$

$$= 3R\lim_{x\to 0}\frac{x^2}{(e^x - 1)^2}\lim_{x\to 0} e^x \tag{3.1.6}$$

$$= 3R \tag{3.1.7}$$

Similarly,

$$\lim_{T\to 0} C_v = 3R\lim_{T\to 0}\left(\frac{h\nu}{k_BT}\right)^2\frac{e^{\frac{h\nu}{k_BT}}}{\left(e^{\frac{h\nu}{k_BT}} - 1\right)^2} \tag{3.1.8}$$

$$= 3R\lim_{x\to\infty}\frac{x^2e^{-x}}{(1 - e^{-x})^2} \tag{3.1.9}$$

$$= 0 \tag{3.1.10}$$

3.2. (a) A diatomic molecule consists of two equal point masses (m) separated by a distance D (called the bond length). Consider a gas of such diatomic molecules. The molecular specific heat at constant volume C_v of this gas changes from $1.5R$ to $2.5R$ at a temperature T_1. The quantum of rotational energy of the molecule is given by $\frac{\hbar^2}{2I}$, where I is the moment of inertia of the molecule. Obtain an expression for D in terms of m and T_1

Solution: First of all, C_v will have three contributions, one from translational, one from rotational, and one from vibrational
In the translational dof, most of the molecules are in non ground state, hence contribute to $\frac{3}{2}R$ to C_v, as predicted classically
For the rotational dof, let E be the spacing between the ground and the first excited state. As we know that there is a $e^{\frac{E}{k_BT}}$ term in the relative number of molecules in the ground and the first excited state, hence we know that if $T \ll \frac{E}{k_B}$, then most of the molecules are in ground state having no energy at all, and thus do not contribute significantly to C_v. As we increase temperature to $T \gg \frac{E}{k_B}$ more and more molecules start to jump to first and higher excited states, and contribute $2 \times \frac{R}{2}$ to C_v.
Hence the C_v increases from $1.5R$ to $2.5R$ at $T_1 \approx \frac{E}{k_B} = \frac{\hbar^2}{2Ik_B} = \frac{\hbar^2}{mD^2k_B}$

(b) C_v of the above diatomic gas changes from $2.5R$ to $3.5R$ at temperature T_2. The quantum of vibration energy is given by $\hbar\omega$, where ω is the angular frequency of vibrations. Obtain an expression for the bond strength (or the spring constant of the bond) in terms of m and T_2

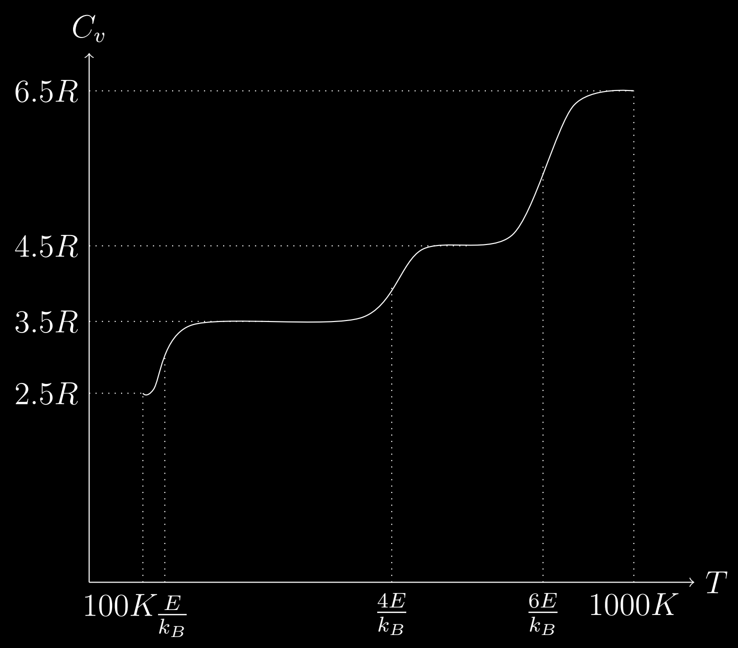
Solution: Using similar logic as above, $T_2 \approx \frac{\hbar\omega}{k_B} = \frac{\hbar}{k_B}\sqrt{\frac{k}{m}}$
$\implies k = \frac{mk_BT_2^2}{\hbar^2}$

3.3. Graphite structure consists of carbon layers arranged in the xy-plane. Each atom in the structure can, in principle, perform simple harmonic motion in 3 mutually perpendicular directions. The restoring forces in the xy-plane and hence the natural frequency of oscillations in the x and y directions are large such that $\hbar\omega_x \gg 300k_B$, $\hbar\omega_y \gg 300k_B$, the thermal energy at room temperature. On the other hand, the restoring force perpendicular to a layer is quite small and hence $\hbar\omega_z \ll 300k_B$. On the basis of this information, find C_v of graphite at 300 K. You may assume that the equipartition theorem is valid in this case.

Solution: As we can imagine, most of the atoms are in the excited state of the vibration perpendicular to plane, because $k_BT \gg \hbar\omega_z$. So that dof contributes R to C_v. On the other hand, most of the atoms are in ground states of vibration in plane, so they do not contribute to C_v
Hence $C_v = R$

3.4. CO_2 is a linear tri-atomic molecule with the carbon atom in the middle connected to an oxygen atom on either side (O−C−O). This molecule has two rotational and four vibrational degrees of freedom. Assume that the excitation energy of the rotational degrees of freedom is very small. The quantum of energy required to excite the lowest vibrational mode is E, and and that for the next mode is $4E$. The next two modes have equal excitation energy of $6E$. Given that $E = 12 \times 10^{-3}$ eV, sketch the molar specific heat of CO_2 (in units of R) from $T = 100K$ to $T = 1000K$

Solution:



4 Phase and Group Velocity

4.1. Two harmonic waves which travel simultaneously along a wire are represented by

$$y_1 = 0.002\cos(8.0x - 400t) \quad \text{and} \quad y_2 = 0.002\cos(7.6x - 380t)$$

where x, y are in meters and t is in sec.

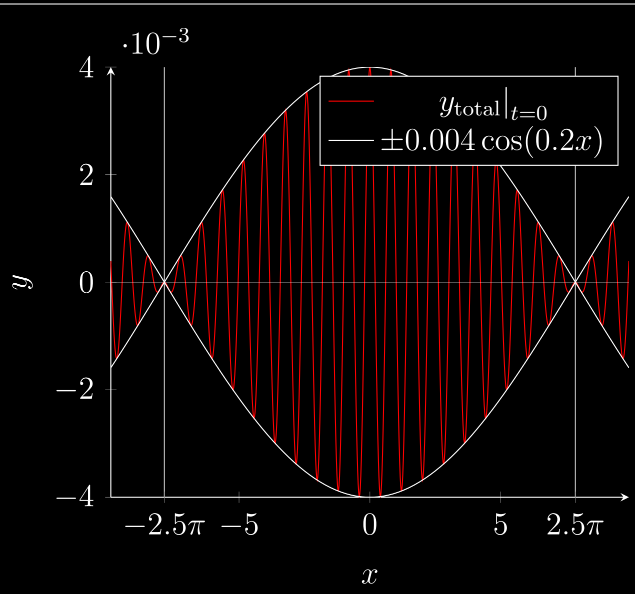
(a) Find the resultant wave and its phase and group velocities

Solution:

$$y_{\text{total}} = y_1 + y_2 \tag{4.1.1}$$

$$= 0.002\,(\cos(8x - 400t) + \cos(7.6x - 380t)) \tag{4.1.2}$$

$$= 0.004\,(\cos(7.8x - 390t)\cos(0.2x - 10t)) \qquad \text{(Using trig identity)} \tag{4.1.3}$$



Thus we see that the envelope is a sinusoid of frequency $\omega = \frac{\Delta\omega}{2} = 10$ Hz and wavenumber $k = \frac{\Delta k}{2} = 0.2\ \text{m}^{-1}$. Thus $v_g = \frac{\Delta\omega}{\Delta k} = 50\ \text{ms}^{-1}$
The wave itself is a sinusoid of frequency $\omega = \omega_{\text{avg}} = 390$ Hz and wavenumber $k = k_{\text{avg}} = 7.8\ \text{m}^{-1}$. Thus $v_p = \frac{\omega_{\text{avg}}}{k_{\text{avg}}} = 50\ \text{ms}^{-1}$

(b) Calculate the range Δx between the zeros of the group wave. Find the product of Δx and Δk?

Solution:

$$\Delta x = \frac{1}{2} \times \frac{2 \times 2\pi}{\Delta k} = 5\pi \text{ m} \tag{4.1.4}$$

$$\Delta x\, \Delta k = 2\pi \tag{4.1.5}$$

4.2. The dispersion relation for a lattice wave propagating in a 1-D chain of atoms of mass m bound together by a force constant β is given by $\omega = \omega_0 \sin\left(\frac{ka}{2}\right)$, where $\omega_0 = \sqrt{\frac{4\beta}{m}}$ and a is the distance between the atoms.

(a) Show that the medium is non- dispersive in the long wavelength limits.

Solution: We have

$$v_g = v_p + k\frac{dv_p}{dk} \tag{4.2.1}$$

For non dispersive medium, we need

$$v_p = v_g \tag{4.2.2}$$

$$\implies v_p = v_p + k\frac{dv_p}{dk} \qquad \text{(From (4.2.1))} \tag{4.2.3}$$

$$\implies k\frac{dv_p}{dk} = 0 \tag{4.2.4}$$

But,

$$v_p = \frac{\omega(k)}{k} = \omega_0 \frac{\sin\left(\frac{ka}{2}\right)}{k} \tag{4.2.5}$$

$$\implies k\frac{dv_p}{dk} = \frac{a\omega_0}{2}\cos\left(\frac{ka}{2}\right) - \frac{a\omega_0}{2}\frac{\sin\left(\frac{ka}{2}\right)}{\frac{ka}{2}} \tag{4.2.6}$$

$$\implies \lim_{k\to 0} k\frac{dv_p}{dk} = \frac{a\omega_0}{2} - \frac{a\omega_0}{2} = 0 \tag{4.2.7}$$

Hence medium is non dispersive in the long wavelength limit

(b) Find the group and phase velocities at $k = \frac{\pi}{a}$.

Solution:

$$v_p = \omega_0 \frac{\sin\left(\frac{\pi}{2}\right)}{\frac{\pi}{a}} = \boxed{\frac{a\omega_0}{\pi}} \tag{4.2.8}$$

$$k\frac{dv_p}{dk}\bigg|_{k=\frac{\pi}{a}} = \frac{a\omega_0}{2}\left(\cos\left(\frac{\pi}{2}\right) - \frac{2}{\pi}\sin\left(\frac{\pi}{2}\right)\right) \tag{4.2.9}$$

$$= -\frac{a\omega_0}{\pi} \tag{4.2.10}$$

$$\boxed{\implies v_g = 0} \qquad \text{(From (4.2.1))} \tag{4.2.11}$$

4.3. Find the group and the phase velocities of the matter wave associated with a free particle under the assumption that the frequency is defined using

(i) the kinetic energy

Solution:

$$v_p = \frac{\omega}{k} = \frac{E}{p} = \boxed{\frac{p}{2m}} \tag{4.3.1}$$

$$v_g = \frac{d\omega}{dk} = \frac{dE}{dp} = \boxed{\frac{p}{m}} \tag{4.3.2}$$

(ii) total relativistic energy

Solution:

$$v_p = \frac{\omega}{k} = \frac{E}{p} \tag{4.3.3}$$
$$= \boxed{\frac{\sqrt{p^2c^2 + m_0^2c^4}}{p}} \tag{4.3.4}$$
$$v_g = \frac{d\omega}{dk} = \frac{dE}{dp} \tag{4.3.5}$$
$$= \frac{d}{dp}\sqrt{p^2c^2 + m_0^2c^4} \tag{4.3.6}$$
$$= \boxed{\frac{pc^2}{E} = \frac{c^2}{v_p}} \tag{4.3.7}$$

4.4. The phase speed v_p of light in a certain wavelength range in a dispersive medium is given by the following expression:

$$v_p = c\left(A + \frac{4\pi^2 B}{\lambda^2}\right)^{-1}$$

where λ is the wavelength, c is the speed of light and A,B are constants.

(a) Find an expression for the group speed in terms of the wave vector $\vec{k}$

Solution:

$$v_p = \frac{c}{A + k^2B} \tag{4.4.1}$$
$$\implies v_g = \frac{c}{A + k^2B} - \frac{2k^2Bc}{(A + k^2B)^2} \qquad \text{(Using (4.2.1))} \tag{4.4.2}$$
$$= \boxed{\frac{c(A - \vec{k}\cdot\vec{k}B)}{(A + \vec{k}\cdot\vec{k}B)^2}} \tag{4.4.3}$$

(b) Taking $A = 1.7$ and $B = \frac{0.01}{4\pi^2}$ $(\mu\text{m})^2$, calculate the group and phase speed of light for a wavelength of 400 nm. Which of the two speeds is physically important and why?

Solution:

$$v_p = \frac{c}{1.7 + \frac{1}{16}} = 0.567c \tag{4.4.4}$$
$$v_g = c\frac{\left(1.7 - \frac{1}{16}\right)}{\left(1.7 + \frac{1}{16}\right)^2} = 0.527c \tag{4.4.5}$$

The reason for v_g being physically important is deep. The wavepacket will be of the form $\Psi(x,t) = E(x,t) \cdot e^{i(x - v_pt)}$, where E is the envelope function. But the thing which is physical are the probability densities of measurement results, which is given by $\bar{\Psi}\Psi = |E|^2$. Therefore the physical measurements depend only on the behaviour of

the envelope, which is governed by v_g.
Even classically, $|E|^2$ represents the intensity of light, which is physical, and the full E field's phase, $e^{i(x-v_pt)}$ doesn't really represent anything physical

4.5. Consider a square 2-D system with small balls (each of mass m) connected by springs. The spring constants along the x- and y-directions are β_x and β_y, respectively. The dispersion relation for this system is given by

$$-\omega^2 m + 2\beta_x(1-\cos(k_x a_x)) + 2\beta_y(1-\cos(k_y a_y)) = 0$$

where $\vec{k} = k_x\,\hat{i} + k_y\,\hat{j}$ is the wave vector and a_x, a_y are the natural distances between the two successive masses along the x- and y-directions, respectively. Find the group velocity and the angle that it makes with the x-axis

Solution: We know that

$$\omega(\vec{k}) = \sqrt{\frac{2\beta_x(1-\cos(k_x a_x)) + 2\beta_y(1-\cos(k_y a_y))}{m}} \tag{4.5.1}$$

$$\implies \vec{v_g} = \nabla_k \omega = \frac{d\omega}{dk_x}\,\hat{i} + \frac{d\omega}{dk_y}\,\hat{j} \tag{4.5.2}$$

$$= \boxed{\frac{\beta_x a_x}{m\omega}\sin(k_x a_x)\,\hat{i} + \frac{\beta_y a_y}{m\omega}\sin(k_y a_y)\,\hat{j}} \tag{4.5.3}$$

$$\implies \varphi = \boxed{\tan^{-1}\left(\frac{\beta_y a_y \sin(k_y a_y)}{\beta_x a_x \sin(k_x a_x)}\right)} \tag{4.5.4}$$

Where φ is the angle made by v_g with the x axis

4.6. Consider an electromagnetic (EM) wave of the form $Ae^{i(kx=wt)}$. Its speed in free space is given by $c = \frac{\omega}{k} = \sqrt{\frac{1}{\epsilon_0\mu_0}}$, where ϵ_0, μ_0 is the electric permittivity, magnetic permeability of free space, respectively.

(a) Find an expression for the speed (v) of EM waves in a medium, in terms of its permittivity ϵ and permeability μ

Solution: Here we want the speed of EM waves themselves, which is
$v_p = \frac{\omega}{k} = \sqrt{\frac{1}{\epsilon\mu}} = \frac{c}{\sqrt{\epsilon_r\mu_r}}$

(b) Suppose the permittivity of the medium depends on the frequency, given by $\epsilon = \epsilon_0\left(1 - \frac{\omega_p^2}{\omega^2}\right)$ where ω_p is a constant called the plasma frequency, find the dispersion relation for the EM waves in a medium. (assume $\mu = \mu_0$)

Solution:

$$\frac{\omega}{k} = \sqrt{\frac{1}{\epsilon\mu}} \tag{4.6.1}$$

$$= \frac{c}{\sqrt{1 - \frac{\omega_p^2}{\omega^2}}} \tag{4.6.2}$$

$$\implies kc = \omega\sqrt{1 - \frac{\omega_p^2}{\omega^2}} \tag{4.6.3}$$

$$\implies k^2c^2 = \omega^2 + \omega_p^2 \tag{4.6.4}$$

$$\implies \omega(k) = \boxed{\sqrt{k^2c^2 - \omega_p^2}} \tag{4.6.5}$$

(c) Consider waves with $\omega = 3\omega_p$. Find the phase and group velocity of the waves. What is the product of group and phase velocities?

Solution:

$$v_p = \frac{\omega}{k} = \boxed{\frac{3\sqrt{2}}{4}c = 1.06c} \tag{4.6.6}$$

$$v_g = \frac{d\omega}{dk} = \boxed{\frac{c^2k}{\omega} = \frac{c^2}{v_p} = \frac{2\sqrt{2}}{3}c = 0.94c} \tag{4.6.7}$$

5 Wave packet, Fourier Theory, HUP

Wave packet and Fourier Theory

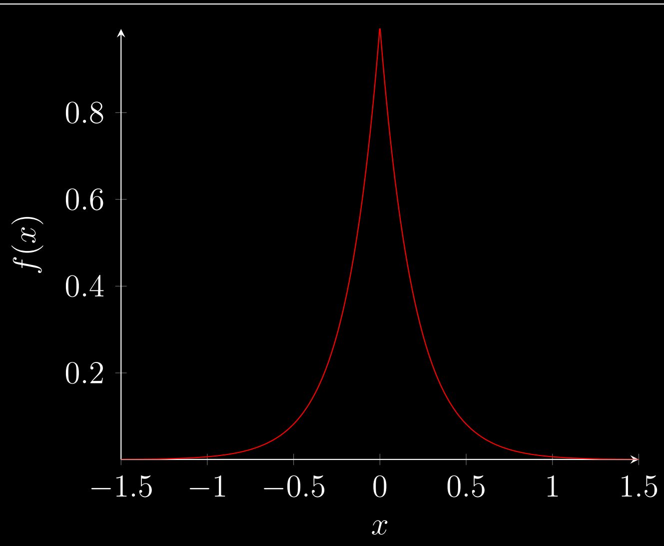
5.1. A wave packet is of the form

$$f(x) = e^{-\alpha|x|}, \qquad -\infty < x < \infty$$

where α is a +ve constant

(a) Plot $f(x)$ versus x

Solution:



(b) Find the values of x at which $f(x)$ attains half of its maximum value

Solution:

$$f_{\text{max}} = f(0) = 1 \tag{5.1.1}$$
$$\implies f(x_{\text{half-width}}) = 0.5 \tag{5.1.2}$$
$$\implies \alpha|x_{\text{half-width}}| = \ln 2 \tag{5.1.3}$$
$$\implies x_{\text{half-width}} = \boxed{\pm\frac{\ln 2}{\alpha}} \tag{5.1.4}$$

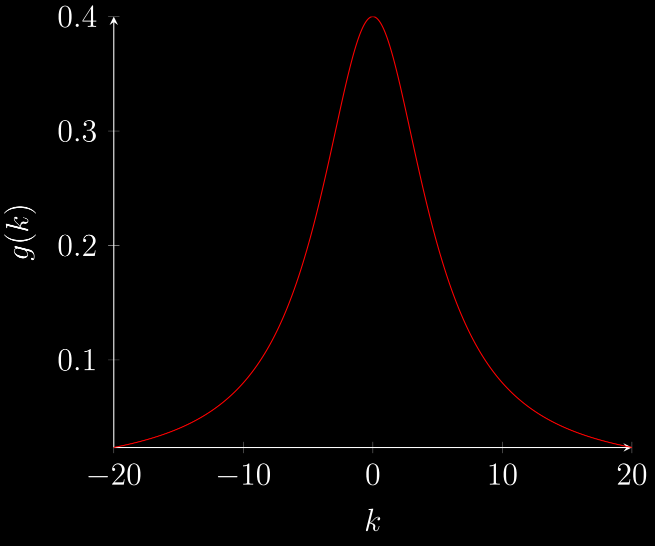
(c) Calculate the Fourier transform of $f(x)$ i.e. $g(k) = \int_{-\infty}^{\infty} f(x)e^{ikx}\,dx$

Solution:

$$g(k) = \int_{x=-\infty}^{\infty} f(x)e^{ikx}\,dx \tag{5.1.5}$$
$$= \int_{x=0}^{\infty} e^{(-\alpha+ik)x}\,dx + \int_{x=-\infty}^{0} e^{(\alpha+ik)x}\,dx \tag{5.1.6}$$
$$= \left(\frac{e^{(-\alpha+ik)x}}{-\alpha+ik} + \frac{e^{(-\alpha-ik)x}}{-\alpha-ik}\right)\Bigg|_{x=0}^{\infty} \tag{5.1.7}$$
$$= \frac{1}{\alpha-ik} + \frac{1}{\alpha+ik} \tag{5.1.8}$$
$$= \boxed{\frac{2\alpha}{\alpha^2+k^2}} \tag{5.1.9}$$

(d) Plot $g(k)$ versus k

Solution:



(e) Find the values of k at which $f(k)$ attains half of its maximum value

Solution:

$$g_{\text{max}} = g(0) = \frac{2}{\alpha} \tag{5.1.10}$$

$$\implies g(k_{\text{half-width}}) = \frac{1}{\alpha} \tag{5.1.11}$$

$$\implies \frac{2\alpha}{\alpha^2 + k^2} = \frac{1}{\alpha} \tag{5.1.12}$$

$$\implies k_{\text{half-width}} = \boxed{\pm\alpha} \tag{5.1.13}$$

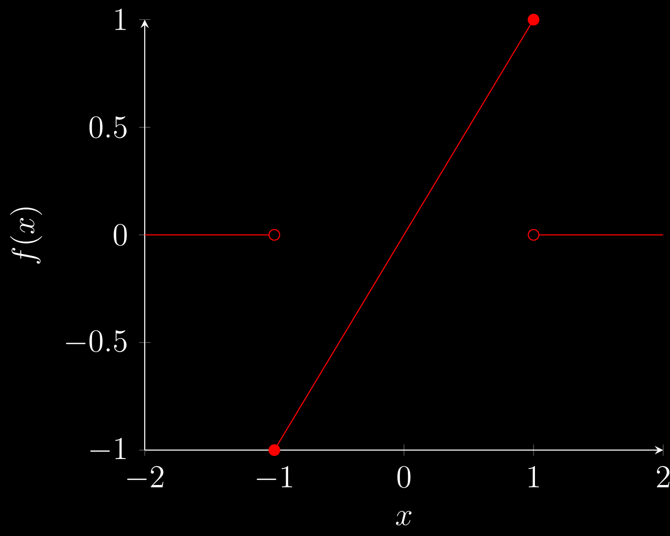
(f) From the values obtained in (b) and (e), find $\Delta x \, \Delta k$

Solution: Taking Δx and Δk as half width at half maxima, we get
$\Delta x \, \Delta k = \frac{\ln 2}{\alpha} \times \alpha = \ln 2$
(We could have taken them as full width at half maxima and got four times this value)

5.2. A wave packet is of the form $f(x) = x$ for $-1 \leq x \leq 1$ and $f(x) = 0$ elsewhere

(a) Plot $f(x)$ vs x

Solution:



(b) Calculate the Fourier transform of $f(x)$

Solution:

$$g(k) = \int_{x=-\infty}^{\infty} f(x)e^{-ikx}\,dx \tag{5.2.1}$$

$$= \int_{x=-1}^{1} xe^{-ikx}\,dx \tag{5.2.2}$$

Integrating by parts

$$= \frac{i}{k}\left(xe^{-ikx}\Big|_{x=-1}^{1} - \int_{x=-1}^{1} e^{-ikx} \right) \tag{5.2.3}$$

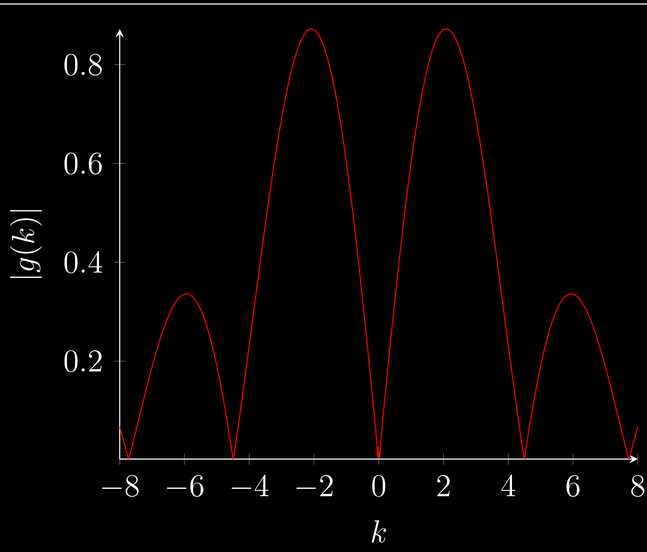
$$= \frac{i}{k}\left(xe^{-ikx} + \frac{1}{ik}e^{-ikx} \right)\Bigg|_{x=-1}^{1} \tag{5.2.4}$$

$$= \frac{2i}{k}\left(\cos k - \frac{\sin k}{k} \right) \tag{5.2.5}$$

$$\tag{5.2.6}$$

(c) Plot $|g(k)|$ versus k

Solution:



(d) At what value of k, $|g(k)|$ attains a minimum value?

