Tutorial – 4

Free particle –

1.) For free particle, $V(x) = 0$

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

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

$$= -k^2\psi(x)$$

$$k = \sqrt{\frac{2mE}{\hbar^2}}$$

Assume $\psi(x) = e^{mx}$

$$\Rightarrow m^2 = -k^2 \Rightarrow m = \pm ik$$

$$\Rightarrow \psi(x)\Big|_{general} = Ce^{ikx} + De^{-ikx}$$

We replace $e^{i\theta} = \cos\theta + i\sin\theta$

$$\text{so } \psi(x) = C(\cos kx + i\sin kx) + D(\cos kx - i\sin kx)$$

$$= i(C-D)\sin kx + (C+D)\cos kx$$

$$= A\sin kx + B\cos kx$$

∴ The 'two' expressions of $\psi(x)$ are equivalent solutions of the TISE of a free particle.

2.) TDSE is given by

$$i\hbar \frac{\partial}{\partial t}\psi(x,t) = E\psi(x,t)$$

$$i\hbar \frac{\partial}{\partial t}\psi(x,t) = E\psi(x,t)$$

In case of free particle,

$$E = \frac{\hbar^2 k^2}{2m} \quad (k \to \text{angular wave number})$$

we are given

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

$$i\hbar \frac{\partial \psi}{\partial t} = i\hbar[-A\omega\cos(kx-\omega t) + B\omega\sin(kx-\omega t)]$$

$$= iE[B\sin(kx-\omega t) - A\cos(kx-\omega t)]$$

But $\text{RHS} = E[A\sin(kx-\omega t) + B\cos(kx-\omega t)]$
$\neq \text{LHS}$

So $\psi(x,t)$ does not obey TDSE.

3.) $\psi = Ae^{ikx} + Be^{-ikx}$

$$\Rightarrow \psi^* = Ae^{-ikx} + Be^{ikx}$$

$$\Rightarrow \psi^* \frac{d\psi}{dx} = (Ae^{-ikx} + Be^{ikx}) \times (ikAe^{ikx} - ikBe^{-ikx})$$

$$= ik(A^2 - ABe^{-2ikx} + ABe^{2ikx} - B^2)$$

$$= ik(A^2-B^2) + ikAB(e^{2ikx} - e^{-2ikx})$$

$$= ik(A^2-B^2) - 2kAB\sin 2kx$$

$$\Rightarrow \frac{\hbar}{m} \tilde{S}\left(\psi^* \frac{d\psi}{dx}\right) = \frac{\hbar k}{m}(A^2 - B^2)$$

Physical significance:

This quantity represents probability current.

4) $\psi(x,t) = Ae^{i(5.02\times10^{11}x - 8\times10^{15}t)}$

$$k = 5.02\times10^{11}\ m^{-1}, \quad \omega = 8\times10^{15}\ s^{-1}$$

$$p = \hbar k = \frac{6.626\times10^{-34}\times5.02\times10^{11}}{2\pi}\ Js/m$$

$$= 5.294\times10^{-25}\ kg\,ms^{-1}$$

$$E = \hbar\omega = 6.626\times10^{-34}\times8\times10^{15}\ J$$

$$= 53.008\times10^{-19}\ J$$

5) $\psi(x) = \begin{cases} A\left(1+\cos\frac{\pi x}{a}\right), & |x|\le a \\ 0, & |x|>a \end{cases}$

$$\int_{-\infty}^{\infty} |\psi|^2 dx = A^2\int_{-a}^{a}\left[1+2\cos\frac{\pi x}{a}+\cos^2\frac{\pi x}{a}\right]dx$$

$$= 2A^2\int_0^a\left(1+2\cos\frac{\pi x}{a}+\frac{1+\cos\frac{2\pi x}{a}}{2}\right)dx$$

$$= A^2\int_0^a\left(3+4\cos\frac{\pi x}{a}+\cos\frac{2\pi x}{a}\right)dx$$

$= 3aA^2$

we see, ψ is continuous and finite and same for $\frac{d\psi}{dx}$, also $\psi = 0$ for $x \to \pm\infty$, ~~it is just not~~ normalised, so it is a physically acceptable wave function.