Solution:

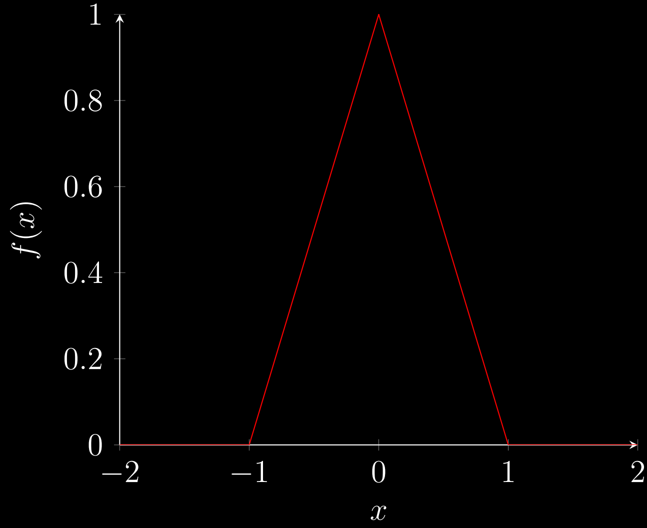
$$|g(k)|_{\text{min}} = 0 \tag{5.2.7}$$
$$\implies \sin(k_{\text{min}}) = k_{\text{min}} \cos(k_{\text{min}}) \tag{5.2.8}$$
$$\implies \tan(k_{\text{min}}) = k_{\text{min}} \tag{5.2.9}$$

Thus, $|g(k)|$ attains a minimum value at the solutions of $\tan k = k$, one of them being $k = 0$

5.3. A triangular pulse is represented by $f(x) = 1 - |x|$ for $-1 \leq x \leq 1$ and $f(x) = 0$ elsewhere

(a) Plot $f(x)$ vs x

Solution:



(b) Calculate the Fourier transform of $f(x)$

Solution:

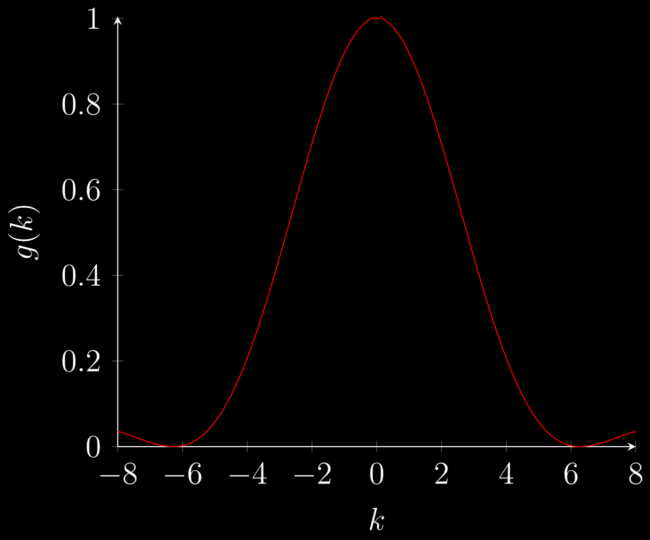
$$g(k) = \int_{x=-\infty}^{\infty} f(x)e^{-ikx}\,dx \tag{5.3.1}$$
$$= \int_{x=0}^{1} (1-x)e^{-ikx}\,dx + \int_{x=-1}^{0} (1+x)e^{-ikx}\,dx \tag{5.3.2}$$
$$= 2\int_{x=0}^{1} (1-x)\cos(kx)\,dx \tag{5.3.3}$$

Integrating by parts

$$= \frac{2}{k}\left((1-x)\sin(kx)\big|_{x=0}^{1} + \int_{x=0}^{1} \sin(kx)\right) \tag{5.3.4}$$
$$= \frac{2}{k}\left((1-x)\sin(kx) - \frac{\cos(kx)}{k}\right)\Bigg|_{x=0}^{1} \tag{5.3.5}$$
$$= \frac{2}{k}\left(\frac{1-\cos k}{k}\right) \tag{5.3.6}$$

(c) Plot $g(k)$ versus k

Solution:



(d) Find the value of k at which $|g(k)|$ attains its maximum value?

Solution: At $g_{\max} = g(0) = 1$

(e) Find the values of k, at which $g(k)$ attains half of this maximum value

Solution:

$$g_{\text{max}} = g(0) = 1 \tag{5.3.7}$$
$$\implies g(k_{\text{half-width}}) = \frac{1}{2} \tag{5.3.8}$$
$$\implies \sqrt{2}\sin\left(\frac{k_{\text{half-width}}}{2}\right) = \pm\frac{k_{\text{half-width}}}{2} \tag{5.3.9}$$

Solving this transcendental equation via a calculator,

$$\implies k_{\text{half-width}} = \pm 2.783 \tag{5.3.10}$$

(f) From the values obtained in (e), find the spread Δk. Calculate the spread Δx using the uncertainty relation $\Delta x\,\Delta k = \frac{1}{2}$

Solution: Taking Δk as half-width at half maxima,

$$\Delta k = 2.783 \tag{5.3.11}$$
$$\implies \Delta x = \frac{1}{2 \times 2.783} = 0.18 \tag{5.3.12}$$

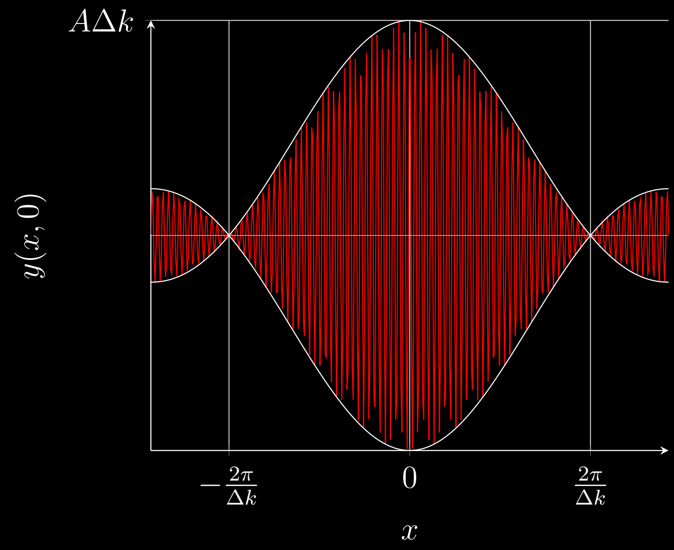
5.4. A wave packet is constructed by superposing waves, their wavelengths varying continuously as

$$y(x,t) = \int A(k)\cos(kx - \omega t)\,dk$$

where $A(k) = A$ for $\left(k_0 - \frac{\Delta k}{2}\right) \leq k \leq \left(k_0 + \frac{\Delta k}{2}\right)$ and $A(k) = 0$ otherwise. Sketch $y(x,t)$ (approximately) and estimate Δx by taking the difference between two values of x for which the central maximum and the nearest minimum is observed in the envelope. Verify uncertainty principle from this.

Solution:

$$y(x,t) = A\int_{k=k_0-\frac{\Delta k}{2}}^{k_0+\frac{\Delta k}{2}} \cos(kx - \omega t)\,dk \tag{5.4.1}$$
$$= A\left.\frac{\sin(kx - \omega t)}{x}\right|_{k=k_0-\frac{\Delta k}{2}}^{k_0+\frac{\Delta k}{2}} \tag{5.4.2}$$
$$= \frac{2A\sin\left(\frac{\Delta k}{2}x\right)}{x}\cos(k_0 x - \omega t) \tag{5.4.3}$$



We can see $\Delta x = \frac{2\pi}{\Delta k}$
$\implies \Delta x\, \Delta k = 2\pi \geq 1$, hence HUP is satisfied

Uncertainty Principle

5.5. Position and momentum of an electron ($E = 1$ keV) are determined simultaneously. Its position is known to an accuracy of only 1 Å along the x-axis. Using uncertainty principle, find the minimum permissible uncertainty in its momentum along the x-axis? From the above data can you determine the uncertainty along the y-axis?

Solution:

$$\Delta x\, \Delta p \geq \frac{\hbar}{2} \tag{5.5.1}$$

$$\implies \Delta p \geq \frac{\hbar}{2}\ \text{Å}^{-1} \tag{5.5.2}$$

$$\implies \Delta p \geq 5.27 \times 10^{-25}\ \text{kg m s}^{-1} \tag{5.5.3}$$

We do not have any information about uncertainty of p or x along the y-axis.

5.6. An electron falls from a height of 10 m and passes through a hole of radius 1 cm. To study the motion of the electron afterwards, should we apply the wave aspect or the particle aspect?

Solution: When the electron is at the hole

$$\frac{\langle p\rangle^2}{2m} = mgh \tag{5.6.1}$$
$$\implies \langle p\rangle = m\sqrt{2gh} \tag{5.6.2}$$
$$\implies \lambda \approx \frac{h}{\langle p\rangle} = \frac{h}{m\sqrt{2gh}} \tag{5.6.3}$$
$$= 5.15 \times 10^{-5} m \tag{5.6.4}$$
$$\implies \text{Fresnel Distance } D = \frac{a^2}{\lambda} \approx 7.8 \text{ m} \tag{5.6.5}$$

Hence, we should apply the wave aspect after 7.8 m distance from the hole, before it we should apply the particle aspect (or ray optics)

5.7. A beam of electron of energy 0.025 eV moving along the x-direction passes through a slit of variable width w placed along the y-axis. Estimate the value of w for which the spot size on a screen kept at a distance of 0.5 m from the slit would be a minimum.

Solution: We know that $\theta_{\text{min}} = \frac{\lambda}{w}$ for Fraunhofer diffraction, where θ is the angle made with respect to the incoming beam direction (you can also get this using Δp_y and Δy). Thus for small w,

$$\text{Spot Size } s = 2 \times \theta_{\text{min}} D = 2 \times \frac{\lambda D}{w} \tag{5.7.1}$$
$$= \frac{2hD}{w\sqrt{2mE}} \tag{5.7.2}$$

But the spot size is just w when w is very large. Thus the minimum spot size is when these two seem to agree

$$\frac{2hD}{w\sqrt{2mE}} \sim w \tag{5.7.3}$$
$$\implies w \sim \sqrt[4]{\frac{4h^2D^2}{2mE}} \approx 88\ \mu\text{m} \tag{5.7.4}$$

5.8. If the average value of momentum $\langle p_x\rangle = 0$, then the x-component of momentum Δp_x is given by $\Delta p_x = \sqrt{\langle p_x^2\rangle}$. Using this relation, estimate the following (use $\Delta x\, \Delta p_x \geq \frac{\hbar}{2}$)

(a) Minimum kinetic energy that a proton and an electron would have if they were confined to a nucleus of approximate diameter 10^{-14} m. This is an argument used against the existence of electron in nuclei.

Solution: Δx will be of the order 10^{-14} m.
Thus Δp_x will be of the order 10^{-20} kg m s^{-1}
Therefore,

$$\langle E^2 \rangle = c^2 \langle p^2 \rangle + m_0^2 c^4 \tag{5.8.1}$$
$$\sim 10^{14} \text{ eV}^2 \tag{5.8.2}$$
$$\implies \langle E \rangle \sim 10 \text{ MeV} \tag{5.8.3}$$

This back of the envelope estimation reveals that the energy is too high to remain stable inside the atom

(b) The ground state energy of a particle of mass m bound by a potential $V = \frac{1}{2}kx^2$

Solution:

$$\langle E \rangle = \frac{1}{2m}\langle p^2 \rangle + \frac{k}{2}\langle x^2 \rangle \tag{5.8.4}$$

Since V is minimum at $x = 0$ and is symmetric about 0, we can safely assume $\langle x \rangle = 0$

$$= \frac{\Delta p^2}{2m} + \frac{k\Delta x^2}{2} \tag{5.8.5}$$
$$\geq \frac{\Delta p^2}{2m} + \frac{k\hbar^2}{8\Delta p^2} \tag{5.8.6}$$

We can minimize the expected Energy by differentiating with Δp and setting to 0

$$\frac{d\langle E \rangle}{d\Delta p} = 0 \tag{5.8.7}$$
$$\implies \frac{\Delta p}{m} - \frac{k\hbar^2}{4\Delta p^3} = 0 \tag{5.8.8}$$
$$\implies \Delta p = \sqrt[4]{\frac{k\hbar^2 m}{4}} \tag{5.8.9}$$

Substituting this in (5.8.6),

$$E_{\text{ground}} = \hbar\left(\frac{1}{4}\sqrt{\frac{k}{m}} + \frac{1}{4}\sqrt{\frac{k}{m}}\right) = \frac{1}{2}\hbar\sqrt{\frac{k}{m}} \tag{5.8.10}$$

Since the actual ground state energy is also $\frac{1}{2}\hbar\sqrt{\frac{k}{m}}$, we have done a pretty good job with our back of the envelope estimation

(c) The radial distance r for which the sum of kinetic and potential energies is minimum in a hydrogen atom.

Solution:

$$\langle E\rangle = \frac{1}{2m}\langle p^2\rangle - \frac{q_e^2}{4\pi\epsilon_0}\langle\frac{1}{r}\rangle \tag{5.8.11}$$
$$\sim \frac{\Delta p^2}{2m} - \frac{q_e^2}{4\pi\epsilon_0}\frac{1}{\Delta r} \tag{5.8.12}$$

Using $\Delta r\,\Delta p \geq \frac{\hbar}{2}$,

$$\geq \frac{\hbar^2}{8m\Delta r^2} - \frac{q_e^2}{4\pi\epsilon_0}\frac{1}{\Delta r} \tag{5.8.13}$$

Minimizing the Expected Energy with respect to Δr

$$\frac{d\langle E\rangle}{d\Delta r} = 0 \tag{5.8.14}$$
$$\implies -\frac{\hbar^2}{4m\Delta r^3} + \frac{q_e^2}{4\pi\epsilon_0}\frac{1}{\Delta r^2} = 0 \tag{5.8.15}$$
$$\implies \Delta r = \frac{\hbar^2\pi\epsilon_0}{mq_e^2} = 0.13\times 10^{-10}\text{ m} \tag{5.8.16}$$

This estimation is not bad considering that the real r is $\frac{4\hbar^2\pi\epsilon_0}{mq_e^2} = 0.53\times 10^{-10}$ m

5.9. Estimate the minimum possible energy (i.e., the ground state energy) consistent with the uncertainty principle for a particle of mass m bound by a potential $V = kx^4$ (use $\Delta x\,\Delta p_x \geq \frac{\hbar}{2}$)

Solution:

$$\langle E\rangle = \frac{1}{2m}\langle p^2\rangle + k\langle x^4\rangle \tag{5.9.1}$$
$$\sim \frac{\Delta p^2}{2m} + k\Delta x^4 \tag{5.9.2}$$
$$\geq \frac{\Delta p^2}{2m} + k\frac{\hbar^4}{16\Delta p^4} \tag{5.9.3}$$

Minimizing the Expected Energy with respect to Δp

$$\frac{d\langle E\rangle}{d\Delta p} = 0 \tag{5.9.4}$$
$$\implies \frac{\Delta p}{m} - \frac{k\hbar^4}{4\Delta p^5} = 0 \tag{5.9.5}$$
$$\implies E_{\text{ground}} \sim \sqrt[3]{\frac{k\hbar^4 m}{4}}\left(\frac{1}{2m} + \frac{1}{4m}\right) \tag{5.9.6}$$
$$= \frac{3}{4}\sqrt[3]{\frac{k\hbar^4}{4m^2}} \tag{5.9.7}$$

5.10. A photon of energy E is emitted as a result of a particular transition.

(a) Find the value of the recoil energy, assuming that the atom recoils with a nonrelativistic speed.

Solution: We begin by momentum as usual

$$p_{a'} = p'_{\lambda} \tag{5.10.1}$$

$$\implies p_{a'} = \frac{E}{c} \tag{5.10.2}$$

$$\implies E_{a'} = \frac{p_{a'}^2}{2m} = \boxed{\frac{E^2}{2mc^2}} \tag{5.10.3}$$

(b) Let the lifetime of the state be of the order of 10^{-8} s. Estimate the natural line width of the emitted line.

Solution: Natural line width refers to the spread in the energies of a line observed in emission/absorption spectrum, and this is nothing but ΔE.
We know that $\Delta E\,\Delta t \geq \frac{\hbar}{2}$, where Δt is the time it takes for the system to change it's observable value considerably. Thus here $\Delta t = 10^{-8}$ s.
$\implies \Delta E \sim \frac{\hbar}{2\Delta t}$ $\boxed{\sim 10^{-8} \text{ eV}}$

(c) Find the value of E for which the recoil energy will be of the same order of magnitude as the natural line width? For order of magnitude calculation take the mass number of the atom as 100.

Solution:

$$\frac{E^2}{2mc^2} \sim 10^{-8} \text{ eV} \tag{5.10.4}$$

$$\implies E \sim 100 \text{ eV} \tag{5.10.5}$$

5.11. Take the hydrogen atoms in thermal equilibrium at a temperature T, for which $k_B T = 0.025$ eV. Let E_1 be the difference in energy between the ground state and the first excited state when the atom is at rest. Let E_2 be the energy of the photon (in the frame of container) required to make this transition when the atom is moving towards the photon

(a) Find $E_1 - E_2$

Solution: We can assume that the translational modes are already activated at these temperatures and the average translational energy is $\frac{3}{2}k_B T$
We begin by conserving momentum and energy (taking note that we conserve the average over all atoms which move towards the incident photon)

$$p_{\mathrm{a}} - \frac{E_2}{c} = p'_{\mathrm{a}} \qquad \text{(Conserving Momentum)}$$

$$\tag{5.11.1}$$

We know that $\frac{\langle p_{\text{a}}\rangle}{m} = v_{\text{mean}} = \sqrt{\frac{8k_BT}{\pi m}}$

$$\langle E_{\text{trans}}\rangle + E_2 = \langle E'_{\text{trans}}\rangle + E_1 \qquad \text{(Conserving Energy)} \tag{5.11.2}$$

We know that $\langle E_{\text{trans}}\rangle = \frac{3}{2}k_BT$

But,

$$\langle E'_{\text{trans}}\rangle = \frac{1}{2m}\langle p'^2_{\text{a}}\rangle \tag{5.11.3}$$

$$= \frac{1}{2m}\langle p^2_{\text{a}}\rangle - \frac{E_2}{mc}\langle p_{\text{a}}\rangle + \frac{E_2^2}{2mc^2} \qquad \text{(Using (5.11.1))} \tag{5.11.4}$$

$$= \langle E_{\text{trans}}\rangle - \frac{E_2}{mc}\langle p_{\text{a}}\rangle + \frac{E_2^2}{2mc^2} \tag{5.11.5}$$

$$= \frac{3}{2}k_BT - E_2\sqrt{\frac{8k_BT}{\pi mc^2}} + \frac{E_2^2}{2mc^2} \tag{5.11.6}$$

$$\implies E_2 = E_1 - E_2\sqrt{\frac{8k_BT}{\pi mc^2}} + \frac{E_2^2}{2mc^2} \tag{5.11.7}$$

$$\implies \left(\frac{E_2}{E_1}\right)^2 - 2\frac{mc^2}{E_1}\left(1 + \sqrt{\frac{8k_BT}{mc^2}}\right)\frac{E_2}{E_1} + \frac{2mc^2}{E_1} = 0 \tag{5.11.8}$$

$$\implies E_2 = 0.99999177E_1 = 10.199916 \text{ eV} \tag{5.11.9}$$

$$\implies E_1 - E_2 = \boxed{0.000084 \text{ eV}} \tag{5.11.10}$$

(b) After the absorption of the photon, find the final velocity of the hydrogen atom

Solution:

$$\frac{\langle p'_{\text{a}}\rangle}{m} = \frac{\langle p_{\text{a}}\rangle}{m} - \frac{E_2}{mc} \qquad \text{(Using (5.11.1))} \tag{5.11.11}$$

$$= \boxed{2466 \text{ m s}^{-1}} \tag{5.11.12}$$

(c) If the lifetime of the first excited state is 10^{-8} s, will the photon with energy E_2 be able to cause a transition, had the atom been at rest? Discuss quantitatively. You are free to make any assumption, provided you justify it

Solution: Had the atom been at rest,

$$\frac{E_2}{c} = p'_a \tag{5.11.13}$$

$$E_2 = E'_{\text{trans}} + E_1 \tag{5.11.14}$$

$$= \frac{E_2^2}{2mc^2} + E_1 \tag{5.11.15}$$

$$\implies \left(\frac{E_2}{E_1}\right)^2 - 2\frac{mc^2}{E_1}\frac{E_2}{E_1} + \frac{2mc^2}{E_1} = 0 \tag{5.11.16}$$

$$\implies E_2 = 10.200000055386 \text{ eV} \tag{5.11.17}$$

Thus the required photon energy is $\sim 10^{-5}$ eV more than the energy supplied. But as we already know, the line width is $\sim 10^{-8}$ eV, thus the difference is more than that is acceptable, hence the photon will not be able to excite the atom at rest

5.12. For a non-relativistic electron, using the uncertainty relation $\Delta x\, \Delta p_x = \frac{\hbar}{2}$

(a) Derive an expression for the minimum kinetic energy when localized in a region of size a

Solution:

$$\Delta x \sim a \tag{5.12.1}$$

$$\implies \Delta p_x \geq \frac{\hbar}{2a} \tag{5.12.2}$$

$$\text{But, } \langle E \rangle = \frac{\langle p_x^2 \rangle}{2m} \tag{5.12.3}$$

$$= \frac{1}{2m}\left(\Delta p_x^2 + \langle p_x \rangle^2\right) \tag{5.12.4}$$

$$\geq \frac{\hbar^2}{8ma^2} \tag{5.12.5}$$

(b) Show that the uncertainty in the measurement of its velocity is the same as the particle velocity if the uncertainty in the position of the particle is equal to its de Broglie wavelength.

Solution:

$$\Delta v_x \geq \frac{\hbar}{2m\lambda} = \frac{v}{4\pi} \sim v \tag{5.12.6}$$

(c) Using the expression in (b), calculate the uncertainty in the velocity of an electron having energy 0.2 keV

Solution:

$$\Delta v_x = \frac{1}{4\pi}\sqrt{\frac{2E}{m}} = 6.7 \times 10^5 \text{ m s}^{-1} \tag{5.12.7}$$

(d) An electron of energy 0.2 keV is passed through a circular hole of radius 10^{-6} m. Find the uncertainty introduced in the angle of emergence in radians (given $\tan\theta \cong \theta$)

Solution:

$$\Delta y \sim 10^{-6} \text{ m} \tag{5.12.8}$$

$$\implies \Delta p_y = \frac{\hbar}{2\Delta y} \tag{5.12.9}$$

$$\implies \Delta\theta \cong \frac{\Delta p_y}{\langle p_x \rangle} = \frac{\hbar}{2\Delta y\sqrt{2Em}} = 4.3 \times 10^{-5} \text{ rad} \tag{5.12.10}$$

6 Wave function and Operators

6.1. If $\phi_n(x)$ are the solutions of time independent Schrödinger equation with energies E_n, show that

$$\psi(x,t) = \sum_n C_n \phi_n(x) e^{-i\frac{E_n}{\hbar}t}$$

is a solution of time dependent Schrödinger equation (C_n are constants). However, show that $\psi(x,0)$ is not a solution of the time independent Schrödinger equation

Solution: According to TISE,

$$-\frac{\hbar^2}{2m}\frac{\partial^2 \phi_n(x)}{\partial^2 x} + V(x)\phi_n(x) = E_n\phi_n(x) \qquad \forall\, n \tag{6.1.1}$$

We need to satisfy the TDSE,

$$-\frac{\hbar^2}{2m}\frac{\partial^2 \psi(x,t)}{\partial^2 x} + V(x)\psi(x,t) = i\hbar\frac{\partial\psi(x,t)}{\partial t} \tag{6.1.2}$$

$$\implies \text{LHS} = \sum_n -\frac{\hbar^2}{2m}\frac{\partial^2 \phi_n(x)}{\partial^2 x} C_n e^{-i\frac{E_n}{\hbar}t} + C_n \sum_n V(x)\phi_n(x) e^{-i\frac{E_n}{\hbar}t} \tag{6.1.3}$$

$$= \sum_n E_n C_n \phi_n(x) e^{-i\frac{E_n}{\hbar}t} \text{ (Using (6.1.1))} \tag{6.1.4}$$

$$\text{RHS} = i\hbar \sum_n C_n\phi_n(x)\frac{\partial e^{i\frac{E_n}{\hbar}t}}{\partial t} \tag{6.1.5}$$

$$= \sum_n E_n C_n \phi_n(x) e^{-i\frac{E_n}{\hbar}t} = \text{LHS} \tag{6.1.6}$$

Hence $\psi(x,t)$ satisfies TDSE
Now to check satisfiability of $\psi(x,0)$ on TISE

$$\text{LHS} = \sum_n -\frac{\hbar^2}{2m} C_n \frac{\partial^2 \phi_n(x)}{\partial^2 x} + \sum_n C_n V(x)\phi_n(x) \tag{6.1.7}$$

$$\text{RHS} = E \sum_n C_n \phi_n(x) \tag{6.1.8}$$

We can see that no single value of E satisfies TISE $\forall\ x$, so $\psi(x,0)$ is **not** a solution of the TISE

6.2. Consider a wave function $\phi_k(x) = \sin(kx)$. Is this an eigenfuction of the operators

$$\hat{p} = -i\hbar\frac{\partial}{\partial x} \quad \text{and} \quad \hat{K} = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}$$

Find the eigenvalues

Solution:

$$\hat{p}\phi_k(x) = -i\hbar\frac{\partial \sin(kx)}{\partial x} \tag{6.2.1}$$

$$= -i\hbar k \cos(kx) \tag{6.2.2}$$

Thus $\phi_k(x)$ is **not** an eigenfunction of $\hat{p}$

$$\hat{K}\phi_k(x) = -\frac{\hbar^2}{2m}\frac{\partial^2 \sin(kx)}{\partial x^2} \tag{6.2.3}$$

$$= \frac{(\hbar k)^2}{2m}\sin(kx) = \frac{(\hbar k)^2}{2m}\phi_k(x) \tag{6.2.4}$$

Thus, $\phi_k(x)$ is an eigenfunction of $\hat{K}$ with eigenvalue $\frac{(\hbar k)^2}{2m}$

6.3. If $\psi_1(x,t)$ and $\psi_2(x,t)$ are solutions of time dependent Schrödinger equation, show that $a\psi_1(x,t) + b\psi_2(x,t)$ is also a solution of the same, where a and b are constants.

Solution:

$$-\frac{\hbar^2}{2m}\frac{\partial^2 \psi_1(x,t)}{\partial^2 x} + V(x)\psi_1(x,t) = i\hbar\frac{\partial \psi_1(x,t)}{\partial t} \tag{6.3.1}$$

$$-\frac{\hbar^2}{2m}\frac{\partial^2 \psi_2(x,t)}{\partial^2 x} + V(x)\psi_2(x,t) = i\hbar\frac{\partial \psi_2(x,t)}{\partial t} \tag{6.3.2}$$

Adding a(6.3.1) + b(6.3.2),

$$-\frac{\hbar^2}{2m}\frac{\partial^2 \psi(x,t)}{\partial^2 x} + V(x)\psi(x,t) = i\hbar\frac{\partial \psi(x,t)}{\partial t} \tag{6.3.3}$$

Where $\psi(x,t) = a\psi_1(x,t) + b\psi_2(x,t)$

6.4. Consider two operators $\hat{O}_1$ and $\hat{O}_2$, defined as:

$$\hat{O}_1 \equiv -i\frac{\partial}{\partial x}, \qquad \hat{O}_2 \equiv \hat{x} - i\frac{\partial}{\partial x}$$

Calculate $O_1\psi(x)$ and $O_2\psi(x)$, where $\psi(x)$ is a function of x. Is $\psi(x)$ an eigen function of the two operators if it has the form $\psi(x) = e^{ikx}$?

Solution:

$$O_1\psi(x) = \boxed{-i\frac{\partial\psi(x)}{\partial x}} \tag{6.4.1}$$

$$O_2\psi(x) = \boxed{x\psi(x) - i\frac{\partial\psi(x)}{\partial x}} \tag{6.4.2}$$

$$\implies O_1 e^{ikx} = k e^{ikx} \tag{6.4.3}$$

$$\implies O_2 e^{ikx} = (x-k)e^{ikx} \tag{6.4.4}$$

Thus, $\psi(x)$ is an eigenfunction of $\hat{O}_1$ with eigenvalue k

6.5. An operator is given by

$$\hat{G} \equiv i\hbar\frac{\partial}{\partial x} + Ax$$

where A is a constant. Find the eigenfunction $\phi(x)$. If this eigen function is subjected to a boundary condition $\phi(a) = \phi(-a)$, find out the eigen values.

Solution: We need to solve the differential equation

$$\hat{G}\phi(x) = \lambda\phi(x) \tag{6.5.1}$$

$$\implies i\hbar\frac{d\phi(x)}{dx} + Ax\phi(x) = \lambda\phi(x) \tag{6.5.2}$$

$$\implies \frac{d\phi(x)}{dx} = \frac{i}{\hbar}(Ax-\lambda)\phi(x) \tag{6.5.3}$$

$$\implies \int \frac{1}{\phi(x)}\, d\phi(x) = \frac{i}{\hbar}\int Ax - \lambda\, dx \tag{6.5.4}$$

$$\implies \ln\phi(x) = \frac{i}{\hbar}\left(\frac{A}{2}x^2 - \lambda x\right) + \ln(C) \tag{6.5.5}$$

Where C is a constant

$$\implies \phi(x) = Ce^{-i\frac{\lambda}{\hbar}x}e^{i\frac{A}{2\hbar}x^2} \tag{6.5.6}$$

Applying the boundary condition $\phi(a) = \phi(-a)$

$$\implies Ce^{-i\frac{\lambda}{\hbar}a}e^{i\frac{A}{2\hbar}a^2} = Ce^{i\frac{\lambda}{\hbar}a}e^{i\frac{A}{2\hbar}a^2} \tag{6.5.7}$$

$$\implies e^{i\frac{2a\lambda}{\hbar}} = 1 \tag{6.5.8}$$

$$\implies \frac{2a\lambda}{\hbar} = 2n\pi \text{ for } n \in \mathbb{N} \tag{6.5.9}$$

$$\implies \lambda_n = \frac{n\pi\hbar}{a} \tag{6.5.10}$$

6.6. Consider a large number (N) of identical experimental set-ups. In each of these, a single particle is described by a wave function $\phi(x) = Ae^{-\frac{x^2}{a^2}}$ at $t = 0$, where A is the normalization constant and a is another constant with the dimension of length. If a measurement of the position of the particle is carried out at time $t = 0$ in all these set-ups, it is found that in 100 of these, the particle is found within an infinitesimal interval of $x = 2a$ to $2a + dx$. Find out, in how many of the measurements, the particle would have been found in the infinitesimal interval of $x = a$ to $a + dx$

Solution:

$$\frac{N_{[2a,2a+dx]}}{N_{[a,a+dx]}} = \frac{P(2a < x < 2a + dx)}{P(a < x < a + dx)} \tag{6.6.1}$$

$$= \frac{|\phi(2a)|^2\,dx}{|\phi(a)|^2\,dx} = e^{-\frac{(2a)^2-a^2}{a^2}} = e^{-6} \tag{6.6.2}$$

$$\implies N_{[a,a+dx]} \approx \boxed{100e^6 \approx 40343} \tag{6.6.3}$$

6.7. $\psi_1(x)$ and $\psi_2(x)$ are the normalized eigenfunctions of an operator $\hat{P}$, with eigen values P_1 and P_2 respectively. If the wave function of a particle is $0.25\psi_1(x) + 0.75\psi_2(x)$ at $t = 0$, find the probability of observing P_1

Solution: Since $\hat{P}$ corresponds to an observable, therefore it is a Hermitian Operator. Thus it's eigenfunctions with distinct eigenvalues must be orthogonal

$$\implies \langle\psi_1|\psi_2\rangle = \langle\psi_2|\psi_1\rangle = 0 \tag{6.7.1}$$

$$\text{And } \langle\psi_1|\psi_1\rangle = \langle\psi_2|\psi_2\rangle = 1 \tag{6.7.2}$$

According to the postulates of QM, the probability of observing P_1 is $\frac{|\langle\psi_1|\psi\rangle|^2}{\langle\psi|\psi\rangle}$ where $\psi(x) = 0.25\psi_1(x) + 0.75\psi_2(x)$

$$\langle\psi_1|\psi\rangle = 0.25\langle\psi_1|\psi_1\rangle + 0.75\langle\psi_1|\psi_2\rangle = 0.25 \tag{6.7.3}$$

$$\langle\psi|\psi\rangle = 0.25^2\langle\psi_1|\psi_1\rangle + 0.75^2\langle\psi_2|\psi_2\rangle \tag{6.7.4}$$

$$+ 0.25 \cdot 0.75\langle\psi_1|\psi_2\rangle + 0.25 \cdot 0.75\langle\psi_2|\psi_1\rangle = 0.25^2 + 0.75^2 \tag{6.7.5}$$

$$\implies \text{Probability of } P_1 = \frac{\langle|\psi_1|\psi\rangle|^2}{\langle\psi|\psi\rangle} = \frac{0.25^2}{0.25^2 + 0.75^2} = \frac{1}{10} \approx 0.1 \tag{6.7.6}$$

6.8. An observable A is represented by the operator $\hat{A}$. Two of its normalized eigen functions are given as $\phi_1(x)$ and $\phi_2(x)$, corresponding to distinct eigenvalues a_1 and a_2, respectively. Another observable B is represented by an operator $\hat{B}$. Two normalized eigenfunctions of this operator are given as $u_1(x)$ and $u_2(x)$ with distinct eigenvalues b_1 and b_2, respectively. The eigenfunctions $\phi_1(x)$ and $\phi_2(x)$ are related to $u_1(x)$ and $u_2(x)$ as

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

At time $t = 0$, a particle is in a state given by $\frac{2}{3}\phi_1 + \frac{1}{3}\phi_2$

(a) Find the values of D, F and P

Solution: We know that ϕ_1, ϕ_2, u_1, u_2 are normalized, and ϕ_1, ϕ_2 are orthogonal and so are u_1, u_2.

We begin by using normalization of ϕ_1

$$\implies \langle\phi_1|\phi_1\rangle = 1 \tag{6.8.1}$$

$$\implies |D|^2\left(9\langle u_1|u_1\rangle + 16\langle u_2|u_2\rangle\right. \tag{6.8.2}$$

$$\left.+12\langle u_2|u_1\rangle + 12\langle u_1|u_2\rangle\right) = 1 \tag{6.8.3}$$

$$\implies 25|D|^2 = 1 \tag{6.8.4}$$

$$\implies D = \boxed{0.2e^{i\theta}} \tag{6.8.5}$$

Where θ is any value $\in [0, 2\pi)$

Now we can use orthogonality of ϕ_1 and ϕ_2

$$\langle\phi_1|\phi_2\rangle = 0 \tag{6.8.6}$$

$$\implies \bar{D}F\left(12\langle u_1|u_1\rangle - 4P\langle u_2|u_2\rangle\right. \tag{6.8.7}$$

$$\left.-\ 3P\langle u_1|u_2\rangle + 16\langle u_2|u_1\rangle\right) = 0 \tag{6.8.8}$$

$$\implies P = \boxed{3} \tag{6.8.9}$$

Finally we use the normalization of ϕ_2

$$\implies \langle\phi_2|\phi_2\rangle = 1 \tag{6.8.10}$$

$$\implies |F|^2\left(16\langle u_1|u_1\rangle + 9\langle u_2|u_2\rangle\right. \tag{6.8.11}$$

$$\left.-12\langle u_2|u_1\rangle - 12\langle u_1|u_2\rangle\right) = 1 \tag{6.8.12}$$

$$\implies 25|F|^2 = 1 \tag{6.8.13}$$

$$\implies F = \boxed{0.2e^{i\phi}} \tag{6.8.14}$$

(b) If a measurement of A is carried out at $t = 0$, what are the possible results and what are their probabilities?

Solution: According to the postulates of QM, the possible results of an A measurement are the eigenvalues a_1 and a_2, and the probability is $\frac{|\langle\phi|\psi\rangle|^2}{\langle\psi|\psi\rangle}$ where ϕ is the corresponding eigenfunction and $\psi = \frac{2}{3}\phi_1 + \frac{1}{3}\phi_2$

$$\langle \phi_1 | \psi \rangle = \frac{2}{3} \tag{6.8.15}$$

$$\langle \phi_2 | \psi \rangle = \frac{1}{3} \tag{6.8.16}$$

$$\langle \psi | \psi \rangle = \frac{4}{9} + \frac{1}{9} = \frac{5}{9} \tag{6.8.17}$$

$$\implies \text{Probability}(a_1) = \frac{\frac{4}{9}}{\frac{5}{9}} = 0.8 \tag{6.8.18}$$

$$\implies \text{Probability}(a_2) = \frac{\frac{1}{9}}{\frac{5}{9}} = 0.2 \tag{6.8.19}$$

(c) Assume that the measurement of A mentioned above yielded a value a_1. If a measurement of B is carried out immediately after this, what would be the possible outcomes and what would be their probabilities?

Solution: According to the postulates of QM, once a_1 is measured, the wavefunction will collapse to ϕ_1. Thus the wavefunction at the moment after measurement is $\phi_1(x)$. Again we repeat the same exercise as above for u_1 and u_2. The possible outcomes are of course b_1 and b_2.

$$\langle u_1 | \phi_1 \rangle = 0.6e^{i\theta} \tag{6.8.20}$$

$$\langle u_2 | \phi_1 \rangle = 0.8e^{i\theta} \tag{6.8.21}$$

$$\langle \phi_1 | \phi_1 \rangle = 1 \tag{6.8.22}$$

$$\implies \text{Probability}(b_1) = 0.36 \tag{6.8.23}$$

$$\implies \text{Probability}(b_2) = 0.64 \tag{6.8.24}$$

(d) If instead of following the above path, a measurement of B was carried out initially at $t = 0$, what would be the possible outcomes and what would be their probabilities?

Solution: Following same steps as above, the possible outcomes are same, b_1 and b_2

$$\psi = \frac{2}{3}\phi_1 + \frac{1}{3}\phi_2 \tag{6.8.25}$$

$$= \left(\frac{2}{5}e^{i\theta} + \frac{4}{15}e^{i\phi}\right) u_1 + \left(\frac{8}{15}e^{i\theta} - \frac{1}{5}e^{i\phi}\right) u_2 \tag{6.8.26}$$

$$\langle u_1|\psi\rangle = \frac{2}{5}e^{i\theta} + \frac{4}{15}e^{i\phi} \tag{6.8.27}$$

$$\langle u_2|\psi\rangle = \frac{8}{15}e^{i\theta} - \frac{1}{5}e^{i\phi} \tag{6.8.28}$$

$$\langle \psi|\psi\rangle = \frac{5}{9} \tag{6.8.29}$$

$$\implies \text{Probability}(b_1) = \frac{9}{5}\left(\frac{4}{25} + \frac{16}{225} + 2\frac{8}{75}\cos(\theta - \phi)\right) \tag{6.8.30}$$

$$= \frac{468}{1125} + \frac{144}{375}\cos(\theta - \phi) \tag{6.8.31}$$

$$\implies \text{Probability}(b_2) = \frac{9}{5}\left(\frac{64}{225} + \frac{1}{25} - 2\frac{8}{75}\cos(\theta - \phi)\right) \tag{6.8.32}$$

$$= \frac{657}{1125} - \frac{144}{375}\cos(\theta - \phi) \tag{6.8.33}$$

(e) Assume that after performing the measurements described in (c), the outcome was b_2. What would be the possible outcomes, if A were measured immediately after this and what would be the probabilities?

Solution: So immediately after measurement the wavefunction collapses to u_2. Now once again the possibilities are a_1 and a_2

$$\langle \phi_1|u_2\rangle = \langle u_2|\phi_1\rangle^* = 0.8e^{-i\theta} \tag{6.8.34}$$

$$\langle \phi_2|u_2\rangle = \langle u_2|\phi_2\rangle^* = -0.6e^{-i\phi} \tag{6.8.35}$$

$$\langle u_2|u_2\rangle = 1 \tag{6.8.36}$$

$$\implies \text{Probability}(a_1) = 0.64 \tag{6.8.37}$$

$$\implies \text{Probability}(a_2) = 0.36 \tag{6.8.38}$$

7 Free Particle

7.1. Consider a particle with one-dimensional wave function

$$\phi(x) = N(a^2 + x^2)^{\frac{-1}{2}} e^{ip_0 x\hbar}$$

where a, p_0, N are real constants.

(a) Find the normalization constant N

Solution:

$$\int_{\mathbb{R}} \phi(x)^* \phi(x)\, dx = 1 \tag{7.1.1}$$

$$\implies N^2 \int_{x=-\infty}^{\infty} \frac{1}{a^2+x^2}\, dx = 1 \tag{7.1.2}$$

$$\implies N^2 \int_{\theta=-\frac{\pi}{2}}^{\frac{\pi}{2}} \frac{a \sec^2\theta}{a^2\sec^2\theta}\, d\theta = 1 \tag{7.1.3}$$

$$\implies \frac{N^2\pi}{a} = 1 \tag{7.1.4}$$

$$\implies N = \sqrt{\frac{a}{\pi}} \tag{7.1.5}$$

(b) Determine the probability of finding the particle in the interval $-\frac{a}{\sqrt{5}} \le x \le \frac{a}{\sqrt{5}}$

Solution:

$$P(-\frac{a}{\sqrt{5}} \le x \le \frac{a}{\sqrt{5}}) = \int_{x=-\frac{a}{\sqrt{5}}}^{\frac{a}{\sqrt{5}}} \phi(x)^*\phi(x)\, dx \tag{7.1.6}$$

$$= \frac{a}{\pi}\int_{x=-\frac{a}{\sqrt{5}}}^{\frac{a}{\sqrt{5}}} \frac{1}{a^2+x^2}\, dx \tag{7.1.7}$$

$$= \frac{a}{\pi}\int_{\theta=-\tan^{-1}\frac{1}{\sqrt{5}}}^{\tan^{-1}\frac{1}{\sqrt{5}}} \frac{1}{a}\, d\theta \tag{7.1.8}$$

$$= \frac{2}{\pi}\tan^{-1}\frac{1}{\sqrt{5}} \approx 0.27 \tag{7.1.9}$$

(c) What is the expectation value of the momentum?

Solution:

$$\langle p\rangle = -i\hbar \int_{\mathbb{R}} \phi(x)^* \frac{\partial\phi(x)}{\partial x}\, dx \tag{7.1.10}$$

$$= -i\hbar\frac{a}{\pi}\int_{x=-\infty}^{\infty} \frac{1}{\sqrt{a^2+x^2}} e^{-ip_0x\hbar}\left(\frac{-x}{\sqrt{a^2+x^2}^3} + \frac{ip_0\hbar}{\sqrt{a^2+x^2}}\right) e^{ip_0x\hbar}\, dx \tag{7.1.11}$$

$$= \frac{-ia\hbar}{\pi}\int_{x=-\infty}^{\infty} p_0\hbar\frac{1}{a^2+x^2}i - \frac{x}{(a^2+x^2)^2}\, dx \tag{7.1.12}$$

$$= \frac{-ia\hbar}{\pi}\left(ip_0\hbar\int_{x=-\infty}^{\infty}\frac{1}{a^2+x^2}\, dx - \int_{x=\infty}^{\infty}\frac{x}{(a^2+x^2)^2}\, dx\right) \tag{7.1.13}$$

$$= p_0\hbar^2 \tag{7.1.14}$$

7.2. Show that

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

and

$$\psi(x) = Ce^{ikx} + De^{-ikx}$$

are equivalent solutions of TISE of a free particle. A, B, C and D can be complex numbers.

Solution: We already know that e^{ikx} and e^{-ikx} are solutions to TISE for a free particle. Hence $\psi(x) = Ce^{ikx} + De^{-ikx}$ is also a solution to the TISE. We can also see that by taking $A = i(C - D)$ and $B = (C + D)$, $\psi(x) = A\sin(kx) + B\cos(kx)$

7.3. A particle with mass m is described by the following wave function:

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

where A, B, k are constants

(a) For a free particle, show that $\psi(x)$ is a solution of the Schrödinger equation and find its energy

Solution: We already saw in Q7.2 that $\psi(x)$ is a solution to TISE
This must be then an energy eigenstate, and we want to find the energy eigenvalue

$$\hat{H}\psi(x) = -A\frac{\hbar^2}{2m}\frac{d^2\sin(kx)}{dx^2} + -B\frac{\hbar^2}{2m}\frac{d^2\cos(kx)}{dx^2} \tag{7.3.1}$$

$$= \frac{\hbar^2k^2}{2m}(A\sin(kx) + B\cos(kx)) \tag{7.3.2}$$

$$= \frac{\hbar^2k^2}{2m}\psi(x) \tag{7.3.3}$$

Therefore the energy eigenvalue is $\frac{\hbar^2k^2}{2m}$

(b) Check whether $\psi(x) = A\sin(kx)$ or $\psi(x) = B\cos(kx)$ is an eigenfunction of the momentum operator.

Solution:

$$\hat{P}(A\sin(kx)) = -i\hbar A\frac{d\sin(kx)}{dx} = -i\hbar kA\cos(kx) \tag{7.3.4}$$

$$\hat{P}(A\cos(kx)) = -i\hbar A\frac{d\cos(kx)}{dx} = i\hbar kA\sin(kx) \tag{7.3.5}$$

Thus none of them are momentum eigenfunctions.

7.4. Show that

$$\Psi(x,t) = A\sin(kx - \omega t) + B\cos(kx - \omega t)$$

does not obey the time-dependant Schrödinger's equation for a free particle

Solution: We have the TDSE,

$$-\frac{\hbar^2}{2m}\frac{\partial^2\psi(x,t)}{\partial x^2} = i\hbar\frac{\partial\psi(x,t)}{\partial t} \tag{7.4.1}$$

$$\text{LHS} = -\frac{\hbar^2}{2m}\frac{\partial^2 A\sin(kx-\omega t) + B\cos(kx-\omega t)}{\partial x^2} \tag{7.4.2}$$

$$= \frac{\hbar^2 k^2}{2m}A\sin(kx-\omega t) + B\cos(kx-\omega t) \tag{7.4.3}$$

$$\text{RHS} = i\hbar\frac{\partial A\sin(kx-\omega t) + B\cos(kx-\omega t)}{\partial t} \tag{7.4.4}$$

$$= -i\hbar(A\cos(kx-\omega t) - B\sin(kx-\omega t)) \neq \text{LHS} \tag{7.4.5}$$

7.5. Find the expectation value of the square of the momentum squared for the particle in the state:

$$\Psi(x,t) = Ae^{i(kx-\omega t)}$$

What conclusion can you draw for this solution?

Solution:

$$\langle P^2\rangle = \frac{\int_{\mathbb{R}}\Psi(x,t)^*\hat{P}\hat{P}\Psi(x,t)\,dx}{\int_{\mathbb{R}}\Psi(x,t)^*\Psi(x,t)}\,dx \tag{7.5.1}$$

$$= \hbar^2 k^2\frac{\int_{\mathbb{R}}\Psi(x,t)^*\Psi(x,t)\,dx}{\int_{\mathbb{R}}\Psi(x,t)^*\Psi(x,t)\,dx} \tag{7.5.2}$$

$$= \hbar^2 k^2 \tag{7.5.3}$$

Conclusion is that this has expected energy equal to energy eigenvalue $\frac{\hbar^2 k^2}{2m}$

7.6. A free proton has a wave function given by

$$\Psi(x,t) = Ae^{i(5.02\times 10^{11}x - 8.00\times 10^{15}t)}$$

The coefficient of x is inverse meters, and the coefficient of t is inverse seconds. Find its momentum and energy.

Solution: We know that $\Psi(x,t)$ is a momentum eigenfunction with momentum eigenvalue $\hbar k = 3.32\times 10^{-22}$ kg ms^{-1}, which is also the value of expected momentum
We also know that $\Psi(x,t)$ is an energy eigenfunction with energy eigenvalue $\hbar\omega = 5.3\times 10^{-18}$ J, which is also the value of expected energy

7.7. The wave function for a particle is given by

$$\phi(x) = Ae^{ikx} + Be^{-ikx}$$

where A and B are real constants. Show that $\phi(x)^*\phi(x)$ is always a positive quantity.

Solution:

$$\begin{aligned}
\phi(x)^*\phi(x) &= (Ae^{-ikx} + Be^{ikx})(Ae^{ikx} + Be^{-ikx}) && (7.7.1)\\
&= A^2 + B^2 + AB(e^{2ikx} + e^{-2ikx}) && (7.7.2)\\
&= A^2 + B^2 + 2AB\cos(2kx) && (7.7.3)\\
&\geq A^2 + B^2 - 2AB && (7.7.4)\\
&= (A-B)^2 \geq 0 && (7.7.5)
\end{aligned}$$

8 Infinite Potential Box

8.1. For a particle in a 1-D box of side L, show that the probability of finding the particle between $x = a$ and $x = a + b$ approaches the classical value $\frac{b}{L}$, if the energy of the particle is very high.