Now, $3aA^2 = 1 \Rightarrow A = \pm \frac{1}{\sqrt{3a}}$

[Take +ve sign]

$\Delta x = a - (-a) = 2a$

$$a(k) = \int_{-\infty}^{\infty} \psi(x) e^{-ikx} dx$$

$$= \frac{1}{\sqrt{3a}} \int_{-a}^{a} \left(1 + \cos\frac{\pi x}{a}\right) e^{-ikx} dx$$

$$= \frac{1}{\sqrt{3a}} \int_{0}^{a} \left(1 + \cos\frac{\pi x}{a}\right)\left(e^{ikx} + e^{-ikx}\right) dx$$

$$= \frac{2}{\sqrt{3a}} \int_{0}^{a} \left(1 + \cos\frac{\pi x}{a}\right) \cos kx \, dx$$

$$= \frac{2}{\sqrt{3a}} \left[\int_{0}^{a} \left(\cos kx + \cos\frac{\pi x}{a} \cos kx\right) dx\right]$$

$$= \frac{2}{\sqrt{3a}} \left[\frac{\sin kx}{k}\Big|_{0}^{a} + \frac{1}{2} \int_{0}^{a} \left[\cos\left(\frac{\pi}{a} + k\right)x + \cos\left(\frac{\pi}{a} - k\right)x\right] dx\right]$$

$$= \frac{2}{\sqrt{3a}}\left[\frac{\sin ka}{k} + \frac{1}{2}\left\{\frac{\sin\left(\frac{\pi}{a}+k\right)a}{\frac{\pi}{a}+k} + \frac{\sin\left(\frac{\pi}{a}-k\right)a}{\frac{\pi}{a}-k}\right\}\right]$$

$$= \frac{1}{\sqrt{3a}}\left(\frac{2\sin ka}{k} - \frac{\sin ka}{\frac{\pi}{a}+k} + \frac{\sin ka}{\frac{\pi}{a}-k}\right)$$

$$= \frac{\sin ka}{\sqrt{3a}}\left[\frac{2}{k} + \frac{2k}{\left(\frac{\pi^2}{a^2}-k^2\right)}\right]$$

$$= \frac{2\sin ka}{\sqrt{3a}}\left[\frac{\pi^2/a^2}{k\left(\pi^2/a^2-k^2\right)}\right]$$

$$= \frac{2\pi^2\sin ka}{\sqrt{3a}\,k(\pi^2-a^2k^2)}$$

$$\Delta k = \frac{2\pi}{a} - \left(-\frac{2\pi}{a}\right) = \frac{4\pi}{a}$$

$$\therefore \Delta x \Delta p = 2a \times \hbar \times \frac{4\pi}{a}$$

$$= 4h > \frac{\hbar}{2}$$

d.) $|x| \le a$ is the classically allowed region. (Think why! ☺)

☆ Particle in a box –

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

Probability of finding the particle between $x = a$ and $x = a+b$

between $x=a$ and $x=a+b$,

$$P = \frac{2}{L}\int_a^{a+b} \sin^2\frac{n\pi x}{L}\,dx$$

$$= \frac{1}{L}\int_a^{a+b}\left(1-\cos\frac{2n\pi x}{L}\right)dx$$

$$= \frac{1}{L}\left[x - \frac{L}{2n\pi}\sin\frac{2n\pi x}{L}\right]_a^{a+b}$$

$$= \frac{1}{L}\left[b - \frac{L}{2n\pi}\left\{\sin\frac{2n\pi(a+b)}{L} - \sin\frac{2n\pi a}{L}\right\}\right]$$

Now, $E = \dfrac{n^2h^2}{8mL^2}$

$E \rightarrow$ very high $\Rightarrow n \rightarrow$ very large

$\Rightarrow \dfrac{L}{2n\pi} \longrightarrow 0$

So $P = \dfrac{b}{L}$

2) Ground state $\Rightarrow n = 1$

$P\left(x=\frac{L}{3} \text{ to } x=\frac{2L}{3}\right)$

$$= \frac{1}{L}\left[x - \frac{L}{2\pi}\sin\frac{2\pi x}{L}\right]_{L/3}^{2L/3}$$

$$= \frac{1}{L}\left[\frac{L}{3} - \frac{L}{2\pi}\left(-\frac{\sqrt{3}}{2} - \frac{\sqrt{3}}{2}\right)\right]$$

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

3.) a.) $\langle x \rangle_n = \int_{-\infty}^{\infty} \psi^* x \psi \, dx$

$$= \int_0^a x |\psi|^2 dx$$

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

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

$$= \frac{1}{a} \left[\frac{a^2}{2} - \int_0^a x \cos \frac{2n\pi x}{L} dx \right]$$

$$= \frac{a}{2}$$

$$\langle p \rangle_n = \int_0^a \sqrt{\frac{2}{a}} \sin \frac{n\pi x}{a} \left(-i\hbar \frac{\partial}{\partial x} \right) \sqrt{\frac{2}{a}} \sin \frac{n\pi x}{a} dx$$

$$= \frac{-2i\hbar}{a} \int_0^a \sin \frac{n\pi x}{a} \frac{n\pi}{a} \cos \frac{n\pi x}{a} dx$$

$$= \frac{-i\hbar n\pi}{a^2} \int_0^a \sin \frac{2n\pi x}{a} dx$$

$$= 0$$

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

$$= \frac{2}{a}\left[\frac{a^3\{4\pi^3 n^3 - 6\pi n\}}{24\pi^3 n^3}\right]$$

$$= \frac{a^2}{6}\left(2 - \frac{3}{\pi^2 n^2}\right)$$

$$\langle p^2\rangle_n = \int_{-\infty}^{\infty} \psi^* \left(-i\hbar \frac{d}{dx}\right)^2 \psi \, dx$$

$$= \frac{-2\hbar^2}{a} \int_0^a \sin\frac{n\pi x}{a} \frac{d^2}{dx^2} \sin\frac{n\pi x}{a} \, dx$$

$$= \frac{2\hbar^2}{a} \int_0^a \sin^2\frac{n\pi x}{a} \, dx \quad \times \frac{n^2\pi^2}{a^2}$$

$$= \frac{\hbar^2}{a} \int_0^a \left(1 - \cos\frac{2n\pi x}{a}\right) dx \quad \times \frac{n^2\pi^2}{a^2}$$

$$= \frac{\hbar^2}{a}\left[x - \frac{a}{2n\pi} \sin\frac{2n\pi x}{a}\right]_0^a \times \frac{n^2\pi^2}{a^2}$$

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

$$= \frac{n^2 h^2}{4a^2}$$

b) $\Delta x_n \Delta p_n = \sqrt{\langle x_n^2\rangle - \langle x_n\rangle^2} \sqrt{\langle p_n^2\rangle - \langle p_n\rangle^2}$

$$= \sqrt{\frac{a^2}{6}\left[2-\frac{3}{\pi^2 n^2}\right]-\frac{a^2}{4}}\;\sqrt{\frac{n^2h^2}{4a^2}}$$

$$= \sqrt{\frac{1}{3}-\frac{1}{2\pi^2 n^2}-\frac{1}{4}} \times \frac{nh}{2}$$

$$= \frac{nh}{2}\sqrt{\frac{1}{12}-\frac{1}{2\pi^2 n^2}}$$

$$= \frac{nh}{2}\sqrt{\frac{2\pi^2 n^2-12}{24\pi^2 n^2}}$$

$$= \frac{\hbar}{2}\sqrt{\frac{2\pi^2 n^2-12}{6}}$$

$$= \frac{\hbar}{2}\sqrt{\frac{\pi^2 n^2}{3}-2}$$

c.) $\langle K\rangle = \frac{\langle p_n^2\rangle}{2m} = \frac{n^2h^2}{8ma^2}$

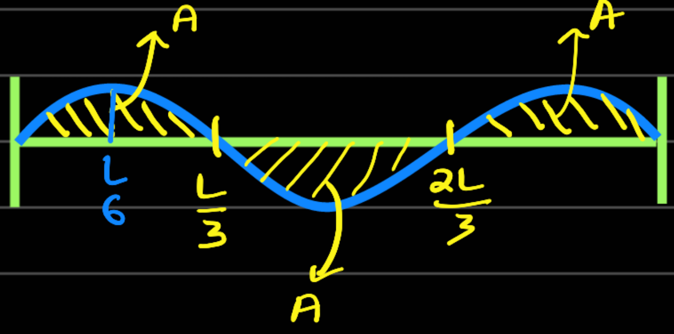
[Don't know how to use expression in (b) to obtain this expression]

4.) Probability $= \frac{2}{L}\int_0^{L/6} \sin^2\frac{3\pi x}{L}\,dx$

$$= \frac{1}{L}\int_0^{L/6}\left(1-\cos 6\pi x/L\right)dx$$

$$= \frac{1}{L}\times\frac{L}{6} = \frac{1}{6}$$

How to 'guess' the answer without performing the integral?



Area of each lobe, due to 'symmetry' is equal $(= A)$.