Solution: Let us assume the particle to be in one of the energy eigenstates $\psi_n(x)$

$$\begin{aligned}
\text{Prob}\,(a < x < a+b) &= \int_{x=a}^{a+b} \psi_n(x)^*\psi_n(x)\,dx && (8.1.1)\\
&= \frac{2}{L}\int_{x=a}^{a+b} \sin^2\left(n\frac{\pi}{L}x\right)\,dx && (8.1.2)\\
&= \frac{1}{L}\int_{x=a}^{a+b} 1 - \cos\left(2n\frac{\pi}{L}x\right)\,dx && (8.1.3)\\
&= \frac{1}{2n\pi}\int_{x=\frac{2n\pi}{L}a}^{\frac{2n\pi}{L}(a+b)} 1 - \cos x\,dx && (8.1.4)\\
&= \frac{1}{2n\pi}\left(\frac{2n\pi}{L}b - \sin\left(\frac{2n\pi}{L}(a+b)\right) + \sin\left(\frac{2n\pi}{L}a\right)\right) && (8.1.5)\\
&\to \frac{b}{L} \qquad \text{as } n\to\infty && (8.1.6)
\end{aligned}$$

8.2. Consider a particle confined to a 1-D box. Find the probability that the particle in its ground state will be in the central one-third region of the box.

Solution:

$$\text{Prob}(\frac{L}{3} < x < \frac{2L}{3}) = \int_{x=\frac{L}{3}}^{\frac{2L}{3}} \psi_1(x)^* \psi_1(x)\, dx \tag{8.2.1}$$

$$= \frac{2}{L} \int_{x=\frac{L}{3}}^{\frac{2L}{3}} \sin^2\left(\frac{\pi}{L}x\right)\, dx \tag{8.2.2}$$

$$= \frac{1}{L} \int_{x=\frac{L}{3}}^{\frac{2L}{3}} 1 - \cos\Big(2n\frac{\pi}{L}x\Big)\, dx \tag{8.2.3}$$

$$= \frac{1}{2\pi} \int_{x=\frac{2\pi}{3}}^{\frac{4\pi}{3}} 1 - \cos x\, dx \tag{8.2.4}$$

$$= \frac{1}{2\pi}\left(\frac{2\pi}{3} - \sin\left(\frac{4\pi}{3}\right) + \sin\left(\frac{2\pi}{3}\right)\right) \tag{8.2.5}$$

$$= \frac{1}{3} + \frac{\sqrt{3}}{2\pi} \tag{8.2.6}$$

8.3. Consider a one dimensional infinite square well potential of length L. A particle is in $n = 3$ state of this potential well. Find the probability that this particle will be observed between $x = 0$ and $x = L/6$. Can you guess the answer without solving the integral? Explain how.

Solution: As we can easily see, $\int_0^{\frac{L}{6}} \sin^2\left(3\frac{\pi}{L}x\right)\, dx = \int_{\frac{L}{6}}^{\frac{L}{3}} \sin^2\left(3\frac{\pi}{L}x\right)\, dx = \cdots$
$\implies \text{Prob}\big(0 < x < \frac{L}{6}\big) = \frac{1}{6}$

8.4. Solve the time independent Schrödinger equation for a particle in a 1-D box, taking the origin at the centre of the box and the ends at $\pm\frac{L}{2}$, where L is the length of the box.

Solution: We have

$$V(x) = \begin{cases} \infty & x < -\frac{L}{2} \\ 0 & -\frac{L}{2} \leq x \leq \frac{L}{2} \\ \infty & x > \frac{L}{2} \end{cases} \tag{8.4.1}$$

Applying TISE

$$\implies \frac{1}{\psi(x)}\frac{d^2\psi(x)}{dt^2} = -k^2 \qquad -\frac{L}{2} \leq x \leq \frac{L}{2} \tag{8.4.2}$$

Where

$$-k^2 = -\frac{2mE}{\hbar^2} \tag{8.4.3}$$

Solving the differential equation, we get

$$\psi(x) = \begin{cases} 0 & x < -\frac{L}{2} \\ A\cos(kx) + B\sin(kx) & -\frac{L}{2} \leq x \leq \frac{L}{2} \\ 0 & x > \frac{L}{2} \end{cases} \tag{8.4.4}$$

Imposing the boundary conditions

Continuity at $x = -\frac{L}{2}$

$$0 = A\cos\left(\frac{kL}{2}\right) - B\sin\left(\frac{kL}{2}\right) \tag{8.4.5}$$

Continuity at $x = \frac{L}{2}$

$$A\cos\left(\frac{kL}{2}\right) + B\sin\left(\frac{kL}{2}\right) = 0 \tag{8.4.6}$$

Using (8.4.5) we get $\tan\left(\frac{kL}{2}\right) = \frac{A}{B}$. Putting this in (8.4.6),

$$B\sin(kL) = 0 \tag{8.4.7}$$

$$\implies B = 0 \text{ or } k = \frac{n\pi}{L} \tag{8.4.8}$$

$$\implies \cot\left(\frac{kL}{2}\right) = 0 \text{ or } k = \frac{n\pi}{L} \tag{8.4.9}$$

$$\implies k = \frac{(2n'+1)\pi}{L} \text{ or } k = \frac{n\pi}{L} \tag{8.4.10}$$

$$\implies k = \frac{n\pi}{L} \tag{8.4.11}$$

Because the second case covers the first case

$$\tan\frac{kL}{2} = 0 \qquad n \text{ even} \tag{8.4.12}$$

$$\cot\frac{kL}{2} = 0 \qquad n \text{ odd} \tag{8.4.13}$$

$$\implies A = 0 \qquad n \text{ even} \tag{8.4.14}$$

$$\implies B = 0 \qquad n \text{ odd} \tag{8.4.15}$$

$$\implies \psi_n(x) = \begin{cases} A\cos\left(n\frac{\pi}{L}x\right) & n \text{ odd} \\ B\sin\left(n\frac{\pi}{L}x\right) & n \text{ even} \end{cases} \tag{8.4.16}$$

Finally we can normalize $\psi(x)$ to get $A = B = \sqrt{\frac{2}{L}}$

$$\psi_n(x) = \begin{cases} \sqrt{\frac{2}{L}}\cos\left(n\frac{\pi}{L}x\right) & n \text{ odd} \\ \sqrt{\frac{2}{L}}\sin\left(n\frac{\pi}{L}x\right) & n \text{ even} \end{cases} \tag{8.4.17}$$

8.5. Consider a particle of mass m in an infinite potential well extending from $x = 0$ to $x = L$. Wavefunction of the particle is given by

$$\psi(x) = A\left(\sin\left(\frac{\pi}{L}x\right) + \sin\left(\frac{2\pi}{L}x\right)\right)$$

where A is the normalization constant

(a) Calculate A

Solution:

$$\int_{\mathbb{R}} \psi(x)^* \psi(x)\, dx = 1 \tag{8.5.1}$$

$$\implies |A|^2 \int_{\mathbb{R}} \sin^2\left(\frac{\pi}{L}x\right) + \sin^2\left(\frac{2\pi}{L}x\right) + \cancelto{0}{2\sin\left(\frac{\pi}{L}x\right)\sin\left(\frac{2\pi}{L}x\right)} = 1 \tag{8.5.2}$$

$$\implies L|A|^2 = 1 \tag{8.5.3}$$

$$\implies A = \frac{e^{i\theta}}{\sqrt{L}} \tag{8.5.4}$$

(b) Calculate the expectation values of x and x^2 and hence the uncertainty Δx

Solution:

$$\langle x\rangle = \int_{\mathbb{R}} \psi(x)^* x \psi(x)\, dx \tag{8.5.5}$$

$$= \frac{1}{L}\int_{x=0}^{L} x\sin^2\left(\frac{\pi}{L}x\right) + x\sin^2\left(\frac{2\pi}{L}x\right) + 2x\sin\left(\frac{\pi}{L}x\right)\sin\left(\frac{2\pi}{L}x\right) \tag{8.5.6}$$

$$= \frac{1}{L}\int_{x=0}^{L} x - x\frac{\cos\left(2\frac{\pi}{L}x\right)}{2} - x\frac{\cos\left(4\frac{\pi}{L}x\right)}{2} + x\cos\left(\frac{\pi}{L}x\right) - x\cos\left(3\frac{\pi}{L}x\right) dx \tag{8.5.7}$$

$$= \frac{1}{L}\int_{x=0}^{L} x + \frac{\sin\left(2\frac{\pi}{L}x\right)}{4\frac{\pi}{L}} + \frac{\sin\left(4\frac{\pi}{L}x\right)}{8\frac{\pi}{L}} - \frac{\sin\left(\frac{\pi}{L}x\right)}{\frac{\pi}{L}} + \frac{\sin\left(3\frac{\pi}{L}x\right)}{3\frac{\pi}{L}}\, dx \tag{8.5.8}$$

$$= \frac{L}{2} - \frac{2L}{\pi^2} + \frac{2L}{9\pi^2} \tag{8.5.9}$$

$$= L\left(\frac{1}{2} - \frac{16}{9\pi^2}\right) \tag{8.5.10}$$

$$\langle x^2\rangle = \int_{\mathbb{R}} \psi(x)^* x^2 \psi(x)\, dx \tag{8.5.11}$$

$$= \frac{1}{L}\int_{x=0}^{L} x^2 \sin^2\left(\frac{\pi}{L}x\right) + x^2 \sin^2\left(\frac{2\pi}{L}x\right) + 2x^2 \sin\left(\frac{\pi}{L}x\right)\sin\left(\frac{2\pi}{L}x\right) \tag{8.5.12}$$

$$= \frac{1}{L}\int_{x=0}^{L} x^2 - x^2\frac{\cos\left(2\frac{\pi}{L}x\right)}{2} - x^2\frac{\cos\left(4\frac{\pi}{L}x\right)}{2} + x^2\cos\left(\frac{\pi}{L}x\right) - x^2\cos\left(3\frac{\pi}{L}x\right) dx \tag{8.5.13}$$

$$= \frac{1}{L}\int_{x=0}^{L} x^2 + x\frac{\sin\left(2\frac{\pi}{L}x\right)}{2\frac{\pi}{L}} + x\frac{\sin\left(4\frac{\pi}{L}x\right)}{4\frac{\pi}{L}} - 2x\frac{\sin\left(\frac{\pi}{L}x\right)}{\frac{\pi}{L}} + 2x\frac{\sin\left(3\frac{\pi}{L}x\right)}{3\frac{\pi}{L}}\, dx \tag{8.5.14}$$

$$= -\frac{1}{L}\left(x\frac{\cos\left(2\frac{\pi}{L}x\right)}{4\frac{\pi^2}{L^2}} + x\frac{\cos\left(4\frac{\pi}{L}x\right)}{16\frac{\pi^2}{L^2}} - 2x\frac{\cos\left(\frac{\pi}{L}x\right)}{\frac{\pi^2}{L^2}} + 2x\frac{\cos\left(3\frac{\pi}{L}x\right)}{9\frac{\pi^2}{L^2}}\right)\Bigg|_{x=0}^{L} \tag{8.5.15}$$

$$+ \frac{1}{L}\int_{x=0}^{L} x^2 + \frac{\cos\left(2\frac{\pi}{L}x\right)}{4\frac{\pi^2}{L^2}} + \frac{\cos\left(4\frac{\pi}{L}x\right)}{16\frac{\pi^2}{L^2}} - 2\frac{\cos\left(\frac{\pi}{L}x\right)}{\frac{\pi^2}{L^2}} + 2\frac{\cos\left(3\frac{\pi}{L}x\right)}{9\frac{\pi^2}{L^2}}\, dx \tag{8.5.16}$$

$$= \frac{L^2}{3} - \frac{L^2}{4\pi^2} - \frac{L^2}{16\pi^2} - \frac{2L^2}{\pi^2} + \frac{2L^2}{9\pi^2} \tag{8.5.17}$$

$$= L^2\left(\frac{1}{3} - \frac{301}{144\pi^2}\right) \tag{8.5.18}$$

$$\Delta x = \sqrt{\langle x^2\rangle - \langle x\rangle^2} \tag{8.5.19}$$

$$= L\sqrt{\frac{1}{3} - \frac{301}{144\pi^2} - \frac{1}{4} - \frac{256}{81\pi^4} + \frac{16}{9\pi^2}} \tag{8.5.20}$$

$$= L\sqrt{\frac{1}{12} - \frac{5}{16\pi^2} - \frac{256}{81\pi^4}} \tag{8.5.21}$$

(c) Calculate the expectation values of p and p^2 and hence the uncertainty Δp

Solution:

$$\langle p\rangle = -i\hbar \int_{\mathbb{R}} \psi(x)^* \frac{d\psi(x)}{dx}\, dx \tag{8.5.22}$$

$$= -i\hbar \int_{x\in\mathbb{R}} \psi(x) d\psi(x) \tag{8.5.23}$$

$$= \frac{-i\hbar}{2}\, \psi(x)^2\Big|_{x=-\infty}^{\infty} \tag{8.5.24}$$

$$= 0 \tag{8.5.25}$$

$$\langle p^2\rangle = -\hbar^2 \int_{\mathbb{R}} \psi(x)^* \frac{d^2\psi(x)}{dx^2}\, dx \tag{8.5.26}$$

$$= -\frac{\hbar^2}{L}\left(-\frac{\pi^2}{L^2}\int_{x=0}^{L} \sin^2\left(\frac{\pi}{L}x\right) dx - \frac{4\pi^2}{L^2}\int_{x=0}^{L} \sin^2\left(\frac{2\pi}{L}x\right) dx \right. \tag{8.5.27}$$

$$\left. - \left(\frac{\pi^2}{L^2} + \frac{4\pi^2}{L^2}\right)\int_{x=0}^{L} \sin\left(\frac{\pi}{L}x\right)\sin\left(\frac{2\pi}{L}x\right) dx\right) \tag{8.5.28}$$

$$= \frac{\hbar^2\pi^2}{L^3}\left(\frac{5L}{2} - \frac{1}{2}\int_{x=0}^{L} \cos\left(\frac{2\pi}{L}x\right) dx - 2\int_{x=0}^{L} \cos\left(\frac{4\pi}{L}x\right)\right. \tag{8.5.29}$$

$$\left. + \frac{5}{2}\int_{x=0}^{L} \cos\left(\frac{\pi}{L}x\right) - \cos\left(\frac{3\pi}{L}x\right) dx\right) \tag{8.5.30}$$

$$= \frac{5\hbar^2\pi^2}{2L^2} \tag{8.5.31}$$

$$\Delta p = \sqrt{\langle p^2\rangle - \langle p\rangle^2} \tag{8.5.32}$$

$$= \sqrt{\frac{5}{2}}\frac{\hbar\pi}{L} \tag{8.5.33}$$

(d) What is the probability of finding the particle in the first excited state, if an energy measurement is made?

Solution: As we know, the probability of finding the particle in first excited state $\psi_2(x)$ upon energy measurement is simply $|\langle\psi_2(x)|\psi(x)\rangle|^2$

$$\langle\psi_2(x)|\psi(x)\rangle = \langle\psi_2(x)|\frac{1}{\sqrt{2}}(\psi_1(x) + \psi_2(x))\rangle = \frac{1}{\sqrt{2}} \tag{8.5.34}$$

$$\implies \text{Probability} = \frac{1}{2} \tag{8.5.35}$$

8.6. Suppose we have 10000 rigid boxes of same length L from $x = 0$ to $x = L$. Each box contains one particle of mass m. All these particles are in the ground state

(a) If a measurement of position of the particle is made in all the boxes at the same time, in how many of them, the particle is expected to be found between $x = 0$ and $\frac{L}{4}$

Solution: Before measurement the wavefunction is $\psi(x) = \sqrt{\frac{2}{L}}\sin(\frac{\pi}{L})x$

$\implies$ Probability$(0 \le x \le \frac{L}{4}) = \int_{x=0}^{\frac{L}{4}} |\psi(x)|^2\,dx$

$$= \frac{2}{L}\int_{x=0}^{\frac{L}{4}} \sin^2\left(\frac{\pi}{L}x\right)\,dx \tag{8.6.1}$$

$$= \frac{1}{L}\int_{x=0}^{\frac{L}{4}} 1 - \cos\left(\frac{2\pi}{L}x\right)dx \tag{8.6.2}$$

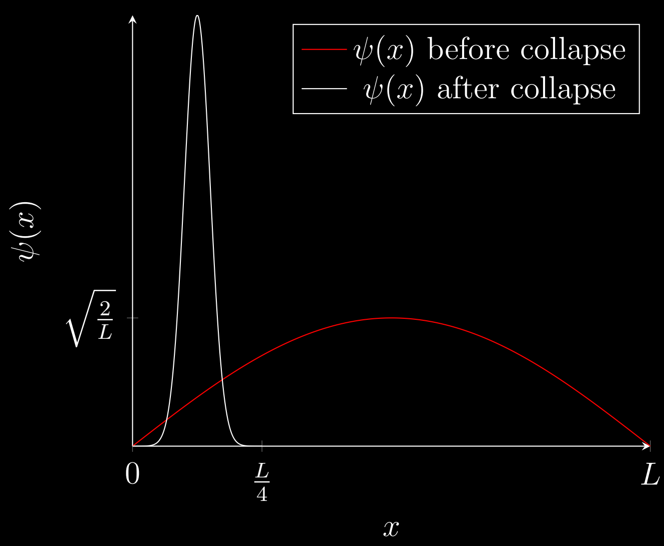
$$= \frac{1}{L}\left(\frac{L}{4} - \frac{L}{2\pi}\right) \tag{8.6.3}$$

$$= 0.091 \tag{8.6.4}$$

$$\implies N(0 \le x \le \frac{L}{4}) = 910 \tag{8.6.5}$$

(b) In a particular box, the particle was found to be between $x = 0$ and $\frac{L}{4}$. Another measurement of the position of the particle is carried out in this box immediately after the first measurement. What is the probability that the particle is again found between $x = 0$ and $\frac{L}{4}$

Solution:



As we can see, upon the first measurement the wavefunction must collapse to a function which is non zero only inside $x \in [0, \frac{L}{4}]$. Thus if we again immediately carry out a measurement, the only non zero values are inside $x \in [0, \frac{L}{4}]$. Therefore the probability for the second measurement to yield a value inside $x \in [0, \frac{L}{4}]$ is 1

8.7. An electron is bound in an infinite potential well extending from $x = 0$ to $x = L$. At time $t = 0$, its normalized wave function is given by

$$\psi(x, 0) = \frac{2}{\sqrt{L}}\sin\left(\frac{3\pi x}{2L}\right)\cos\left(\frac{\pi x}{2L}\right)$$

(a) Calculate $\psi(x, t)$ at a later time t.

Solution: First we need to decompose $\psi(x,0)$ into energy eigenstates

$$\psi(x,0) = \frac{2}{\sqrt{L}}\sin\left(\frac{3\pi x}{2L}\right)\cos\left(\frac{\pi x}{2L}\right) \tag{8.7.1}$$

$$= \frac{1}{\sqrt{L}}\left(\sin\left(\frac{\pi}{L}x\right) + \sin\left(2\frac{\pi}{L}x\right)\right) \tag{8.7.2}$$

$$= \frac{1}{\sqrt{2}}\left(\psi_1(x) + \psi_2(x)\right) \tag{8.7.3}$$

$$\implies \psi(x,t) = \frac{1}{\sqrt{2}}\left(\psi_1(x)e^{-i\frac{E_1}{\hbar}t} + \psi_2(x)e^{-i\frac{E_2}{\hbar}t}\right) \tag{8.7.4}$$

$$= \frac{1}{\sqrt{L}}\left(\sin\left(\frac{\pi}{L}x\right)e^{-i\frac{\hbar\pi^2}{2mL^2}t} + \sin\left(2\frac{\pi}{L}x\right)e^{-i\frac{2\hbar\pi^2}{mL^2}t}\right) \tag{8.7.5}$$

(b) Calculate the probability of finding the electron between $x = L/4$ and $x = L/2$ at time t.

Solution:

$$\text{Prob}\left(\frac{L}{4} < x < \frac{L}{2}\right) = \int_{x=\frac{L}{4}}^{\frac{L}{2}} \psi(x,t)^*\psi(x,t)\,dx \tag{8.7.6}$$

$$= \frac{1}{L}\int_{x=\frac{L}{4}}^{\frac{L}{2}} \sin^2\left(\frac{\pi}{L}x\right) + \sin^2\left(2\frac{\pi}{L}x\right)\,dx \tag{8.7.7}$$

$$+ \frac{1}{L}\int_{x=\frac{L}{4}}^{\frac{L}{2}} \sin\left(\frac{\pi}{L}x\right)\sin\left(2\frac{\pi}{L}x\right)\left(e^{i\frac{3\hbar\pi^2}{2mL^2}t} + e^{-i\frac{3\hbar\pi^2}{2mL^2}t}\right)\,dx \tag{8.7.8}$$

$$= \frac{\pi+2}{8\pi} + \frac{1}{8} + \frac{4-\sqrt{2}}{3\pi}\cos\left(\frac{3\hbar\pi^2}{2mL^2}t\right) \tag{8.7.9}$$

$$\tag{8.7.10}$$

8.8. A speck of dust ($m = 1\ \mu$g) is trapped to roll inside a tube of length $L = 1.0\ \mu$m. The tube is capped at both ends and the motion of the speck is considered to be along the length of the tube.

(a) Modeling this as a 1-D infinite square well, determine the value of the quantum number n if the speck has an energy of 1 μJ

Solution: Assuming the particle is in one of the energy eigenstates,

$$n^2\frac{\hbar^2\pi^2}{2mL^2} = E \tag{8.8.1}$$

$$\implies n = \frac{L}{\hbar\pi}\sqrt{2mE} \approx 4.27 \times 10^{21} \tag{8.8.2}$$

(b) What is the probability of finding this speck within 0.1 μm of the center of the tube ($0.45 < x < 0.55$)

Solution: Using (9.6.4)

$$\text{Prob}\,(a < x < a+b) = \frac{1}{2n\pi}\left(\frac{2n\pi}{L}b - \sin\left(\frac{2n\pi}{L}(a+b)\right) + \sin\left(\frac{2n\pi}{L}a\right)\right) \tag{8.8.3}$$

$$\approx \frac{1}{10} \tag{8.8.4}$$

(c) How much energy is needed to excite this speck to an energy level next to 1 μJ? Compare this excitation energy with the thermal energy at room temperature ($T = 300K$).

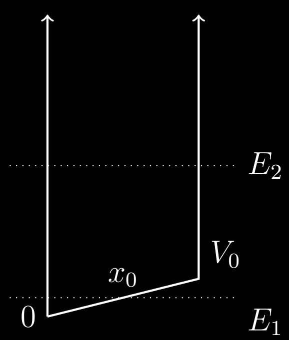
Solution:

$$\Delta E \approx 2n\frac{\hbar^2\pi^2}{2mL^2} = \frac{2E}{n} = 4.7 \times 10^{-28}\ \text{J} \tag{8.8.5}$$

Thermal energy at room temperature

$$= 1.5k_BT = 6.2 \times 10^{-21}\ \text{J} \tag{8.8.6}$$

8.9. Consider a particle bound inside an infinite well whose floor is sloping (variation is small) as shown in the figure. Without solving the Schrodinger equation (provide proper justification for your answers)



(a) Sketch a plausible wave function when the energy is E_1, assuming that it has no nodes.

Solution: We will use here what is commonly called the **WKB** approximation. We know that

$$V(x) = \begin{cases} \infty & x < 0 \\ \frac{x}{L}V_0 & 0 \le x \le L \\ \infty & x > L \end{cases} \tag{8.9.1}$$

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

$$\frac{1}{\psi(x)}\frac{d^2\psi(x)}{dx^2} = \begin{cases} -k(x)^2 & 0 < x < x_0 \\ \kappa(x)^2 & x_0 \le x < L \end{cases} \tag{8.9.2}$$

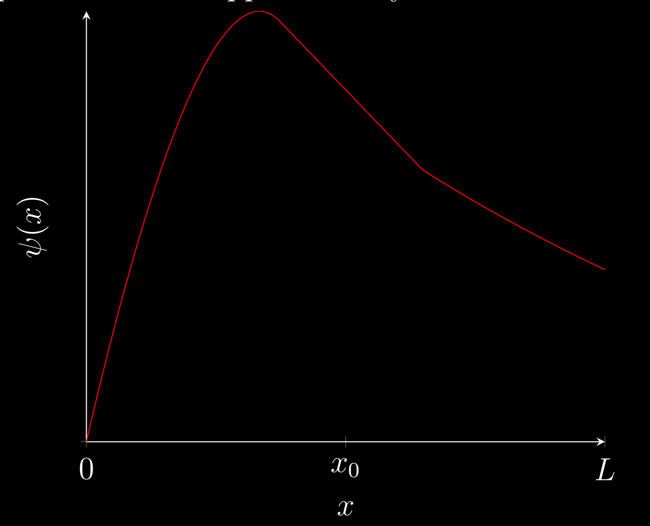
Where

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

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.

$$\implies \psi(x) \approx \begin{cases} A\sin(k(x)x) & 0 < x < x_0 - \epsilon \\ ?? & x_0 - \epsilon \leq x \leq x + \epsilon \\ Be^{-\kappa(x)x} & x_0 + \epsilon < x < L \end{cases} \tag{8.9.3}$$

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

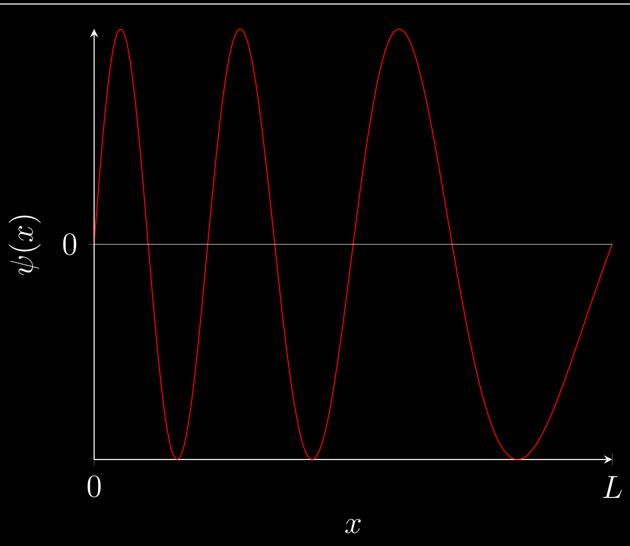


(b) Sketch the wave function with 5 nodes when the energy is E_2

Solution: Using similar logic as above, we have

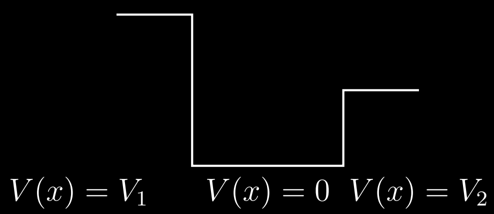
$$\psi(x) \approx A\sin(k(x)x) \qquad 0 < x < L \tag{8.9.4}$$

Since $V(x)$ is increasing as we increase x, therefore the wavelength $\frac{2\pi}{k(x)}$ will also increase as we increase x. The graph is thus approximately



9 Finite Potential Well

9.1. Consider an asymmetric finite potential well of width L, with a barrier V_1 on one side and a barrier V_2 on the other side (figure below). Obtain the energy quantization condition for the bound states in such a well. From this condition derive the energy quantization conditions for a semi-infinite potential well (when $V_1 \to \infty$ and V_2 is finite)



Solution: We can write the potential as

$$V(x) = \begin{cases} V_1 & x < 0 \\ 0 & 0 \leq x \leq L \\ V_2 & x > L \end{cases} \tag{9.1.1}$$

We are looking for a bound state, i.e. an energy eigenstate whose energy eigenvalue $E < V(\pm\infty) \implies E < V_2$ (WLOG we assume $V_2 < V_1$)

Let us first solve the TISE differential equation regionwise which we will patch together by imposing boundary conditions

$$\frac{1}{\psi(x)}\frac{d^2\psi(x)}{dx^2} = \begin{cases} \kappa_1^2 & x < 0 \\ -k^2 & 0 \leq x \leq L \\ \kappa_2 & x > L \end{cases} \tag{9.1.2}$$

$$\psi(x) = \begin{cases} 0 & x \to -\infty \\ Ae^{\kappa_1 x} + Be^{-\kappa_1 x} & x < 0 \\ C\cos(kx) + D\sin(kx) & 0 \leq x \leq L \\ Fe^{\kappa_2 x} + Ge^{-\kappa_2 x} & x > L \\ 0 & x \to \infty \end{cases} \tag{9.1.3}$$

Where

$$\kappa_1^2 = \frac{2m(V_1 - E)}{\hbar^2}$$
$$-k^2 = \frac{-2mE}{\hbar^2}$$
$$\kappa_2^2 = \frac{2m(V_2 - E)}{\hbar^2}$$

Since $\psi(x)$ cannot blow up at $\pm\infty$, $B = F = 0$
Since we want our solution to be fully real, we can safely take A, C, D, G to be real
Now to impose boundary conditions

Continuity and Differentiability at $x = 0$

$$A = C \tag{9.1.4}$$
$$A\kappa_1 = Dk \tag{9.1.5}$$

Continuity and Differentiability at $x = L$

$$C\cos(kL) + D\sin(kL) = Ge^{-\kappa_2 L} \tag{9.1.6}$$
$$-k(C\sin(kL) - D\cos(kL)) = -\kappa_2 Ge^{-\kappa_2 L} \tag{9.1.7}$$

We put the values of C and D from (9.1.4) and (9.1.5) and write $\frac{(9.1.7)}{(9.1.6)}$

$$\frac{\sin(kL) - \frac{\kappa_1}{k}\cos(kL)}{\cos(kL) + \frac{\kappa_1}{k}\sin(kL)} = \frac{\kappa_2}{k} \tag{9.1.8}$$
$$\implies \frac{\tan(kL) - \frac{\kappa_1}{k}}{1 + \frac{\kappa_1}{k}\tan(kL)} = \frac{\kappa_2}{k} \tag{9.1.9}$$
$$\implies \tan(kL) = \frac{\frac{\kappa_1}{k} + \frac{\kappa_2}{k}}{1 - \frac{\kappa_1}{k}\frac{\kappa_2}{k}} \tag{9.1.10}$$
$$\implies \tan(kL) = \tan\left(\tan^{-1}\left(\frac{\kappa_1}{k}\right) + \tan^{-1}\left(\frac{\kappa_2}{k}\right)\right) \tag{9.1.11}$$
$$\implies \tan^{-1}\left(\frac{\kappa_1}{k}\right) + \tan^{-1}\left(\frac{\kappa_2}{k}\right) = kL \pm n\pi \tag{9.1.12}$$
$$\implies \tan^{-1}\left(\sqrt{\frac{k_1^2}{k^2} - 1}\right) + \tan^{-1}\left(\sqrt{\frac{k_2^2}{k^2} - 1}\right) = kL \pm n\pi \tag{9.1.13}$$

Where

$$k_1 = \sqrt{\frac{2mV_1}{\hbar^2}} \tag{9.1.14}$$

$$k_2 = \sqrt{\frac{2mV_2}{\hbar^2}} \tag{9.1.15}$$

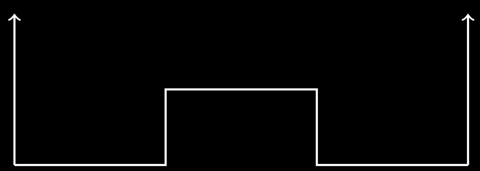
This was the quantization condition we were looking for. You can use any equation from (9.1.9)-(9.1.13) as the answer. We will solve this equation numerically to get the value of k, and hence E which are valid

To find the condition for semi-infinite well, we will use $V_1 \to \infty \implies k_1 \to \infty \implies \tan^{-1}\left(\sqrt{\frac{k_1^2}{k^2} - 1}\right) \to \frac{\pi}{2}$

$$\implies \tan^{-1}\left(\sqrt{\frac{k_2^2}{k^2} - 1}\right) = kL \pm (2n' + 1)\frac{\pi}{2} \tag{9.1.16}$$

$$\implies \sqrt{\frac{k_2^2}{k^2} - 1} = \cot(kL) \tag{9.1.17}$$

9.2. A particle of mass m is bound in a double well potential shown in the figure below. Its energy eigenstate $\psi(x)$ has energy eigenvalue $E = V_0$, where V0 is the energy of the plateau in the middle of the potential well. It is known that $\psi(x) = C$, a constant in the plateau region.



$V(x) = \infty$ $V(x) = 0$ $V(x) = V_0$ $V(x) = 0$ $V(x) = \infty$

(a) Obtain $\psi(x)$ in the regions $-2L \le x \le -L$ and $L \le x \le 2L$ and the relation between the wave number k and L

Solution: Again, we write the potential as

$$V(x) = \begin{cases} \infty & x < -2L \\ 0 & -2L \le x < -L \\ V_0 & -L \le x \le L \\ 0 & L < x \le 2L \\ \infty & x > 2L \end{cases} \tag{9.2.1}$$

Next we can solve the TISE differential equation regionwise and patch them using boundary conditions, keeping in mind that we are looking for the stationary state with energy eigenvalue $E = V_0$, if at all that exists

$$\frac{1}{\psi(x)}\frac{d^2\psi(x)}{dx^2} = \begin{cases} -k^2 & -2L \le x < -L \\ 0 & -L \le x \le L \\ -k^2 & L < x \le 2L \end{cases} \tag{9.2.2}$$

$$\implies \psi(x) = \begin{cases} 0 & x < -2L \\ A\cos(kx) + B\sin(kx) & -2L \le x < -L \\ Dx + C & -L \le x \le L \\ F\cos(kx) + G\sin(kx) & L < x \le 2L \\ 0 & x > 2L \end{cases} \tag{9.2.3}$$

Where

$$-k^2 = -\frac{2mE}{\hbar^2} \tag{9.2.4}$$

Imposing boundary conditions

Continuity at $x = -2L$

$$0 = A\cos(2kL) - B\sin(2kL) \tag{9.2.5}$$

Continuity and Differentiability at $x = -L$

$$A\cos(kL) - B\sin(kL) = -DL + C \tag{9.2.6}$$

$$k(A\sin(kL) + B\cos(kL)) = D \tag{9.2.7}$$

Continuity and Differentiability at $x = L$

$$DL + C = F\cos(kL) + G\sin(kL) \tag{9.2.8}$$

$$D = k(-F\sin(kL) + G\cos(kL)) \tag{9.2.9}$$

Continuity at $x = 2L$

$$F\cos(2kL) + G\sin(2kL) = 0 \tag{9.2.10}$$

Thus now we have 6 equations and 6 variables, with an additional normalization constraint. Thus we will get a set of k, and thus E which will satisfy these. If $E = V_0$ is not one of them, then we don't have solution with $E = V_0$ at all. And we additionally need the condition such that this wavefunction $Dx + C$ is constant in the middle region (as specified in the question). If this condition is not satisfied for $E = V_0$, then again we do not have any solution in which $\psi(x)$ is constant in the middle region. Thus $\implies D = 0$

From (9.2.5) and (9.2.10) we get

$$\tan(2kL) = \frac{A}{B} = \frac{-F}{G} \tag{9.2.11}$$

Putting in (9.2.6), (9.2.7), (9.2.8), (9.2.9),

$$B\sin(kL) = C\cos(2kL) \tag{9.2.12}$$
$$B\cos(kL) = 0 \tag{9.2.13}$$
$$C\cos(2kL) = -G\sin(kL) \tag{9.2.14}$$
$$0 = G\cos(kL) \tag{9.2.15}$$

Thus we get $\cos(kL) = 0 \implies \boxed{kL = \frac{(2n+1)\pi}{2}}$. This was the condition we were looking for. This also makes total sense if we look at the problem physically
We also get $\tan(2kL) = 0 \implies A = F = 0$, and $-B = G = (-1)^n C$
Thus our wavefunction becomes

$$\psi(x) = \begin{cases} 0 & x < -2L \\ (-1)^{n+1} C\sin\left(\frac{(2n+1)}{2}\pi\frac{x}{L}\right) & -2L \le x < -L \\ C & -L \le x \le L \\ (-1)^n C\sin\left(\frac{(2n+1)}{2}\pi\frac{x}{L}\right) & L < x \le 2L \\ 0 & x > 2L \end{cases} \tag{9.2.16}$$

Since the boundary conditions are satisfied fully, the necessary and sufficient condition for such a solution to exist is $\frac{\sqrt{2mV_0}}{\hbar}L = \frac{(2n+1)\pi}{2}$

(b) Determine C in terms of L

Solution: To find $\psi(x)$ fully we must also impose the normalization condition

$$2C^2\int_{x=L}^{2L}\sin^2\left(\frac{2n+1}{2}\pi\frac{x}{L}\right)dx + 2C^2L = 1 \tag{9.2.17}$$
$$\implies 3C^2L = 1 \tag{9.2.18}$$
$$\implies C = \sqrt{\frac{1}{3L}} \tag{9.2.19}$$

$$\implies \psi(x) = \begin{cases} 0 & x < -2L \\ -(-1)^n\sqrt{\frac{1}{3L}}\sin\left(\frac{(2n+1)}{2}\pi\frac{x}{L}\right) & -2L \le x < -L \\ \sqrt{\frac{1}{3L}} & -L \le x \le L \\ (-1)^n\sqrt{\frac{1}{3L}}\sin\left(\frac{(2n+1)}{2}\pi\frac{x}{L}\right) & L < x \le 2L \\ 0 & x > 2L \end{cases} \tag{9.2.20}$$

(c) Assume the bound particle to be an electron and $L = 1$ Å. Calculate the two lowest values of V_0 (in eV) for which such a solution exists.

Solution: As solved above, the necessary and sufficient condition for such a solution to exist is $\frac{\sqrt{2mV_0}}{\hbar}L = \frac{(2n+1)\pi}{2}$

$$\implies V_0 = \frac{(2n+1)^2\pi^2\hbar^2}{8mL^2} \tag{9.2.21}$$

Thus the two lowest values of V_0 are obtained by putting $n = 0$ and $n = 1$, giving us $V_0 = 9.34$ eV, $V_0 = 84$ eV

(d) For the smallest allowed k, calculate the expectation values for x, x^2, p, p^2 and show that the uncertainty principle is obeyed.

Solution: The smallest allowed value of k is for $n = 0$

$$\implies \psi(x) = \begin{cases} 0 & x < -2L \\ -\sqrt{\frac{1}{3L}}\sin\left(\frac{\pi}{2}\frac{x}{L}\right) & -2L \le x < -L \\ \sqrt{\frac{1}{3L}} & -L \le x \le L \\ \sqrt{\frac{1}{3L}}\sin\left(\frac{\pi}{2}\frac{x}{L}\right) & L < x \le 2L \\ 0 & x > 2L \end{cases} \tag{9.2.22}$$

$$\langle x\rangle = \int_{x=-2L}^{x=-L} \frac{1}{3L} x \sin^2\left(\frac{\pi x}{2L}\right) dx + \int_{x=L}^{x=2L} \frac{1}{3L} x \sin^2\left(\frac{\pi x}{2L}\right) dx + \int_{x=-L}^{x=L} \frac{1}{3L} x \, dx \tag{9.2.23}$$

$$= 0 \tag{9.2.24}$$

$$\langle x^2\rangle = \int_{x=-2L}^{x=-L} \frac{1}{3L} x^2 \sin^2\left(\frac{\pi x}{2L}\right) dx + \int_{x=L}^{x=2L} \frac{1}{3L} x^2 \sin^2\left(\frac{\pi x}{2L}\right) dx + \int_{x=-L}^{x=L} \frac{1}{3L} x^2 \, dx \tag{9.2.25}$$

$$= \frac{2}{3L}\left(\int_{x=L}^{x=2L} x^2 \sin^2\left(\frac{\pi x}{2L}\right) dx + \int_{x=0}^{x=L} x^2 \, dx\right) \tag{9.2.26}$$

$$= 2L^2\left(\frac{1}{2} - \frac{1}{\pi^2}\right) \tag{9.2.27}$$

$$\langle p\rangle = \int_{x=-2L}^{x=-L} \frac{-i\pi\hbar}{6L^2} \sin\left(\frac{\pi x}{2L}\right) \cos\left(\frac{\pi x}{2L}\right) dx + \int_{x=L}^{x=2L} \frac{-i\pi\hbar}{6L^2} \sin\left(\frac{\pi x}{2L}\right) \cos\left(\frac{\pi x}{2L}\right) dx \tag{9.2.28}$$

$$= 0 \tag{9.2.29}$$

$$\langle p^2\rangle = \int_{x=-2L}^{x=-L} \frac{\pi^2\hbar^2}{12L^3} \sin^2\left(\frac{\pi x}{2L}\right) dx + \int_{x=L}^{x=2L} \frac{\pi^2\hbar^2}{12L^3} \sin^2\left(\frac{\pi x}{2L}\right) dx \tag{9.2.30}$$

$$= \frac{\pi^2\hbar^2}{6L^3} \int_{x=L}^{x=2L} \sin^2\left(\frac{\pi x}{2L}\right) dx \tag{9.2.31}$$

$$= \frac{\pi^2\hbar^2}{12L^2} \tag{9.2.32}$$

$$\implies \Delta x \Delta p = \sqrt{\langle x^2\rangle\langle p^2\rangle} \tag{9.2.33}$$

$$= \sqrt{\frac{\pi^2}{12} - \frac{1}{6}}\hbar = 0.81\hbar > 0.5\hbar \tag{9.2.34}$$

9.3. You are given an arbitrary potential $V(x)$ and the corresponding orthogonal and normalized bound-state solutions to the time independent Schrodinger's equation $\psi_n(x)$, with the corresponding energy eigenvalues E_n. At time t = 0, the system is in the state, $\psi(x,0) = A(\psi_1(x) + \psi_2(x) + \psi_4(x))$

(a) Find the value of A

Solution: We start with normalization of ψ at $t = 0$

$$\langle\psi|\psi\rangle = 1 \tag{9.3.1}$$

$$\implies 3|A|^2 = 1 \tag{9.3.2}$$

$$\implies A = \frac{1}{\sqrt{3}} \tag{9.3.3}$$

(In general $A = \frac{e^{i\theta}}{\sqrt{3}}$ but we will force our stationary states to be real, which we can always do)

(b) What is the wave function at time $t > 0$

Solution: We already have our decomposition of ψ into energy eigenstates, hence time evolution is trivial

$$\psi(x,t) = \frac{1}{\sqrt{3}}(\psi_1(x)e^{-i\frac{E_1}{\hbar}t} + \psi_2(x)e^{-i\frac{E_2}{\hbar}t} + \psi_4(x)e^{-i\frac{E_4}{\hbar}t}) \tag{9.3.4}$$

(c) What is the expectation value of the energy at time $t > 0$

Solution:

$$\langle E\rangle = \langle \psi(x,t)|H\psi(x,t)\rangle \tag{9.3.5}$$

$$= \frac{E_1 + E_2 + E_4}{3} \tag{9.3.6}$$

9.4. A finite square well (height = 30 eV, width = $2a$, from $-a$ to a), has six bound states 3, 7, 12, 17, 21, and 24 eV. If instead, the potential is semi infinite, with an infnite wall at x = 0, how many bound states will exist and what are the energies associated with it? Justify your answer

Solution: For the finite well the potential is

$$V_1(x) = \begin{cases} V_0 & x < -a \\ 0 & -a \leq x \leq a \\ V_0 & x > a \end{cases} \tag{9.4.1}$$

For the semi infinite well the potential is

$$V_2(x) = \begin{cases} \infty & x < 0 \\ 0 & 0 \leq x \leq a \\ V_0 & x > a \end{cases} \tag{9.4.2}$$

where $V_0 = 30$ eV
Now we can see that for $x > 0$, $V_1(x) = V_2(x)$. We also know that $\psi^{(2)}(x) = 0$ for $x < 0$, where $\psi^{(2)}(x)$ is any stationary state for $V_2(x)$. Therefore any stationary state $\psi^{(1)}(x)$ for the finite well should also match a stationary state $\psi^{(2)}(x)$ for $x \geq 0$, as long as $\psi^{(1)}(0) = 0$, since the differential equation for both $V_1(x)$ and $V_2(x)$ are same for the region $x > 0$. We know that $\psi^{(1)}(x) = 0$ for the odd states, which will thus have energies 7, 17, 24 eV. Thus those are the energies for $V_2(x)$ as well, and thus the semi infinite well will have 3 bound states

9.5. A particle with energy E is bound in a finite square well potential with height U and width $2L$ (from $-L$ to L)

(a) If E < U, obtain the energy quantization condition for the symmetric wave functions in terms of k and α, where $k = \frac{\sqrt{2mE}}{\hbar}$ and $\alpha = \frac{\sqrt{2m(U-E)}}{\hbar}$

Solution: We can write the potential as

$$V(x) = \begin{cases} U & x < -L \\ 0 & -L \leq x \leq L \\ U & x > L \end{cases} \tag{9.5.1}$$

We are looking for a bound state, i.e. an energy eigenstate whose energy eigenvalue $E < V(\pm\infty) \implies E < U$

Let us first solve the TISE differential equation regionwise which we will patch together by imposing boundary conditions

$$\frac{1}{\psi(x)}\frac{d^2\psi(x)}{dx^2} = \begin{cases} \alpha^2 & x < -L \\ -k^2 & -L \leq x \leq L \\ \alpha_2 & x > L \end{cases} \tag{9.5.2}$$

$$\psi(x) = \begin{cases} 0 & x \to -\infty \\ Ae^{\alpha x} + Be^{-\alpha x} & x < -L \\ C\cos(kx) + D\sin(kx) & -L \leq x \leq L \\ Fe^{\alpha x} + Ge^{-\alpha x} & x > L \\ 0 & x \to \infty \end{cases} \tag{9.5.3}$$

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 $x = -L$

$$Ae^{-\alpha L} = C\cos(kL) \tag{9.5.4}$$

$$\alpha Ae^{-\alpha L} = kC\sin(kL) \tag{9.5.5}$$

Continuity and Differentiability at $x = L$

$$C\cos(kL) = Ae^{-\alpha L} \tag{9.5.6}$$

$$kC\sin(kL) = \alpha Ae^{-\alpha L} \tag{9.5.7}$$

We have two redundant equations, so the assumption of symmetric solution was consistent

Let us write $\frac{(9.5.5)}{(9.5.4)}$

$$\tan kL = \frac{\alpha}{k} \tag{9.5.8}$$

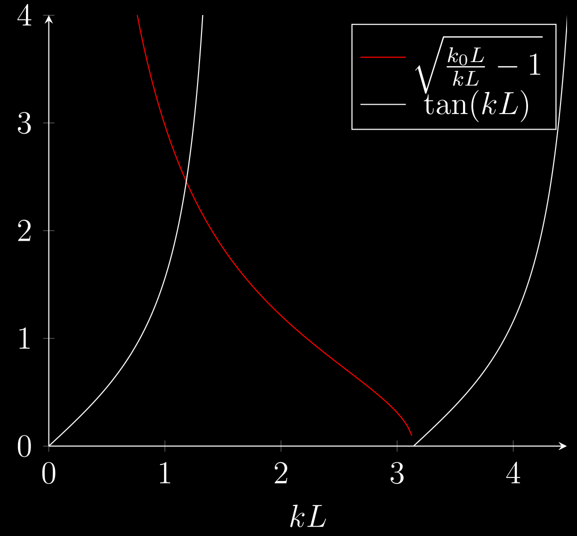
Thus this is the quantization condition we were looking for

(b) Apply this result to an electron trapped inside a defect site in a crystal. Modeling this defect as a finite square well potential with height 5 eV and width 200 pm, calculate the ground state energy

Solution: 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 $k_0 = \frac{\sqrt{2mU}}{\hbar}$, 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 $kL = 1.081 \implies E = \frac{\hbar^2(kL)^2}{2mL^2} = 1.1$ eV

(c) Calculate the total number of bound states with symmetric wave-function

Solution:



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 $\lceil \frac{k_0L}{\pi} \rceil = \lceil \frac{\sqrt{2mU}L}{\hbar\pi} \rceil$

9.6. A potential $V(x)$ is defined over a region R, which consists of two sub regions R_1 and R_2 ($R = R_1 \bigcup R_2$). This potential has two normalized energy eigenfunctions $\Psi_1(x)$ and $\Psi_2(x)$ with energy eigenvalues E_1 and E_2 ($E_1 \neq E_2$), respectively. $\psi_1(x) = 0$ outside region R_1 and $\psi_2(x) = 0$ outside region R_2

(a) Suppose the regions R_1 and R_2 do not overlap, show that the particle will stay there forever, if it is in the region R_1

Solution: The wavefunction $\Psi(x, 0)$ for the particle at $t = 0$ can be written as

$$\Psi(x, 0) = a\Psi_1(x) + b\Psi_2(x) \tag{9.6.1}$$

Since the particle is in region R_1 at $t = 0$, $\Psi(x, 0) = 0 \ \forall x \in R_2$
Since $R_1 \bigcap R_2 = \phi \implies b = 0$, $a = 1$
Thus the wavefunction evolved to some time t is

$$\Psi(x, t) = \Psi_1(x)e^{-i\frac{E_1}{\hbar}t} \tag{9.6.2}$$

which is again $= 0$ in region R_2

(b) If the initial state is $\Psi(x,0) = \frac{1}{\sqrt{2}}(\Psi_1(x) + \Psi_2(x))$, show that the probability density $|\Psi(x,t)|^2$ is independant of time

Solution:

$$\Psi(x,t) = \frac{1}{\sqrt{2}}(\Psi_1(x)e^{-i\frac{E_1}{\hbar}t} + \Psi_2(x)e^{-i\frac{E_2}{\hbar}t}) \tag{9.6.3}$$

$$\begin{aligned}\implies |\Psi(x,t)|^2 = \Psi(x,t)^*\Psi(x,t) &= \frac{1}{2}\left(|\Psi_1(x)|^2 + |\Psi(x)|^2\right.\\ &\left.+ \Psi_1(x)^*\Psi_2(x)e^{i\frac{E_1-E_2}{\hbar}t} + \Psi_2(x)^*\Psi_1(x)e^{i\frac{E_2-E_1}{\hbar}t}\right)\end{aligned} \tag{9.6.4}$$

$$= \frac{1}{2}\left(|\Psi_1(x)|^2 + |\Psi(x)|^2\right) \tag{9.6.5}$$

$\because R_1 \bigcap R_2 = \phi$, $\Psi_1(x)^*\Psi_2(x) = \Psi_1(x)\Psi_2(x)^* = 0$

$$\implies \frac{d|\Psi(x,t)|^2}{dt} = 0 \tag{9.6.6}$$

(c) If the regions R_1 and R_2 overlap, show that the probability density $|\Psi(x,t)|^2$ oscillate in time for the initial state given in (b)

Solution: From (9.6.4)

$$|\psi(x,t)|^2 = \frac{1}{2}\left(|\Psi_1(x)|^2 + |\Psi(x)|^2 + \mathrm{Re}\left[\Psi_1(x)^*\Psi_2(x)e^{i\frac{E_1-E_2}{\hbar}t}\right]\right) \tag{9.6.7}$$

$$\begin{aligned}&= \frac{1}{2}\left(|\Psi_1(x)|^2 + |\Psi(x)|^2\right.\\ &\left.+ \mathrm{Re}\left[\Psi_1(x)^*\Psi_2(x)\right]\cos\left(\frac{E_1-E_2}{\hbar}t\right) - \mathrm{Im}\left[\Psi_1(x)^*\Psi_2(x)\right]\sin\left(\frac{E_1-E_2}{\hbar}t\right)\right)\end{aligned} \tag{9.6.8}$$

10 Step Potential

10.1. A potential barrier is defined by $V = 0$ for $x < 0$ and $V = V_0$ for $x > 0$. Particles with energy $E < V_0$ approaches the barrier from the left

(a) Find the value of $x = x_0$ $(x_0 > 0)$, for which the probability density is $\frac{1}{e}$ times the probability density at $x = 0$.