Area from 0 to $\frac{L}{6} = \frac{A}{2}$

Now, $A + A + A = 1$

[A is probability, and $\sum$ probability $= 1$]

$$\Rightarrow A = \frac{1}{3}$$

$$\Rightarrow \frac{A}{2} = \frac{1}{6}$$

5) a) $\psi(x,t) = \sin\frac{\pi x}{a} e^{-i\omega t}$

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

$$\Rightarrow \hbar\omega = \frac{\hbar^2}{2m} \times \frac{\pi^2}{a^2} \psi + V(x)\psi$$

$$\Rightarrow V(x) = \hbar\omega - \frac{h^2}{8ma^2}$$

b) First normalise $\psi(x,t)$.

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

$$\Rightarrow A \int_0 \sin \frac{\pi x}{a}\, dx = 1$$

$$\Rightarrow A = \sqrt{\frac{2}{a}}$$

Now, $$\frac{2}{a} \int_{a/4}^{3a/4} \sin^2 \frac{\pi x}{a}\, dx$$

$\cos \frac{2\pi x}{a}$

$$= \frac{1}{a}\left[\frac{a}{2} + \frac{a}{\pi}\right]$$

$$= \frac{1}{2} + \frac{1}{\pi}$$

Q6 is done at the end

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

$$\Rightarrow \frac{d^2\psi}{dx^2} = -\frac{2mE}{\hbar^2}\psi$$

$$= -k^2\psi \qquad \left[k = \frac{2mE}{\hbar^2}\right]$$

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

$$\psi\left(-\frac{L}{2}\right) = 0 = \psi\left(\frac{L}{2}\right)$$

$$\Rightarrow -A\sin\frac{kL}{2} + B\cos\frac{kL}{2} = 0 = A\sin\frac{kL}{2} + B\cos\frac{kL}{2}$$

$$\Rightarrow A\sin\frac{kL}{2} = 0 \quad \Rightarrow A = 0 \quad \text{OR } k = \frac{2n\pi}{L}$$

If $A = 0 \Rightarrow B\cos\frac{kL}{2} = 0 \Rightarrow k = (2n-1)\frac{\pi}{L}$

So $\psi(x) = \sqrt{\frac{2}{L}} \cos \frac{(2n-1)\pi x}{L}$ $(n \in N)$

$\left(B = \sqrt{\frac{2}{L}} \text{ upon normalisation}\right)$

If $K = \frac{2n\pi}{L}$

$\Rightarrow B \cos \frac{2n\pi}{L} \times \frac{L}{2} = 0$

$\Rightarrow B \cos n\pi = 0 \Rightarrow B = 0$

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

Normalisation: $\int_{-L/2}^{L/2} |\psi(x)|^2 dx = 1$

$\Rightarrow A^2 \int_{-L/2}^{L/2} \sin^2 \frac{2n\pi x}{L} dx = 1$

$\Rightarrow A = \sqrt{\frac{2}{L}}$

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

8) $\psi(x) = A\left(\sin \frac{\pi x}{L} + \sin \frac{2\pi x}{L}\right)$ $x \in [0, L]$

a) Now, $A^2 \int_0^L \left(\sin \frac{\pi x}{L} + \sin \frac{2\pi x}{L}\right)^2 dx = 1$

$\Rightarrow A^2 \int_0^L \left(\sin^2 \frac{\pi x}{L} + 2 \sin \frac{\pi x}{L} \sin \frac{2\pi x}{L} + \sin^2 \frac{2\pi x}{L}\right) dx$

$= 1$

$\Rightarrow A^2 L = 1$

$\Rightarrow A = \frac{1}{}$

$\sqrt{L}$

b.) $$\langle x \rangle = \int_0^L \psi^* x \psi \, dx$$

$$= \frac{1}{L} \int_0^L x \left(\sin\frac{\pi x}{L} + \sin\frac{2\pi x}{L} \right)^2 dx$$

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

$$\langle x^2 \rangle = \frac{1}{L} \int_0^L \left[x \left(\sin\frac{\pi x}{L} + \sin\frac{2\pi x}{L} \right) \right]^2 dx$$

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

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

$$= L \sqrt{\frac{1}{3} - \frac{301}{144\pi^2} - \left(\frac{1}{2} - \frac{16}{9\pi^2} \right)^2}$$

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

$$= L \sqrt{\frac{1}{12} - \frac{45}{144\pi^2} - \frac{256}{81\pi^4}}$$

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

c.) $$\langle p \rangle = \frac{1}{L} \int_0^L \left(\sin\frac{\pi x}{L} + \sin\frac{2\pi x}{L} \right) \times -i\hbar \frac{d}{dx} \left(\sin\frac{\pi x}{L} + \sin\frac{2\pi x}{L} \right) dx$$

L

$$= \frac{-i\hbar\pi}{L^2} \int_0 \left(\sin\frac{\pi x}{L} + \sin\frac{2\pi x}{L}\right)\left(\cos\frac{\pi x}{L} + 2\cos\frac{2\pi x}{L}\right)dx$$

$$= 0$$

$$\langle p^2 \rangle = \frac{1}{L}\int_0^L \left(\sin\frac{\pi x}{L} + \sin\frac{2\pi x}{L}\right)\left(-i\hbar\frac{\partial}{\partial x}\right)^2 \left(\sin\frac{\pi x}{L} + \sin\frac{2\pi x}{L}\right)dx$$

$$= \frac{\hbar^2\pi^2}{L^3}\int_0^L \left(\sin\frac{\pi x}{L} + \sin\frac{2\pi x}{L}\right)\left(\sin\frac{\pi x}{L} + 4\sin\frac{2\pi x}{L}\right)dx$$

$$= \frac{5\hbar^2\pi^2}{2L^2} = \frac{5h^2}{8L^2}$$

$$\Delta p = \sqrt{\langle p^2\rangle - \langle p\rangle^2} = \frac{h}{2L}\sqrt{\frac{5}{2}}$$

d.) $\psi(x) = \frac{1}{\sqrt{L}}\sin\frac{\pi x}{L} + \frac{1}{\sqrt{L}}\sin\frac{2\pi x}{L}$

Perform the operation

$$\int_0^L \phi_2^*(x)\,\psi(x)\,dx$$

$$= \int_0^L \left(\sqrt{\frac{2}{L}}\sin\frac{2\pi x}{L}\right)\left(\frac{1}{\sqrt{L}}\sin\frac{\pi x}{L} + \frac{1}{\sqrt{L}}\sin\frac{2\pi x}{L}\right)dx$$

$$= \frac{\sqrt{2}}{L}\int_0^L \left(\sin\frac{2\pi x}{L}\sin\frac{\pi x}{L} + \sin^2\frac{2\pi x}{L}\right)dx$$

$$= \frac{1}{\ldots}$$

$\sqrt{2}$

Probability of finding the particle in 1st excited state $= \left(\frac{1}{\sqrt{2}}\right)^2 = \frac{1}{2}$

6.) $\psi(x) = \sqrt{\frac{2}{a}} \sin\frac{\pi x}{a}$

$\phi_1(x) = \sqrt{\frac{1}{2a}} \sin\frac{\pi x}{4a}$

$\phi_2(x) = \sqrt{\frac{1}{2a}} \sin\frac{\pi x}{2a}$

a.) Perform $\left|\int_0^a \phi_1^* \psi \, dx\right|^2$

$$= \left|\frac{1}{a}\int_0^a \sin\frac{\pi x}{4a} \sin\frac{\pi x}{a} \, dx\right|^2$$

$$= \frac{1}{4a^2}\left|\int_0^a \left[\cos\left(\frac{3\pi x}{4a}\right) - \cos\left(\frac{5\pi x}{4a}\right)\right] dx\right|^2$$

$$= \frac{1}{4a^2}\left|\left[\frac{4a}{3\pi} \sin\frac{3\pi}{4} - \frac{4a}{5\pi} \sin\frac{5\pi}{4}\right]\right|^2$$

$$= \frac{1}{4}\left|\frac{4}{3\pi\sqrt{2}} + \frac{4}{5\pi\sqrt{2}}\right|^2$$

$$= \frac{1}{4} \times \frac{16}{2\pi^2}\left|\frac{1}{3} + \frac{1}{5}\right|^2$$

$$= \frac{2}{\pi^2} \times \frac{64}{225} = \frac{128}{225\pi^2}$$

b.) Perform $\left|\int_0^a \phi_2^*(x) \, \psi(x) \, dx\right|^2$

$$= \left| \frac{1}{a} \int_0^a \sin\frac{\pi x}{2a} \sin\frac{\pi x}{a} \right|^2$$

$$= \frac{1}{4a^2} \left| \int_0^a \left[\cos\frac{\pi x}{2a} - \cos\frac{3\pi x}{2a} \right] dx \right|^2$$

$$= \frac{1}{4a^2} \left| \frac{2a}{\pi} \sin\frac{\pi}{2} - \frac{2a}{3\pi} \sin\frac{3\pi}{2} \right|^2$$

$$= \left| \frac{1}{\pi} + \frac{1}{3\pi} \right|^2$$

$$= \frac{16}{9\pi^2}$$