Solution: The step potential can be written like

$$V(x) = \begin{cases} 0 & x < 0 \\ V_0 & x \geq 0 \end{cases} \tag{10.1.1}$$

Thus we can write the TISE for energy eigenvalue $E < V_0$ as

$$\frac{1}{\psi(x)}\frac{d^2\psi(x)}{dx^2} = \begin{cases} -k^2 & x < 0 \\ \kappa^2 & x \geq 0 \end{cases} \tag{10.1.2}$$

$$\implies \psi(x) = \begin{cases} Ae^{ikx} + Be^{-ikx} & x < 0 \\ Ce^{\kappa x} + De^{-\kappa x} & x \geq 0 \end{cases} \tag{10.1.3}$$

Where

$$-k^2 = -\frac{2mE}{\hbar^2} \tag{10.1.4}$$

$$\kappa^2 = \frac{2m(V_0 - E)}{\hbar^2} \tag{10.1.5}$$

We must have $C = 0$ such that $\psi(x)$ does not blow up at infinity.
We could impose the boundary conditions at this point but that would not lead to anything useful or relevant to the question itself. We finally want the probability density at $x \geq 0$

$$\implies \text{ProbDens}(x) = \psi(x)^*\psi(x) \tag{10.1.6}$$

$$= |C|^2 e^{-2\kappa x} \tag{10.1.7}$$

$$\text{We want } \frac{\text{ProbDens}(x_0)}{\text{ProbDens}(0)} = \frac{1}{e} \tag{10.1.8}$$

$$\implies e^{-2\kappa x_0} = \frac{1}{e} \tag{10.1.9}$$

$$\implies x_0 = \frac{1}{2\kappa} = \boxed{\frac{\hbar}{\sqrt{8m(V_0 - E)}}} \tag{10.1.10}$$

(b) Take the maximum allowed uncertainty Δx for the particle to be localized in the classically forbidden region as x_0. Find the uncertainty this would cause in the energy of the particle. Can then one be sure that its energy E is less than V_0?

Solution: We want to analyse what happens to the wavefunction, and hence the particle if it was originally in the energy eigenstate with eigenvalue $E < V_0$, and a position observation leads us to find the position result as $x > 0$
Of course our position detector will not be perfect, and won't perform a perfect position measurement.
Hence after the measurement the wavefunction will collapse to a state **close to** the position eigenstate (a delta function), i.e. it will collapse to a gaussian packet instead, one with $\sigma_x = \Delta x = x_0$. Thus is an assumption of the physical imperfection of our detector
This collapsed wavefunction is **no longer** an energy eigenstate, hence it does **not** have any energy eigenvalue, and the expectation of energy is certainly **not** $E < V_0$

Instead this collapsed wavefunction will be composed of a spread in energies, with

$$\Delta E = \sqrt{\langle E^2 \rangle - \langle E \rangle^2} \tag{10.1.11}$$
$$\sim \frac{\Delta p^2}{2m} = \frac{\hbar^2}{8m^2 \Delta x^2} \tag{10.1.12}$$
$$= V_0 - E \tag{10.1.13}$$

Therefore the energy has enough spread such that it takes up the expectation of energy well above V_0

10.2. A potential barrier is defined by $V = 0$ eV for $x < 0$ and $V = 7$ eV for $x > 0$. . A beam of electrons with energy 3 eV collides with this barrier from left. Find the value of x for which the probability of detecting the electron will be half the probability of detecting it at $x = 0$.

Solution: This is the same as the setup of Q10.1, where $V_0 = 7$ eV, $E = 3$ eV
Using the same formulation as above,

$$\text{We want } x_0 \text{ such that } \frac{\text{ProbDens}(x_0)}{\text{ProbDens}(0)} = \frac{1}{2} \tag{10.2.1}$$
$$\implies e^{-2\kappa x_0} = \frac{1}{2} \tag{10.2.2}$$
$$\implies x_0 = \frac{\log 2}{2\kappa} = \frac{\hbar \log 2}{\sqrt{8m(V_0 - E)}} \tag{10.2.3}$$
$$= 0.33 \text{ Å} \tag{10.2.4}$$

10.3. A beam of particles of energy E and de Broglie wavelength λ, traveling along the positive x-axis in a potential free region, encounters a one-dimensional potential barrier of height $V = E$ and width L.

(a) Obtain an expression for the transmission coefficient.

Solution: We have the potential function

$$V(x) = \begin{cases} 0 & x < 0 \\ E & 0 \leq x < L \\ 0 & x \geq L \end{cases} \tag{10.3.1}$$

Thus we can write the TISE for the energy eigenstate with eigenvalue E as

$$\frac{1}{\psi(x)}\frac{d^2\psi(x)}{dx^2} = \begin{cases} -k^2 & x < 0 \\ 0 & 0 \leq x < L \\ -k^2 & x \geq L \end{cases} \tag{10.3.2}$$

$$\implies \psi(x) = \begin{cases} Ae^{-ikx} + Be^{ikx} & x < 0 \\ Cx + D & 0 \leq x < L \\ Fe^{-ikx} + Ge^{ikx} & x \geq L \end{cases} \tag{10.3.3}$$

Where

$$-k^2 = -\frac{2mE}{\hbar^2} \tag{10.3.4}$$

We want to analyse the case where the particle is coming in from $x < 0$ and getting reflected and transmitted. Hence $F = 0$.
Imposing the boundary conditions,

Continuity and Differentiability at $x = 0$

$$A + B = D \tag{10.3.5}$$

$$ik(-A + B) = C \tag{10.3.6}$$

Continuity and Differentiability at $x = L$

$$CL + D = Ge^{ikL} \tag{10.3.7}$$

$$C = ikGe^{ikL} \tag{10.3.8}$$

From (10.3.7) and (10.3.8)

$$D = Ge^{ikL}(1 - ikL) \tag{10.3.9}$$

Putting C and D from (10.3.8) and (10.3.9) into (10.3.5) and (10.3.6)

$$A + B = Ge^{ikL}(1 - ikL) \tag{10.3.10}$$

$$-A + B = Ge^{ikL} \tag{10.3.11}$$

$$\implies B = G(1 - \frac{ikL}{2}) \tag{10.3.12}$$

We know that the transmission coefficient $T = \frac{|G|^2}{|B|^2}$

$$\implies T = \frac{1}{1 + \frac{k^2L^2}{4}} \tag{10.3.13}$$

$$= \frac{1}{1 + \frac{mEL^2}{2\hbar^2}} \tag{10.3.14}$$

(b) Find the value of L (in terms of λ) for which the reflection coefficient will be half.

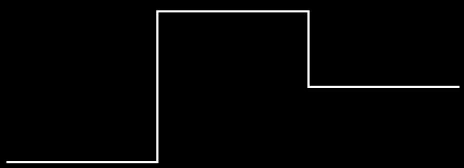
Solution: We know that if $R = \frac{1}{2} \implies T = \frac{1}{2}$
Using the result (10.3.13),

$$\implies \frac{1}{1 + \frac{k^2L^2}{4}} = \frac{1}{2} \tag{10.3.15}$$

$$\implies kL = 4 \tag{10.3.16}$$

$$\implies L = \frac{2\lambda}{\pi} \tag{10.3.17}$$

10.4. A beam of particles of energy $E < V_0$ is incident on a barrier (see figure below) of height $2V_0$. It is claimed that the solution is $\psi_I = Ae^{-k_1x}$ for region I ($0 < x < L$) and $\psi_{II} = Be^{-k_2x}$ for region II ($x > L$), where $k_1 = \sqrt{\frac{2m(2V_0-E)}{\hbar^2}}$ and $k_2 = \sqrt{\frac{2m(V_0-E)}{\hbar^2}}$. Is this claim correct? Justify your answer.



$V(x) = 0$ $V(x) = 2V_0$ $V(x) = V_0$

Solution: If we apply boundary conditions to the purported solution, we will get

Continuity and Differentiability at $x = L$

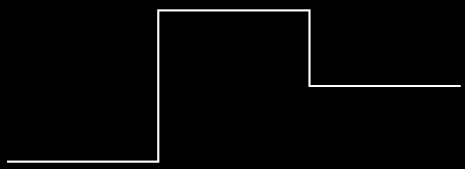
$$Ae^{-ik_1L} = Be^{-ik_2L}Ak_1e^{-ik_1L} \qquad = Bk_2e^{-ik_2L} \tag{10.4.1}$$

$$\implies k_1 = k_2 \tag{10.4.2}$$

$$\implies V_0 = 0 \tag{10.4.3}$$

Thus the only possibility is if both the regions have same potential height, which is not what happens. Hence the claim is incorrect

10.5. A beam of particles of mass m and energy $9V_0$ (V_0 is a positive constant with the dimension of energy) is incident from left on a barrier, as shown in figure below. $V = 0$ for $x < 0$, $V = 5V_0$ for $x \leq d$ and $V = nV_0$ for $x > d$. Here n is a number, positive or negative and $d = \frac{\pi\hbar}{\sqrt{8mV_0}}$. It is found that the transmission coefficient from $x < 0$ region to $x > d$ region is 0.75.



$V(x) = 0$ $V(x) = 5V_0$ $V(x) = nV_0$

(a) Find n. Are there more than one possible values for n?

Solution: We have the potential function

$$V(x) = \begin{cases} 0 & x < 0 \\ 5V_0 & 0 \leq x < d \\ nV_0 & x \geq d \end{cases} \tag{10.5.1}$$

Thus we can write the TISE for the energy eigenstate with eigenvalue $9V_0$ as

$$\frac{1}{\psi(x)}\frac{d^2\psi(x)}{dx^2} = \begin{cases} -k_1^2 & x < 0 \\ -k_2^2 & 0 \leq x < d \\ -k_3^2 & x \geq d \end{cases} \tag{10.5.2}$$

$$\implies \psi(x) = \begin{cases} Ae^{-ik_1x} + Be^{ik_1x} & x < 0 \\ Ce^{-ik_2x} + De^{ik_2x} & 0 \leq x < d \\ Fe^{-ik_3x} + Ge^{ik_3x} & x \geq d \end{cases} \tag{10.5.3}$$

Where

$$-k_1^2 = -\frac{18mV_0}{\hbar^2} \tag{10.5.4}$$

$$-k_2^2 = -\frac{8mV_0}{\hbar^2} \tag{10.5.5}$$

$$-k_3^2 = -\frac{2mV_0(9-n)}{\hbar^2} \tag{10.5.6}$$

Now according to the ansatz of the question, $F = 0$
First we take note that $k_2d = \pi \implies e^{ik_2d} = -1$.
Let us impose boundary conditions

Continuity and Differentiability at $x = 0$

$$A + B = C + D \tag{10.5.7}$$

$$k_1(-A + B) = k_2(-C + D) \tag{10.5.8}$$

Continuity and Differentiability at $x = d$

$$-(C + D) = Ge^{ik_3d} \qquad \text{(Using } e^{ik_2d} = -1) \tag{10.5.9}$$

$$-k_2(-C + D) = k_3Ge^{ik_3d} \tag{10.5.10}$$

Due to the fact that $k_2 d$ being a multiple of π has significantly reduced the calculation effort for us. We now directly get

$$A + B = -Ge^{ik_3 d} \tag{10.5.11}$$

$$-A + B = -\frac{k_3}{k_1} Ge^{ik_3 d} \tag{10.5.12}$$

$$\implies B = -\frac{k_1 + k_3}{2k_1} Ge^{ik_3 d} \tag{10.5.13}$$

We know that that $T = \frac{k_3 |G|^2}{k_1 |B|^2} = 0.75$

$$\implies T = \frac{4k_3 k_1}{(k_1 + k_3)^2} = 0.75 \tag{10.5.14}$$

$$\implies \frac{16\frac{k_3}{k_1}}{\left(1 + \frac{k_3}{k_1}\right)^2} = 3 \tag{10.5.15}$$

$$\implies 3\left(\frac{k_3}{k_1}\right)^2 - 10\frac{k_3}{k_1} + 3 = 0 \tag{10.5.16}$$

$$\implies \frac{k_3}{k_1} = 3 \text{ or } \frac{k_3}{k_1} = \frac{1}{3} \tag{10.5.17}$$

Putting in the values of k_1 and k_3

$$\implies \frac{9}{9 - n} = 9 \text{ or } \frac{9}{9 - n} = \frac{1}{9} \tag{10.5.18}$$

$$\implies \boxed{n = 8} \text{ or } \boxed{n = -72} \tag{10.5.19}$$

(b) Find the un-normalized wave function in all the regions in terms of the amplitude of the incident wave for each possible value of n.

Solution: Solving for A, B, C, D using the boundary condition equations,

$$B = -\frac{k_1 + k_3}{2k_1} Ge^{ik_3 d} \tag{10.5.20}$$

$$A = -\frac{k_1 - k_3}{2k_1} Ge^{ik_3 d} \tag{10.5.21}$$

$$D = -\frac{k_2 + k_3}{2k_2} Ge^{ik_3 d} \tag{10.5.22}$$

$$C = -\frac{k_2 - k_3}{2k_2} Ge^{ik_3 d} \tag{10.5.23}$$

For $n = 8$, $k_3 d = \frac{\pi}{2} \implies e^{ik_3 d} = i$
For $n = -72$, $k_3 d = \frac{9\pi}{2} \implies e^{ik_3 d} = i$.

Thus for both values of n, $e^{ik_3 d} = i$. Thus the above equations become

$$G = i\frac{2k_1}{k_1 + k_3}B \tag{10.5.24}$$

$$A = \frac{k_1 - k_3}{k_1 + k_3}B \tag{10.5.25}$$

$$D = \frac{k_1(k_2 + k_3)}{k_2(k_1 + k_3)}B \tag{10.5.26}$$

$$C = \frac{k_1(k_2 - k_3)}{k_2(k_1 + k_3)}B \tag{10.5.27}$$

Since we cannot normalize our wavefunction, and it can be scaled by any constant, we can set $B = 1$ WLOG

Thus our wavefunction becomes

$$\psi(x) = \begin{cases} e^{ik_1 x} + \frac{k_1 - k_3}{k_1 + k_3}e^{-ik_1 x} & x < 0 \\ \frac{k_1(k_2+k_3)}{k_2(k_1+k_3)}e^{ik_2 x} + \frac{k_1(k_2-k_3)}{k_2(k_1+k_3)}e^{-ik_2 x} & 0 \le x < d \\ -\frac{2k_1}{k_1+k_3}e^{ik_3(x-d)} & x \ge d \end{cases} \tag{10.5.28}$$

(c) Is there a phase change between the incident and the reflected beam at $x = 0$? If yes, determine the phase change for each possible value of n. Give your answers by explaining all the steps and clearly writing the boundary conditions used

Solution: As we can see, for $n = 8$, $k_1 > k_3$, hence A has the same sign as B. Therefore no phase change

If $n = -72$, $k_1 < k_3$, hence A has the opposite sign as B, therefore there is a phase change of π rad.

10.6. A monoenergetic parallel beam of non-relativistic neutrons of energy E is incident on an infinite metal surface. Within the metal, the neutrons experience a uniform negative potential V . The incident beam makes an angle θ with respect to the surface normal. Find the fraction of the incident beam that is reflected.

Solution: Let us assume that the x-axis perpendicular to the metal surface, and y-axis along the metal surface.

Our potential looks like

$$V(x, y) = \begin{cases} 0 & x < 0, \forall y \in \mathbb{R} \\ -V & x \ge 0, \forall y \in \mathbb{R} \end{cases} \tag{10.6.1}$$

We can write the TISE for an energy eigenstate with eigenvalue E as

$$\frac{1}{\psi(x, y)}\nabla^2\psi(x, y) = \begin{cases} -\frac{2mE}{\hbar^2} & x < 0, \forall y \in \mathbb{R} \\ -\frac{2m(E+V)}{\hbar^2} & x \ge 0, \forall y \in \mathbb{R} \end{cases} \tag{10.6.2}$$

Assuming an ansatz where there is an incident and reflected part, and a transmitted part, we know that the solution to this is

$$\psi(x,y) = \begin{cases} Ae^{ik_{1x}x+ik_{1y}y} + Be^{-ik_{1x}x+ik_{1y}y} & x<0,\ \forall y \in \mathbb{R} \\ Ce^{ik_{2x}x+ik_{2y}y} & x \geq 0,\ \forall y \in \mathbb{R} \end{cases} \tag{10.6.3}$$

Where

$$k_{1x}^2 + k_{1y}^2 = \frac{2mE}{\hbar^2} \tag{10.6.4}$$

$$k_{2x}^2 + k_{2y}^2 = \frac{2m(E+V)}{\hbar^2} \tag{10.6.5}$$

According to the ansatz of our question, $\frac{k_{1y}}{k_{1x}} = \tan\theta$, as $k_{1x}\,\hat{\imath} + k_{1y}\,\hat{\jmath}$ is the direction the incident wave travels in region $x<0$, i.e. outside the metal
Imposing boundary conditions

Continuity at $x=0$

$$(A+B)e^{ik_{1y}y} = Ce^{ik_{2y}y} \qquad \forall y \in \mathbb{R} \tag{10.6.6}$$

Continuity of $\nabla\psi(x,y)$ at $x=0$

$$k_{1x}(A-B)e^{ik_{1y}y}\,\hat{\imath} + k_{1y}(A+B)e^{ik_{1y}y}\,\hat{\jmath} = k_{2x}Ce^{ik_{2y}y}\,\hat{\imath} + k_{2y}Ce^{ik_{2y}y}\,\hat{\jmath} \qquad \forall y \in \mathbb{R} \tag{10.6.7}$$

The only way for (10.6.6) to be true $\forall y \in \mathbb{R}$ is if $k_{1y} = k_{2y}$ and $A+B=C$
Putting this in (10.6.7) gives us

$$k_{1x}(A-B) = k_{2x}C \tag{10.6.8}$$

$$\implies A = \frac{k_{1x}+k_{2x}}{2k_{1x}}C \tag{10.6.9}$$

$$B = \frac{k_{1x}-k_{2x}}{2k_{1x}}C \tag{10.6.10}$$

Thus the fraction that gets reflected is $R = \frac{|B|^2}{|A|^2}$.
Since we know that $\frac{k_{1y}}{k_{1x}} = \tan\theta$, we know that $k_{1x} = \frac{\sqrt{2mE}}{\hbar^2}\cos\theta$, $k_{1y} = \frac{\sqrt{2mE}}{\hbar^2}\sin\theta$
We also know that $k_{2y} = k_{1y} = \frac{\sqrt{2mE}}{\hbar^2}\sin\theta$
Thus we can see that $k_{2x} = \frac{\sqrt{2m(E\cos^2\theta+V)}}{\hbar}$
Putting all of this in R, we get

$$R = \frac{|B|^2}{|A|^2} = \frac{(k_{1x}-k_{2x})^2}{(k_{1x}+k_{2x})^2} \tag{10.6.11}$$

$$= \frac{(\sqrt{E}\cos\theta - \sqrt{E\cos^2\theta+V})^2}{(\sqrt{E}\cos\theta + \sqrt{E\cos^2\theta+V})^2} \tag{10.6.12}$$

10.7. A scanning tunneling microscope (STM) can be approximated as an electron tunneling into a step potential [$V(x) = 0$ for $x \leq 0$, $V(x) = V_0$ for $x > 0$]. The tunneling current (or probability) in an STM reduces exponentially as a function of the distance from the sample. Considering only a single electron-electron interaction, an applied voltage of 5 V and the sample work function of 7 eV, calculate the amplification in the tunneling current if the separation is reduced from 2 atoms to 1 atom thickness (take approximate size of an atom to be 3 Å)

Solution:

$$V(x) = \begin{cases} 0 & x \geq 0 \\ V_0 & x > 0 \end{cases} \tag{10.7.1}$$

We can write the TISE for energy eigenstate with eigenvalue E as

$$\frac{1}{\psi(x)}\frac{d^2\psi(x)}{dx^2} = \begin{cases} -k^2 & x < 0 \\ \kappa^2 & x \geq 0 \end{cases} \tag{10.7.2}$$

$$\implies \psi(x) = \begin{cases} Ae^{ikx} + Be^{-ikx} & x < 0 \\ Ce^{\kappa x} + De^{-\kappa x} & x \geq 0 \end{cases} \tag{10.7.3}$$

Where

$$-k^2 = -\frac{2mE}{\hbar^2} \tag{10.7.4}$$

$$\kappa^2 = \frac{2m(V_0 - E)}{\hbar^2} \tag{10.7.5}$$

Here $V_0 = 7$ eV, and the energy eigenvalue is $E = 5$ eV
Because the wavefunction cannot blow up at infinity $C = 0$
If the seperation between the start of the step potential and the microscope is d , then the tunneling current is proportional to $|\psi(d)|^2$

$$\implies \frac{\text{Current}_{1\text{ atom}}}{\text{Current}_{2\text{ atom}}} = e^{2\kappa d} = 78.25 \tag{10.7.6}$$

Where $d = 3$ Å= thickness of atom

11 Harmonic Oscillator and Degenerate states

11.2. Vibrations of the hydrogen molecule can be modeled as a simple harmonic oscillator with the spring constant $k = 1.13 \times 10^3$ Nm^{-2} and mass $m = 1.67 \times 10^{-27}$ kg.

(a) What is the vibrational frequency of this molecule?

Solution: We know that the hydrogen molecule is diatomic and hence the effective mass of the Quantum Harmonic Oscillator is $\mu = \frac{m_H}{2}$

$$k = \mu\omega^2 \tag{11.2.1}$$
$$\implies \omega = \sqrt{\frac{k}{\mu}} \tag{11.2.2}$$
$$= 1.16 \times 10^{15} \text{ Hz} \tag{11.2.3}$$

(b) What are the energy and the wavelength of the emitted photon when the molecule makes transition between its third and second excited states?

Solution: We know that the energy eigenvalues of the QHO is $\left(n + \frac{1}{2}\right)\hbar\omega$. Thus the energy difference between the third and the second excited states is $\hbar\omega$

$$\implies E_\gamma = \hbar\omega = 0.76 \text{ eV} \tag{11.2.4}$$
$$\implies \lambda = \frac{2\pi c}{\omega} = 1.62\ \mu\text{m} \tag{11.2.5}$$

11.4. Determine the expectation value of the potential energy for a quantum harmonic oscillator in the ground state. Use this to calculate the expectation value of the kinetic energy

Solution: We know the ground state eigenfunction for the harmonic oscillator

$$\psi(x) = \left(\frac{\alpha}{\pi}\right)^{\frac{1}{4}} e^{-\alpha\frac{x^2}{2}} \tag{11.4.1}$$

Where

$$\alpha = \frac{m\omega}{\hbar} \tag{11.4.2}$$

We thus calculate the expectation value of Potential Energy as follows

$$\implies \langle V \rangle = \int_{x=-\infty}^{\infty} \psi(x)^* V(x) \psi(x)\, dx \tag{11.4.3}$$
$$= \frac{m\omega^2}{2}\sqrt{\frac{\alpha}{\pi}} \int_{x=-\infty}^{\infty} x^2 e^{-\alpha x^2}\, dx \tag{11.4.4}$$
$$= -\frac{m\omega^2}{4\alpha}\sqrt{\frac{\alpha}{\pi}} \int_{x=-\infty}^{\infty} x\left(-2\alpha x e^{-\alpha x^2}\right) dx \tag{11.4.5}$$

Integrating by parts

$$= -\frac{m\omega^2}{4\alpha}\sqrt{\frac{\alpha}{\pi}} \left(x e^{-\alpha x^2}\Big|_{x=-\infty}^{\infty} - \int_{x=-\infty}^{\infty} e^{-\alpha x^2}\, dx \right) \tag{11.4.6}$$
$$= \frac{m\omega^2}{4\alpha} = \frac{\hbar\omega}{4} \tag{11.4.7}$$

This aligns perfectly with classical results, since the expectation of potential energy is exactly half the total expected energy

$$\implies \langle KE \rangle = \langle V \rangle = \frac{\hbar\omega}{4} \tag{11.4.8}$$

11.5. A diatomic molecule behaves like a quantum harmonic oscillator with the force constant $k = 12$ Nm^{-1} and mass $m = 5.6 \times 10^{-26}$ kg

(a) What is the wavelength of the emitted photon when the molecule makes the transition from the third excited state to the second excited state?

Solution: Along the lines of Q11.2b

$$\omega = \sqrt{\frac{k}{\mu}} \tag{11.5.1}$$

$$= 1.46 \times 10^{13} \text{ Hz} \tag{11.5.2}$$

$$\implies \lambda = \frac{2\pi c}{\omega} = 0.13 \text{ mm} \tag{11.5.3}$$

(b) Find the ground state energy of vibrations for this diatomic molecule.

Solution:

$$E_0 = \frac{\hbar\omega}{2} = 4.8 \text{ meV} \tag{11.5.4}$$

11.6. A two-dimensional isotropic harmonic oscillator has the Hamiltonian

$$H = -\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2}\right) + \frac{1}{2}k(x^2 + y^2)$$

(a) Show that the energy levels are given by

$$E_{n_x n_y} = \hbar\omega(n_x + n_y + 1)$$
$$n_x, n_y \in \{0, 1, 2 \cdots\}$$
$$\omega = \sqrt{\frac{k}{m}}$$

Solution: We can attack the problem using variable separation.
We assume a form separable in the x, y variables

$$\psi(x, y) = \psi_x(x)\psi_y(y) \tag{11.6.1}$$

Putting in TISE

$$H\psi(x,y) = E\psi(x,y) \tag{11.6.2}$$

$$\implies -\frac{\hbar^2}{2m}\psi_y(y)\frac{\partial^2\psi_x(x)}{\partial x^2} - \frac{\hbar^2}{2m}\psi_x(x)\frac{\partial^2\psi_y(y)}{\partial y^2} + \frac{1}{2}kx^2\psi_x(x)\psi_y(x) + \frac{1}{2}ky^2\psi_x(x)\psi_y(y)$$
$$= E\psi_x(x)\psi_y(y) \tag{11.6.3}$$

$$\implies -\frac{\hbar^2}{2m\psi_x(x)}\frac{\partial^2\psi_x(x)}{\partial x^2} + \frac{1}{2}kx^2$$
$$= -\left(-\frac{\hbar^2}{2m\psi_y(y)}\frac{\partial^2\psi_y(y)}{\partial y^2} + \frac{1}{2}ky^2 - E\right) \tag{11.6.4}$$

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

$$-\frac{\hbar^2}{2m\psi_x(x)}\frac{\partial^2\psi_x(x)}{\partial x^2} + \frac{1}{2}kx^2 = E_x \tag{11.6.5}$$

$$-\frac{\hbar^2}{2m\psi_y(y)}\frac{\partial^2\psi_y(y)}{\partial y^2} + \frac{1}{2}ky^2 = E - E_x \tag{11.6.6}$$

We already know the solutions to (11.6.5) and (11.6.6)

$$E_x = \left(n_x + \frac{1}{2}\right)\hbar\omega \tag{11.6.7}$$

$$E - E_x = \left(n_y + \frac{1}{2}\right)\hbar\omega \tag{11.6.8}$$

$$\implies E = (n_x + n_y + 1)\,\hbar\omega \tag{11.6.9}$$

We need not worry about the general E eigenstate (which will be a linear combination of separable E eigenstates), because they by definition will have eigenvalue E, which we already found

(b) What is the degeneracy of each level?

Solution: 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 $n+1$ $(n_x = 0, 1 \cdots, n)$
Therefore the degeneracy of energy E will be $\frac{E}{\hbar\omega}$

11.7. Consider the Hamiltonian of a two-dimensional anisotropic harmonic oscillator

$$H = \frac{p_1^2}{2m} + \frac{p_2^2}{2m} + \frac{1}{2}m\omega_1^2q_1^2 + \frac{1}{2}m\omega_2^2q_2^2 \qquad \omega_1 \neq \omega_2$$

(a) Exploit the fact that the Schrödinger eigenvalue equation can be solved by separating the variables and find a complete set of eigenfunctions of H and the corresponding eigenvalues.

Solution: Proceeding as exactly as in Q11.6a, we get

$$-\frac{\hbar^2}{2m\psi_{q_1}(q_1)}\frac{\partial^2\psi_{q_1}(q_1)}{\partial q_1^2}+\frac{1}{2}m\omega_1^2q_1^2=E_{q_1} \tag{11.7.1}$$

$$-\frac{\hbar^2}{2m\psi_{q_2}(q_2)}\frac{\partial^2\psi_{q_2}(q_2)}{\partial q_2^2}+\frac{1}{2}m\omega_2^2q_2^2=E-E_{q_1} \tag{11.7.2}$$

We already know the solution to these differential equations

$$\psi_{q_1}^{(n_1)}(q_1)=\left(\frac{m\omega_1}{\pi\hbar}\right)^{\frac{1}{4}}\frac{1}{\sqrt{2^{n_1}(n_1)!}}H_{n_1}\left(\sqrt{\frac{m\omega_1}{\hbar}}q_1\right)e^{-\frac{m\omega_1}{\hbar}\frac{q_1^2}{2}} \tag{11.7.3}$$

$$\psi_{q_2}^{(n_2)}(q_2)=\left(\frac{m\omega_2}{\pi\hbar}\right)^{\frac{1}{4}}\frac{1}{\sqrt{2^{n_2}(n_2)!}}H_{n_2}\left(\sqrt{\frac{m\omega_2}{\hbar}}q_2\right)e^{-\frac{m\omega_2}{\hbar}\frac{q_2^2}{2}} \tag{11.7.4}$$

Where $H_n(x)$ is the n^{th} Hermite polynomial, and

$$E_{q_1}=\left(n_1+\frac{1}{2}\right)\hbar\omega_1 \tag{11.7.5}$$

$$E_{q_2}=E-E_{q_1}=\left(n_2+\frac{1}{2}\right)\hbar\omega_2 \tag{11.7.6}$$

$$\implies E=\left(n_1\omega_1+n_2\omega_2+\frac{\omega_1+\omega_2}{2}\right)\hbar \tag{11.7.7}$$

The most general E eigenstate is of course

$$\psi_E(q_1,q_2)=\sum_{E_{q_1}+E_{q_2}=E}c_{n_1n_2}\psi_{q_1}^{(n_1)}(q_1)\psi_{q_2}^{(n_2)}(q_2) \tag{11.7.8}$$

(b) Assume that $\frac{\omega_1}{\omega_2}=\frac{3}{4}$. Find the first two degenerate energy levels. What can one say about the degeneracy of energy levels when the ratio between ω_1 and ω_2 is not a rational number

Solution: When $\frac{\omega_1}{\omega_2}=\frac{3}{4}$, finding out the degeneracy amounts to finding the number of integer solutions to $3n_1+4n_2=n$, which amounts to solving Diophantine equations Finding the degeneracy for the first two energy levels

First State

$$E=(6n_1+8n_2+7)\frac{\hbar\omega_2}{8}=\frac{13}{8}\hbar\omega_2 \tag{11.7.9}$$

This has degeneracy 1, as only $n_x=1$, $n_y=0$ is possible

Second State

$$E=(6n_1+8n_2+7)\frac{\hbar\omega_2}{8}=\frac{15}{8}\hbar\omega_2 \tag{11.7.10}$$

This has degeneracy 1, as only $n_x = 0$, $n_y = 1$ is possible

$$ \tag{11.7.11} $$

If we are asked to find the first energy that has degeneracy 2, that will be

First Energy($n_x = 4$, $n_y = 0$ and $n_x = 0$, $n_y = 3$ are possible)

$$E = \frac{31}{8}\hbar\omega_2 \tag{11.7.12}$$

In general, for the ratio not being a rational number, we will not have any degeneracy for any energy

12 Statistical Mechanics and Density of States

12.1 Statistical Mechanics

12.1.1. A national powerball lottery uses two sets of balls. The first set consists of 59 sequentially numbered balls and the second set consists of 35 sequentially numbered balls. Assume equal probability of choosing any ball and that all the balls are differently numbered. Five balls are chosen without replacement from the set of 59. Then one ball is chosen from the set of 35. Calculate the number of ways these six balls can be chosen (and thus your probability of winning the grand powerball prize).

Solution: The ways of choosing 5 out of 59 distinguishable balls without replacement is $\binom{59}{5}$
The ways of choosing 1 ball out of 35 distinguishable balls is 35
$\implies$ the ways of drawing 6 balls is $\binom{59}{5} \times 35 = 175223510$
The probability of winning the grand prize is hence $\frac{1}{175223510} = 5.7 \times 10^{-9}$

12.1.2. Suppose we have 20 coins and we flip all of them together

(a) Considering all the coins to be independent of each other, how many possible outcomes (no. of microstates) do you expect with such a flipping?

Solution: Every coin can choose to land as either heads or tails, so there are 2^20 possibilities

(b) How many ways are there for obtaining 12 heads and 8 tails?

Solution: We simply need to choose which coins we need as heads, giving us the number as $\binom{20}{12}$

(c) What is the probability of obtaining 12 heads and 8 tails regardless of the order? They are called macrostates.

Solution: The probability is of course $\frac{\text{Num. of ways 12H}}{\text{All num of ways}} = \frac{\binom{20}{12}}{2^{20}} = 0.12$

12.1.3. Three indistinguishable particles (say electrons) are to be arranged in three different energy levels of energy 0, E and $2E$, with respective degeneracies (ignore spin degeneracy) 2, 10 and 20. The total energy available is 3E. What are the possible distributions and what are their probabilities?

Solution: If the number of particles with energy 0, E, $2E$ are n_0, n_E and n_{2E} respectively, then we have $En_E + 2En_{2E} = 3E \implies n_E + 2n_{2E} = 3$, and $n_0 + n_E + n_{2E} = 3$. Subtracting the two equations give us $n_{2E} = n_0$. From this we can easily get the possible distributions

$(n_0, n_E, n_{2E}) = (0, 3, 0)$

$$\text{Prob} \propto \binom{10}{3} = 120 \tag{12.1.3.1}$$

$(n_0, n_E, n_{2E}) = (1, 1, 1)$

$$\text{Prob} \propto \binom{2}{1}\binom{10}{1}\binom{20}{1} = 400 \tag{12.1.3.2}$$

$$\implies \text{Prob}(0, 3, 0) = \frac{120}{120 + 400} = 0.23 \tag{12.1.3.3}$$

$$\text{Prob}(1, 1, 1) = \frac{400}{120 + 400} = 0.77 \tag{12.1.3.4}$$

12.1.4. Consider a particle confined to a 3D harmonic oscillator potential, $V(x, y, z) = \frac{1}{2}m\omega^2(x^2 + y^2 + 4z^2)$

(a) Calculate the ground state energy of the particle.

Solution: The allowed energy levels are $E = (n_x + n_y + 2n_z + 2)\hbar\omega$, for integer $n_x, n_y, n_z \geq 0$
Hence the ground state is $2\hbar\omega$

(b) What is the degeneracy of the state with energy, $E = 7\hbar\omega$?

Solution: We need to calculate the integer solutions to $n_x + n_y + 2n_z = 5$. For $n_z = 0$ there are 5 possibilities, for $n_z = 1$ there are 3, for $n_z = 2$ there is just 1. Hence the total number is $5 + 3 + 1 = 9$

12.1.5. A certain thermodynamic system has non-degenerate energy levels, with energies 0, E, $3E$, $5E$ and $9E$. Suppose that there are four particles, with total energy $U = 9E$. Identify the possible distribution of particles and evaluate their microstates when

(a) The particles are distinguishable

Solution: As before, $n_E+3n_{3E}+5n_{5E}+9n_{9E}=9$ and $n_0+n_E+n_{3E}+n_{5E}+n_{9E}=4$.
$\implies 2n_{3E}+4n_{5E}+8n_{9E}=5+n_0$
We thus have the possibilities

$(n_0, n_E, n_{3E}, n_{5E}, n_{9E})$=$(3, 0, 0, 0, 1)$

$$\text{Prob} \propto 1 \times \frac{4!}{3!} = 4 \tag{12.1.5.1}$$

$(n_0, n_E, n_{3E}, n_{5E}, n_{9E})$=$(1, 1, 1, 1, 0)$

$$\text{Prob} \propto 1 \times 4! = 24 \tag{12.1.5.2}$$

$(n_0, n_E, n_{3E}, n_{5E}, n_{9E})$=$(1, 0, 3, 0, 0)$

$$\text{Prob} \propto 1 \times \frac{4!}{3!} = 4 \tag{12.1.5.3}$$

$$\implies \text{Prob}(3, 0, 0, 0, 1) = \frac{4}{4+24+4} = 0.125 \tag{12.1.5.4}$$

$$\text{Prob}(1, 1, 1, 1, 0) = \frac{24}{4+24+4} = 0.75 \tag{12.1.5.5}$$

$$\text{Prob}(1, 0, 3, 0, 0) = \frac{4}{4+24+4} = 0.125 \tag{12.1.5.6}$$

(b) The particles are identical bosons

Solution: We have the possibilities

$(n_0, n_E, n_{3E}, n_{5E}, n_{9E})$=$(3, 0, 0, 0, 1)$

$$\text{Prob} \propto 1 \tag{12.1.5.7}$$

$(n_0, n_E, n_{3E}, n_{5E}, n_{9E})$=$(1, 1, 1, 1, 0)$

$$\text{Prob} \propto 1 \tag{12.1.5.8}$$

$(n_0, n_E, n_{3E}, n_{5E}, n_{9E})$=$(1, 0, 3, 0, 0)$

$$\text{Prob} \propto 1 \tag{12.1.5.9}$$

$$\implies \text{Prob}(3, 0, 0, 0, 1) = \frac{1}{3} \tag{12.1.5.10}$$

$$\text{Prob}(1, 1, 1, 1, 0) = \frac{1}{3} \tag{12.1.5.11}$$

$$\text{Prob}(1, 0, 3, 0, 0) = \frac{1}{3} \tag{12.1.5.12}$$

(c) the particles are identical fermions

Solution: We have the possibilities

$(n_0, n_E, n_{3E}, n_{5E}, n_{9E})$=$(3, 0, 0, 0, 1)$

$$\text{Prob} \propto 0 \tag{12.1.5.13}$$

$(n_0, n_E, n_{3E}, n_{5E}, n_{9E})$=$(1, 1, 1, 1, 0)$

$$\text{Prob} \propto 1 \tag{12.1.5.14}$$

$(n_0, n_E, n_{3E}, n_{5E}, n_{9E})$=$(1, 0, 3, 0, 0)$

$$\text{Prob} \propto 0 \tag{12.1.5.15}$$

$$\implies \text{Prob}(3, 0, 0, 0, 1) = 0 \tag{12.1.5.16}$$

$$\text{Prob}(1, 1, 1, 1, 0) = 1 \tag{12.1.5.17}$$

$$\text{Prob}(1, 0, 3, 0, 0) = 0 \tag{12.1.5.18}$$

12.1.6. In how many ways three electrons can occupy ten states (include spin degeneracy)? Is the number same as the way in which three persons can occupy ten chairs in a room? State the reason. In case the number is different, find the other number also.

Solution: If we count spin degeneracy, then that is equivalent to having 20 degenerate states. The number of ways then becomes $\binom{20}{3} = 1140$
For the number of ways of 3 people occupying 10 chairs, the people aren't indistinguishable (in contrast to electrons) hence we need to permute them also. The number then becomes $\binom{10}{3}3! = 720$

12.1.7. The energy of a particle in a 3-D cubical box is given by

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

If these levels are going to be occupied by electrons, write the energy values corresponding to the five lowest levels, taking into account the spin degeneracy. If three electrons occupy these states, find out the possible distributions which would yield a total energy of $\frac{18\pi^2\hbar^2}{2mL^2}$. Also find out the probability for each distributions.

Solution: 5 lowest levels energies with respective degeneracies

(n_x, n_y, n_z)=$(1, 1, 1)$. Degeneracy $g_0 = 1 \times 2 = 2$

$$E_0 = \frac{3\pi^2\hbar^2}{2mL^2} \tag{12.1.7.1}$$

(n_x, n_y, n_z)=$(2, 1, 1)$ or $(1, 2, 1)$ or $(1, 1, 2)$. Degeneracy $g_1 = 3 \times 2 = 6$

$$E_1 = \frac{6\pi^2\hbar^2}{2mL^2} \tag{12.1.7.2}$$

(n_x, n_y, n_z)=$(1, 2, 2)$ or $(2, 1, 2)$ or $(2, 2, 1)$. Degeneracy $g_2 = 3 \times 2 = 6$

$$E_2 = \frac{9\pi^2\hbar^2}{2mL^2} \tag{12.1.7.3}$$

(n_x, n_y, n_z)=$(3, 1, 1)$ or $(1, 3, 1)$ or $(1, 1, 3)$. Degeneracy $g_3 = 3 \times 2 = 6$

$$E_3 = \frac{11\pi^2\hbar^2}{2mL^2} \tag{12.1.7.4}$$

(n_x, n_y, n_z)=$(2, 2, 2)$. Degeneracy $g_4 = 1 \times 2 = 2$

$$E_4 = \frac{12\pi^2\hbar^2}{2mL^2} \tag{12.1.7.5}$$

Again, proceeding as before, $3n_0+6n_1+9n_2+11n_3+12n_4 = 18$ and $n_0+n_1+n_2+n_3+n_4 = 3$. We can clearly see $n_3 = 0$
$\implies n_2 + 2n_4 = n_0$ We can thus find the possibilities

$(n_0, n_1, n_2, n_3, n_4)$=$(2, 0, 0, 0, 1)$

$$\text{Prob} \propto \binom{2}{2}\binom{2}{1} = 2 \tag{12.1.7.6}$$

$(n_0, n_1, n_2, n_3, n_4)$=$(1, 1, 1, 0, 0)$

$$\text{Prob} \propto \binom{2}{1}\binom{6}{1}\binom{6}{1} = 72 \tag{12.1.7.7}$$

$(n_0, n_1, n_2, n_3, n_4)$=$(0, 3, 0, 0, 0)$

$$\text{Prob} \propto \binom{6}{3} = 20 \tag{12.1.7.8}$$

$$\implies \text{Prob}(2, 0, 0, 0, 1) = \frac{2}{2 + 72 + 20} = 0.021 \tag{12.1.7.9}$$

$$\text{Prob}(1, 1, 1, 0, 0) = \frac{72}{2 + 72 + 20} = 0.766 \tag{12.1.7.10}$$

$$\text{Prob}(0, 3, 0, 0, 0) = \frac{20}{2 + 72 + 20} = 0.213 \tag{12.1.7.11}$$

12.1.8. Consider a system of five particles trapped in a 1D harmonic oscillator potential.

(a) What are the microstates of the ground state of this system for classical particles, identical Bosons and identical spin half Fermions

Solution: Let the wavefunction of the system be denoted as $\psi(x_1, x_2, x_3, x_4, x_5)$. Let the i^{th} normalized QHO state for a single particle be written as $\psi_i(x)$. We are now in a capacity to write the microstates (eigenfunctions) having the ground state energy of this system

Classical particles (ground state energy eigenvalue $\frac{5}{2}\hbar\omega$)

$$\psi(x_1, x_2, x_3, x_4, x_5) = \psi_0(x_1)\psi_0(x_2)\psi_0(x_3)\psi_0(x_4)\psi_0(x_5) \tag{12.1.8.1}$$

Bosons (Notice that the function is symmetric to exchange), (ground state energy eigenvalue $\frac{5}{2}\hbar\omega$)

$$\psi(x_1, x_2, x_3, x_4, x_5) \tag{12.1.8.2}$$
$$= \frac{1}{\sqrt{120}} \sum_{(p_1,p_2,p_3,p_4,p_5)=\text{perm}(1,2,3,4,5)} \psi_0(x_{p_1})\psi_0(x_{p_2})\psi_0(x_{p_3})\psi_0(x_{p_4})\psi_0(x_{p_5}) \tag{12.1.8.3}$$

The case for fermions is a little bit more complex. We need to realize that we now also have to take into account the spin configuration. Our system wavefunction then will be $\phi(x_1, x_2, x_3, x_4, x_5, s_1, s_2, s_3, s_4, s_5)$. Let $\alpha(s)$ be the "up" spin wavefunction, and $\beta(s)$ be the "down" spin wavefunction.
To write our ground state wavefunction we need to use slater's determinants (which ensures antisymmetricity to exchange). There are two possibilities (hence 2 microstates), each with energy eigenvalue $\frac{13}{2}\hbar\omega$:

2 fermions "up" and "down" in ψ_0, 2 "up" and "down" in ψ_1, 1 "up" in ψ_2

$$\psi(x_1, x_2, x_3, x_4, x_5, s_1, s_2, s_3, s_4, s_5)$$
$$= \frac{1}{\sqrt{120}} \begin{vmatrix} \psi_0(x_1)\alpha(s_1) & \psi_0(x_1)\beta(s_1) & \psi_1(x_1)\alpha(s_1) & \psi_1(x_1)\beta(s_1) & \psi_2(x_1)\alpha(s_1) \\ \psi_0(x_2)\alpha(s_2) & \psi_0(x_2)\beta(s_2) & \psi_1(x_2)\alpha(s_2) & \psi_1(x_2)\beta(s_2) & \psi_2(x_2)\alpha(s_2) \\ & & \vdots & & \\ \psi_0(x_5)\alpha(s_5) & \psi_0(x_5)\beta(s_5) & \psi_1(x_5)\alpha(s_5) & \psi_1(x_5)\beta(s_5) & \psi_2(x_5)\alpha(s_5) \end{vmatrix} \tag{12.1.8.4}$$

2 fermions "up" and "down" in ψ_0, 2 "up" and "down" in ψ_1, 1 "down" in ψ_2

$$\psi(x_1, x_2, x_3, x_4, x_5, s_1, s_2, s_3, s_4, s_5)$$
$$= \frac{1}{\sqrt{120}} \begin{vmatrix} \psi_0(x_1)\alpha(s_1) & \psi_0(x_1)\beta(s_1) & \psi_1(x_1)\alpha(s_1) & \psi_1(x_1)\beta(s_1) & \psi_2(x_1)\beta(s_1) \\ \psi_0(x_2)\alpha(s_2) & \psi_0(x_2)\beta(s_2) & \psi_1(x_2)\alpha(s_2) & \psi_1(x_2)\beta(s_2) & \psi_2(x_2)\beta(s_2) \\ & & \vdots & & \\ \psi_0(x_5)\alpha(s_5) & \psi_0(x_5)\beta(s_5) & \psi_1(x_5)\alpha(s_5) & \psi_1(x_5)\beta(s_5) & \psi_2(x_5)\beta(s_5) \end{vmatrix} \tag{12.1.8.5}$$

(b) Suppose that the system is excited and has one unit of energy ($\hbar\omega$) above the corresponding ground state energy in each of the three cases. Calculate the number of microstates for each of the three cases

Solution:

Classical particles: 5 microstates (each with energy eigenvalue $\frac{7}{2}\hbar\omega$)

$$\psi(x_1,x_2,x_3,x_4,x_5) = \psi_1(x_1)\psi_0(x_2)\psi_0(x_3)\psi_0(x_4)\psi_0(x_5) \tag{12.1.8.6}$$
$$\text{OR} \tag{12.1.8.7}$$
$$\psi(x_1,x_2,x_3,x_4,x_5) = \psi_0(x_1)\psi_1(x_2)\psi_0(x_3)\psi_0(x_4)\psi_0(x_5) \tag{12.1.8.8}$$
$$\text{OR} \tag{12.1.8.9}$$
$$\psi(x_1,x_2,x_3,x_4,x_5) = \psi_0(x_1)\psi_0(x_2)\psi_1(x_3)\psi_0(x_4)\psi_0(x_5) \tag{12.1.8.10}$$
$$\text{OR} \tag{12.1.8.11}$$
$$\psi(x_1,x_2,x_3,x_4,x_5) = \psi_0(x_1)\psi_0(x_2)\psi_0(x_3)\psi_1(x_4)\psi_0(x_5) \tag{12.1.8.12}$$
$$\text{OR} \tag{12.1.8.13}$$
$$\psi(x_1,x_2,x_3,x_4,x_5) = \psi_0(x_1)\psi_0(x_2)\psi_0(x_3)\psi_0(x_4)\psi_1(x_5) \tag{12.1.8.14}$$

Bosons: 1 microstate (with energy eigenvalue $\frac{7}{2}\hbar\omega$). Notice that even if you have the second term in each product to be ψ_1, that is already covered in the sum since it covers all permutations. Hence only 1 microstate possible

$$\psi(x_1,x_2,x_3,x_4,x_5) \tag{12.1.8.15}$$
$$= \frac{1}{\sqrt{120}} \sum_{(p_1,p_2,p_3,p_4,p_5)=\text{perm}(1,2,3,4,5)} \psi_1(x_{p_1})\psi_0(x_{p_2})\psi_0(x_{p_3})\psi_0(x_{p_4})\psi_0(x_{p_5}) \tag{12.1.8.16}$$

Fermions: 4 microstates (each with energy eigenvalue $\frac{15}{2}\hbar\omega$)

2 fermions "up" and "down" in ψ_0, 1 "up" in ψ_1, 2 "up" and "down" in ψ_2

$$\psi(x_1,x_2,x_3,x_4,x_5,s_1,s_2,s_3,s_4,s_5)$$
$$= \frac{1}{\sqrt{120}} \begin{vmatrix} \psi_0(x_1)\alpha(s_1) & \psi_0(x_1)\beta(s_1) & \psi_1(x_1)\alpha(s_1) & \psi_2(x_1)\alpha(s_1) & \psi_2(x_1)\beta(s_1) \\ & & \vdots & & \\ \psi_0(x_5)\alpha(s_5) & \psi_0(x_5)\beta(s_5) & \psi_1(x_5)\alpha(s_5) & \psi_2(x_5)\alpha(s_5) & \psi_2(x_5)\beta(s_5) \end{vmatrix} \tag{12.1.8.17}$$

2 fermions "up" and "down" in ψ_0, 1 "down" in ψ_1, 2 "up" and "down" in ψ_2

$$\psi(x_1,x_2,x_3,x_4,x_5,s_1,s_2,s_3,s_4,s_5)$$
$$= \frac{1}{\sqrt{120}} \begin{vmatrix} \psi_0(x_1)\alpha(s_1) & \psi_0(x_1)\beta(s_1) & \psi_1(x_1)\beta(s_1) & \psi_2(x_1)\alpha(s_1) & \psi_2(x_1)\beta(s_1) \\ & & \vdots & & \\ \psi_0(x_5)\alpha(s_5) & \psi_0(x_5)\beta(s_5) & \psi_1(x_5)\beta(s_5) & \psi_2(x_5)\alpha(s_5) & \psi_2(x_5)\beta(s_5) \end{vmatrix} \tag{12.1.8.18}$$

2 fermions "up" and "down" in ψ_0, 2 "up" and "down" in ψ_1, 1 "up" in ψ_3

$$\psi(x_1, x_2, x_3, x_4, x_5, s_1, s_2, s_3, s_4, s_5) = \frac{1}{\sqrt{120}} \begin{vmatrix} \psi_0(x_1)\alpha(s_1) & \psi_0(x_1)\beta(s_1) & \psi_1(x_1)\alpha(s_1) & \psi_1(x_1)\beta(s_1) & \psi_3(x_1)\alpha(s_1) \\ & & \vdots & & \\ \psi_0(x_5)\alpha(s_5) & \psi_0(x_5)\beta(s_5) & \psi_1(x_5)\alpha(s_5) & \psi_1(x_5)\beta(s_5) & \psi_3(x_5)\alpha(s_5) \end{vmatrix} \tag{12.1.8.19}$$

2 fermions "up" and "down" in ψ_0, 2 "up" and "down" in ψ_1, 1 "down" in ψ_3

$$\psi(x_1, x_2, x_3, x_4, x_5, s_1, s_2, s_3, s_4, s_5) = \frac{1}{\sqrt{120}} \begin{vmatrix} \psi_0(x_1)\alpha(s_1) & \psi_0(x_1)\beta(s_1) & \psi_1(x_1)\alpha(s_1) & \psi_1(x_1)\beta(s_1) & \psi_3(x_1)\beta(s_1) \\ & & \vdots & & \\ \psi_0(x_5)\alpha(s_5) & \psi_0(x_5)\beta(s_5) & \psi_1(x_5)\alpha(s_5) & \psi_1(x_5)\beta(s_5) & \psi_3(x_5)\beta(s_5) \end{vmatrix} \tag{12.1.8.20}$$

(c) Suppose that the temperature of this system is low, so that the total energy is low (but above the ground state), describe in a couple of sentences, the difference in the behavior of the system of identical bosons from that of the system of classical particles

Solution: For a given total energy, because of the distinguishability of classical particles, there are far many more possible microstates than in the case of bosons. There are far more ways of sending a particle up in energy for classical case than for bosonic case.
Hence the system of bosons will have more particles in lower energies than classical system

12.2 Density of States and Fermi Energy

12.2.1. A system has one state with energy 0, four states with energy $2E$ and eight states with energy $3E$. Six electrons are to be distributed among these states such that their total energy is $12E$. Consider a configuration (j, m, n) in which j electrons are in 0 energy state, m electrons are in 2E energy state and n electrons are in $3E$ state

(a) Calculate the total number of microstates for the configuration $(1, 3, 2)$

Solution: We are dealing with fermions here. Number of electrons having each energy is $(n_1, n_2, n_3) = (1, 3, 2)$. Degeneracy of each energy is (including spin degeneracy) $(g_1, g_2, g_3) = (1 \times 2, 4 \times 2, 8 \times 2)$

$$\implies N_{\text{micro}}(1,3,2) = \prod_{i=1}^{3} \binom{g_i}{n_i} \tag{12.2.1.1}$$

$$= \frac{2!}{1!1!} \times \frac{8!}{3!5!} \times \frac{16!}{2!14!} \tag{12.2.1.2}$$

$$= 13440 \tag{12.2.1.3}$$

(b) Find the ratio of probability of occurrence of a configuration $(2,0,4)$ to that of a configuration $(1,3,2)$

Solution: Proceeding as above

$$N_{\text{micro}}(2,0,4) = \prod_{i=1}^{3} \binom{g_i}{n_i} \tag{12.2.1.4}$$

$$= \frac{2!}{2!0!} \times \frac{8!}{0!8!} \times \frac{16!}{4!12!} \tag{12.2.1.5}$$

$$= 1820 \tag{12.2.1.6}$$

$$\implies \frac{\text{Prob}(2,0,4)}{\text{Prob}(1,3,2)} = \frac{N_{\text{micro}}(2,0,4)}{N_{\text{micro}}(1,3,2)} = \frac{1820}{13440} = 0.135 \tag{12.2.1.7}$$

12.2.2. The spin independent energy levels of a carbon nanotube are described by those of a 1D infinite potential well. In a carbon nanotube of length 1 μm, electrons occupy all the energy levels up to 0.1 eV

(a) Calculate the number of electrons in the carbon nanotube

Solution: The spin independent part of the wavefunction of each particle is descibed by 1D particle in a box wavefunctions.
But each wavefunction for a particular spin independent part will have 2 possibilities for the spin part, "up" and "down"
Hence the degeneracy of each energy level is 2
We know that the electrons occupy all energy levels upto 0.1 eV. This is only possible at $T = 0$, and if the fermi energy is $E_f = 0.1$ eV
The number of particles will then simply be the number of states below 0.1 eV, times 2.
If E_F is the n^{th} state then $E_F = n^2 \frac{\hbar^2\pi^2}{2mL^2} \implies N = 2n = 2 \times \frac{\sqrt{2mE_F}}{\hbar\pi} L = 1034$

(b) Calculate the density of states $g(E)$ at the Fermi energy E_F in units of [(eV)$^{-1}$(μm)$^{-1}$]

Solution: We simply need the number of states having energies between E_F and $E_F + dE$. For each n between $\frac{\sqrt{2mE_F}}{\hbar\pi}L$ and $\frac{\sqrt{2m(E_F+dE)}}{\hbar\pi}L = \frac{\sqrt{2mE_F}}{\hbar\pi}L + \frac{1}{2}\frac{\sqrt{2mE_F}}{\hbar\pi}L\,\frac{dE}{E_F}$,

we have 2 states.
Thus we have $\frac{\sqrt{2m}}{\hbar\pi\sqrt{E_F}}L\,dE$ states between E_F and $E_F + dE$
Thus we have $\frac{\sqrt{2m}}{\hbar\pi\sqrt{E_F}}\,dE$ states between E_F and E_F+dE per unit length of container
Thus the density of states is $g(E_F)\,dE = \frac{\sqrt{2m}}{\hbar\pi\sqrt{E_F}}\,dE$
Thus $g(E_F) = 5173\ (\text{eV})^{-1}(\mu\text{m})^{-1}$

12.2.3. Consider a non-interacting Fermi gas of N particles in 2D, confined in a square area $A = L^2$

(a) Derive a formula for the density of states $g(E)$

Solution: Looking at k-space (the state space indexed by (k_x, k_y)), we know that the valid states are arranged in a grid/lattice, with the minimal k-space volume between 4 closest grid points being $\frac{\pi^2}{L^2}$.
Therefore the number of gridpoints enclosed inside a k-space volume V_k is $\frac{V_k L^2}{\pi^2}$
We want the number of states between E and $E+dE$. This corresponds to a quarter ring (because all gridpoints in second, third, fourth quadrants are duplicates of first quadrant states) with radius $k = \sqrt{\frac{2mE}{\hbar^2}}$ and thickness $dk = \sqrt{\frac{m}{2\hbar^2 E}}dE$.
This corresponds to a k-space volume $V_k = \frac{\pi k\,dk}{2} = \frac{\pi m}{2\hbar^2}\,dE$
Hence the number of states (including spin) having energies between E and $E+dE$ is $\frac{2V_k L^2}{\pi^2} = \frac{mL^2}{\hbar^2\pi}\,dE$
Hence the density of states is $g(E)\,dE = \frac{m}{\hbar^2\pi}\,dE$

(b) Find the Fermi energy E_F (in terms of N and A) and show that the average energy per particle $\frac{E}{N}$ at $T = 0$ is $\frac{E_F}{2}$

Solution: As we know, the Fermi energy is simply defined as the highest occupied energy at $T = 0$. We also know that $f_{\text{FD},T}(E) = \frac{1}{e^{\frac{E-E_F}{k_B T}}+1}$, which at $T = 0$ becomes

$$f_{\text{FD},0}(E) = \begin{cases} 1 & E < E_F \\ 0 & E \geq E_F \end{cases} \tag{12.2.3.1}$$

$$\implies \frac{N}{A} = \int_{E=0}^{\infty} f_{\text{FD},0}(E) g(E)\,dE \tag{12.2.3.2}$$

$$= \int_{E=0}^{E_F} g(E)\,dE \tag{12.2.3.3}$$

$$= \int_{E=0}^{E_F} \frac{m}{\hbar^2\pi}\,dE \tag{12.2.3.4}$$

$$= \frac{mE_F}{\hbar^2\pi} \tag{12.2.3.5}$$

$$\implies E_F = \frac{N\pi\hbar^2}{mA} \tag{12.2.3.6}$$

Let us find the average energy per particle

$$\frac{N}{A}\langle E\rangle = \int_{E=0}^{\infty} E f_{\mathrm{FD},0}(E) g(E)\, dE \tag{12.2.3.7}$$

$$= \int_{E=0}^{E_F} E \frac{m}{\pi\hbar^2}\, dE \tag{12.2.3.8}$$

$$= \frac{mE_F^2}{2\pi\hbar^2} \tag{12.2.3.9}$$

$$= \frac{NE_F}{2A} \quad \text{Using (12.2.3.6)} \tag{12.2.3.10}$$

$$\implies \langle E\rangle = \frac{E_F}{2} \tag{12.2.3.11}$$

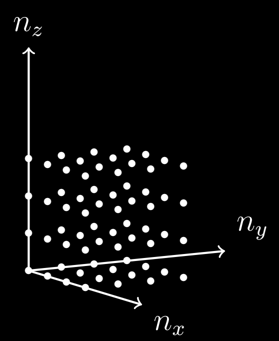
12.2.4. Consider a particle confined to a potential, $V(x, y, z) = \frac{1}{2}m\omega^2(x^2 + y^2 + 4z^2)$

(a) Find the degeneracy of the state with energy $E = 7\hbar\omega$

Solution: Same as 12.1.4b

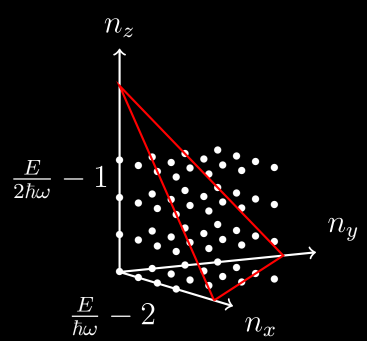
(b) For E $= n\hbar\omega$ ($n \gg 1$), calculate the density of states $g(n)$.

Solution: The energy can be $E = (n_x + n_y + n_z + 2)\hbar\omega$
We need to find the number of states with energies between $n\omega$ and $(n + dn)\omega$.
To do that, let us plot the valid states in n space.



Here each of the points corresponds to a state having energy $(n_x + n_y + 2n_z + 2)\hbar\omega$

Let us plot the surface made by all points such that $(n_x + n_y + 2n_z + 2)\hbar\omega$ is constant $= E = n\hbar\omega$



As we can see, this forms a triangular pyramid of volume $\frac{1}{3}$Base Area $\times$ Height $=$ $\frac{1}{6}\left(\frac{E}{\hbar\omega}-2\right)^2\left(\frac{E}{2\hbar\omega}-1\right)=\frac{(n-2)^3}{12}$
Thus the volume between the two surfaces corresponding to n and $n+dn$ is $\frac{(n-2)^2}{4}\,dn$
This volume will contain $\frac{(n-2)^2}{4}\,dn$ points corresponding to states
Thus the number of states having energies between $n\hbar\omega$ and $(n+dn)\hbar\omega$ is $\frac{(n-2)^2}{4}\,dn$
$g(n)\,dn=\frac{(n-2)^2}{4}\,dn\approx\frac{n^2}{4}\,dn$

12.2.5. Consider a gas of N identical bosons confined by an isotropic 3D harmonic potential. The energy levels in this potential are $\varepsilon = nhf$, where n is a non-negative integer and f is classical oscillation frequency. The degeneracy of the level is $\frac{(n+1)(n+2)}{2}$. Find the density of states for atoms confined by this potential. You may assume $n \gg 1$.

Solution: We are already given the degeneracy (a nice exercise is to prove that the given degeneracy expression is correct)
We need to find the density of states, or number of states with "near" degeneracy, that is, the number of states with energies between nhf and $(n+dn)hf$.
We know that all the energies between nhf and $(n+dn)hf$ will have degeneracy $\frac{(n+1)(n+2)}{2}$, since $dn \ll n$
The number of integers between n and $n+dn$ are dn. Thus there are dn valid energy levels between nhf and $(n+dn)hf$. Thus total number of states is $\frac{(n+1)(n+2)}{2}\,dn$
Thus the density of states is $g(n)\,dn \approx \frac{n^2}{2}\,dn$.
The density of states in energy form is $g(E)\,dE = \frac{E^2}{2(hf)^3}\,dE$

12.2.6. Mass M_s of the Sun is 2×10^{30} kg. Ignore electron spin in this problem.

(a) Estimate the number of electrons (N_s) in the Sun

Solution: Since the sun is entirely composed of ionized Hydrogen (basically proton) and a corresponding electron which are almost free, the number of protons (and thus N_s) in the sun is $\frac{M_s}{M_H} = 1.2\times 10^{57}$

(b) Consider a white dwarf star having N_s electrons, contained in a sphere of radius 2×10^7 m. Assuming these electrons to be nonrelativistic, estimate the Fermi energy (in eV) of this star.

Solution: We will model the white dwarf as a region of constant potential. Hence the energy structure will be same as that of 3D particle in a box
We have our possible energy levels as $E=\frac{\hbar^2\pi^2}{2mL^2}(n_x^2+n_y^2+n_z^2)$. Thus each point (n_x, n_y, n_z) in n space corresponds to a state.
Now, the Fermi energy E_F is defined by the energy such that the number of states below that energy is $\frac{N}{V}$
The volume contained within an eighth sphere in n space with radius $n=\frac{\sqrt{2mE_F}L}{\hbar\pi}$ is $\frac{\pi n^3}{6}=\frac{(2mE_F)^{\frac{3}{2}}}{6\hbar^3\pi^2}V$.

Thus the number of states and hence electrons (at $T = 0$) below E_F is $N = \frac{(2mE_F)^{\frac{3}{2}}}{6\hbar^3\pi^2}V$
Thus $E_F = (\frac{6\pi^2 N}{V})^{\frac{2}{3}}\frac{\hbar^2}{2m} = 62.5$ KeV

(c) Consider another star of volume V . All its electrons, N in number, are extremely relativistic such that the electron rest mass energy $m_e c^2 \ll pc$ where p is the momentum of the electron. Obtain an expression for the Fermi energy of this star.

Solution: Here we have the possible energy levels as $E = \hbar kc = \frac{\pi\hbar c}{L}\sqrt{n_x^2 + n_y^2 + n_z^2}$.
The volume contained within an eighth sphere in n space with radius $n = \frac{E_F}{\hbar\pi c}L$ is $\frac{\pi n^2}{6} = \frac{E_F^3}{6\hbar^3\pi^2 c^3}V$.
Thus the number of states and hence electrons (at $T = 0$) is $N = \frac{E_F^3}{6\hbar^3\pi^2 c^3}V$
Thus $E_F = (\frac{6\pi^2 N}{V})^{\frac{1}{3}}\hbar c$

12.2.7. Use Bose-Einstein Statistics and the density of state expression, with suitable modifications, if any, to derive Planck's formula of black body radiation.

Solution: As done in Q12.2.3a, we can derive the density of states as (use the relation $k = \frac{2\pi}{c}\nu$)

$$g(\nu)\, d\nu = \frac{8\pi}{c^3}\nu^2\, d\nu \tag{12.2.7.1}$$

We can use the formula $f_{\text{BE}}(E) = \frac{1}{e^{\frac{E}{k_B T}} - 1}$ to find the average energy contribution of each energy level

$$\tag{12.2.7.2}$$

$$U(\nu)\, d\nu = h\nu f_{\text{BE}}(h\nu) g(\nu)\, d\nu \tag{12.2.7.3}$$

$$= \frac{8\pi\nu^2}{c^3}\frac{h\nu}{e^{\frac{h\nu}{k_B T}} - 1}\, d\nu \tag{12.2.7.4}$$

12.2.8. Show that the kinetic energy of a 3D gas of N free electrons at 0 K is $\frac{3}{5}NE_F$

Solution: Since there is no potential, the kinetic energy is the total energy
We only need to find the total energy at $T = 0$

First we need the density of states, which we can calculate along similar lines to 12.2.3a

$$g(E)\,dE = \frac{\sqrt{2m^3}}{\pi^2\hbar^3}\sqrt{E}\,dE \quad (12.2.8.1)$$

$$\implies E_{\text{tot}} = V\int_{E=0}^{E_F} Eg(E)\,dE \quad (12.2.8.2)$$

$$= \frac{\sqrt{2m^3}V}{\pi^2\hbar^3}\frac{2}{5}E_F^{\frac{5}{2}} \quad (12.2.8.3)$$

But

$$N = V\int_{E=0}^{E_F} g(E)\,dE \quad (12.2.8.4)$$

$$\implies N = \frac{\sqrt{2m^3}V}{\pi^2\hbar^3}\frac{2}{3}E_F^{\frac{3}{2}} \quad (12.2.8.5)$$

$$\implies E_{\text{tot}} = KE = \frac{3}{5}NE_F \quad (12.2.8.6)$$

12.2.9. (a) Using the Fermi Dirac (FD) Statistics, find the probability that a state is occupied if its energy is higher than ε_F by $0.1k_BT$, $1.0k_BT$, $2.0k_BT$ and $10.0k_BT$, where ε_F is the Fermi Energy. How good is the approximation in neglecting 1 in the denominator of FDS for an energy equal to $10k_BT$.

Solution:

$$f_{\text{FD}}(0.1k_BT) = \frac{1}{e^{0.1}+1} = 0.475 \quad (12.2.9.1)$$

$$f_{\text{FD}}(1.0k_BT) = \frac{1}{e^{1.0}+1} = 0.269 \quad (12.2.9.2)$$

$$f_{\text{FD}}(2.0k_BT) = \frac{1}{e^{2.0}+1} = 0.119 \quad (12.2.9.3)$$

$$f_{\text{FD}}(10.0k_BT) = \frac{1}{e^{10.0}+1} = 4.5398\times 10^{-5} \quad (12.2.9.4)$$

If we neglect 1 in the denominator for $10k_BT$, we get

$$f_{\text{FD}}(10.0k_BT) = e^{-10} = 4.5399\times 10^{-5} \quad (12.2.9.5)$$

Hence the approximation is correct to within 0.002% margin of error

(b) In the Fermi Dirac distribution, substitute $\varepsilon = \varepsilon_F + \delta$. Compute δ for the probability of occupancy equal to 0.25 and 0.75.

Solution:

$f_{\text{FD}}(\varepsilon) = 0.25$

$$\frac{1}{e^{\frac{\delta}{k_B T}} + 1} = 0.25 \tag{12.2.9.6}$$

$$\implies e^{\frac{\delta}{k_B T}} = 3 \tag{12.2.9.7}$$

$$\implies \delta = k_B T \ln 3 \tag{12.2.9.8}$$

$f_{\text{FD}}(\varepsilon) = 0.75$

$$\frac{1}{e^{\frac{\delta}{k_B T}} + 1} = 0.75 \tag{12.2.9.9}$$

$$\implies e^{\frac{\delta}{k_B T}} = \frac{1}{3} \tag{12.2.9.10}$$

$$\implies \delta = -k_B T \ln 3 \tag{12.2.9.11}$$

(c) Show that for a distribution system governed by FD distribution, the probability of occupation of a state with energy higher than ε_F by an amount ΔE is equal to the probability that a state with energy lower than ε_F by ΔE is unoccupied.

Solution:

$$\text{Prob}_{\text{unocc}}(\epsilon_F - \Delta E) = 1 - \frac{1}{e^{\frac{-\Delta E}{k_B T}} + 1} \tag{12.2.9.12}$$

$$= \frac{e^{\frac{-\Delta E}{k_B T}}}{e^{\frac{-\Delta E}{k_B T}} + 1} \tag{12.2.9.13}$$

$$= \frac{1}{e^{\frac{\Delta E}{k_B T}} + 1} \tag{12.2.9.14}$$

$$= \text{Prob}_{\text{occ}}(\epsilon_F + \Delta E) \tag{12.2.9.15}$$

12.2.10. The Fermi energy of Cu is 7.04 eV. Calculate the velocity and de Broglie wavelength of electrons at the Fermi level of Cu. Can these electrons be diffracted by a crystal?

Solution:

$$v = \sqrt{\frac{2E_F}{m}} = 1.6 \times 10^6 \text{ ms}^{-1} \tag{12.2.10.1}$$

$$\lambda = \frac{h}{mv} = 4.63 \text{ Å} \tag{12.2.10.2}$$

Since the wavelength is comparable to atomic spacing, these electrons can be diffracted by a crystal

12.2.11. Show that the fraction of electrons within $k_B T$ of the Fermi energy is $1.5\frac{k_B T}{\varepsilon_F}$, under the assumption that the temperature is so low that the probability of occupancy of levels is not altered from the one at $T = 0$ K. Calculate numerically the value of this fraction for copper ($\varepsilon_F = 7.04$ eV) at 300 K and 1360 K (approximate melting point of Cu). This fraction is of interest because it is a rough measure of the percentage of electrons excited to higher energy states at a temperature T. Find roughly the electronic contribution to specific heat of Cu using this expression.

Solution: First we need the density of states, which we can calculate along similar lines to 12.2.3a

$$g(E)\,dE = \frac{\sqrt{2m^3}}{\pi^2\hbar^3}\sqrt{E}\,dE \tag{12.2.11.1}$$

Using this we can find ε_F in terms of number of electrons N by inspecting $f_{\mathrm{FD},0}(E)$

$$\begin{aligned} N &= V\int_{E=0}^{\infty} f_{\mathrm{FD},0}(E)g(E)\,dE && (12.2.11.2)\\ &= V\frac{\sqrt{2m^3}}{\pi^2\hbar^3}\int_{E=0}^{\varepsilon_F}\sqrt{E}\,dE && (12.2.11.3)\\ &= \frac{\sqrt{8m^3\varepsilon_F^3}}{3\pi^2\hbar^3}V && (12.2.11.4)\end{aligned}$$

We now find the fraction of electrons within k_BT of ε

$$\begin{aligned} f &= V\frac{f_{\mathrm{FD},0}(\varepsilon_F^-)g(\varepsilon_F)k_BT}{N} && (12.2.11.5)\\ &= \frac{3k_BT}{2\varepsilon_F} && (12.2.11.6)\end{aligned}$$

For Cu this can be calculated to be

$$\begin{aligned} f_{300\ \mathrm{K}} &= 0.55\% && (12.2.11.7)\\ f_{1360\ \mathrm{K}} &= 2.5\% && (12.2.11.8)\end{aligned}$$

Thus as we increase the temperature a little bit from $T = 0$, this fraction of electrons jump from levels below ε_F to levels above ε_F. The electron at $\varepsilon_F - k_BT$ jumps to $\varepsilon + k_BT$, gaining $2k_BT$. The electron at ε_F does not gain any energy. Hence on an average each electron gains $\frac{3}{2}k_BT$ The total energy gained is this

$$\begin{aligned} E_{\text{electronic}} &= \frac{Nf}{V}\frac{3k_BT}{2} && (12.2.11.9)\\ &= \frac{9Nk_B^2T^2}{4V\varepsilon_F} && (12.2.11.10)\\ \implies C_{v\text{electronic}} &= \frac{9}{2}R\frac{k_BT}{\varepsilon_F} && (12.2.11.11)\end{aligned}$$