Q.1. If a free particle of mass m is confined to a one-dimensional region $0 \leq x \leq a$. The energy eigen states and eigen values of the particle are

$$X_n = \sqrt{\frac{2}{a}} \sin \frac{n\pi x}{a}$$

$$E_n = \frac{n^2 \pi^2 \hbar^2}{2ma^2} \qquad n = 1, 2, 3 \ldots$$

Now, assume the normalized wave function of the particle at $t = 0$ is

$$\Psi(x,0) = \sqrt{\frac{8}{5a}} \left[1 + \cos\frac{\pi x}{a}\right] \sin\frac{\pi x}{a}$$

Find wave function at any time, $\Psi(x,t)$

a) Find wave function at any time, $\Psi(x,t)$

b) Calculate the average energy at $t = 0$, and $t = t_0$

c) what is the probability that the particle is found in the left half of the box.

Ans:

$$\Psi(x,0) = \sqrt{\frac{8}{5a}} \left[\sin\frac{\pi x}{a} + \cos\frac{\pi x}{a} \sin\frac{\pi x}{a}\right]$$

$$= \sqrt{\frac{8}{5a}} \left[\sin\frac{\pi x}{a} + \frac{1}{2}\sin\frac{2\pi x}{a}\right]$$

Now we know general time dependent state:

$$\Psi(x,t) = \sum A_n X_n e^{-\frac{iE_n t}{\hbar}}$$

Therefore: $\Psi(x,0) = \sum A_n X_n = \sum A_n \sqrt{\frac{2}{a}} \sin\frac{n\pi x}{a}$

Therefore: $A_1 = \frac{2}{\sqrt{5}}, \quad A_2 = \frac{1}{\sqrt{5}}, \quad A_3 = A_4 = \cdots 0$

$$\Psi(x,t) = \sqrt{\frac{8}{5a}} \left[\sin\frac{\pi x}{a} e^{-\frac{iE_1 t}{\hbar}} + \frac{1}{2}\sin\frac{2\pi x}{a} e^{-\frac{iE_2 t}{\hbar}}\right]$$

b) Average energy at $t = 0$.

$$\langle H \rangle = \int_0^a \psi^*(x,0)\, \hat{H}\, \Psi(x,0)\, dx$$

$$= \int_0^a \frac{8}{5a}\left[\sin\frac{\pi x}{a} + \frac{1}{2}\sin\frac{2\pi x}{a}\right] \hat{H} \left[\sin\frac{\pi x}{a} + \frac{1}{2}\sin\frac{2\pi x}{a}\right] dx$$

$$= \sum_n |A_n|^2 E_n = \frac{4}{5}E_1 + \frac{1}{5}E_2$$

$$= \frac{4E_1 + E_2}{5} = \left(\frac{4\pi^2\hbar^2}{2ma^2} + \frac{4\pi^2\hbar^2}{2ma^2}\right)\frac{1}{5}$$

$$= \frac{8\pi^2\hbar^2}{10ma^2}$$

Average energy at $t = t_0$ should also be the same.

c)

$$P = \int_0^{a/2} \Psi^*(x,t)\, \Psi(x,t)\, dx$$

$$= \int_0^{a/2} \frac{8}{5a}\left[\sin\frac{\pi x}{a} e^{+\frac{iE_1 t}{\hbar}} + \frac{1}{2}\sin\frac{2\pi x}{a} e^{+\frac{iE_2 t}{\hbar}}\right] \times \left[\sin\frac{\pi x}{a} e^{-\frac{iE_1 t}{\hbar}} + \frac{1}{2}\sin\frac{2\pi x}{a} e^{-\frac{iE_2 t}{\hbar}}\right] dx$$

$$e^{\frac{i}{\hbar}(E_1 - E_2)t}$$

$$= \frac{8}{5a}\int_0^{a/2} \left\{\sin^2\frac{\pi x}{a} + \frac{1}{2}\sin\frac{\pi x}{a}\sin\frac{2\pi x}{a} + \frac{1}{2}\sin\frac{2\pi x}{a}\sin\frac{\pi x}{a} e^{\frac{i}{\hbar}(E_2 - E_1)t} + \frac{1}{4}\sin^2\frac{2\pi x}{a}\right\} dx$$

$$= \frac{8}{5a}\int_0^{\frac{a}{2}} \left\{\sin^2\frac{\pi x}{a} + \frac{1}{4}\sin^2\frac{2\pi x}{a} + \sin\frac{\pi x}{a}\sin\frac{2\pi x}{a}\cos\underbrace{\frac{(E_1 - E_2)}{\hbar}}_{\omega}t\right\} dx$$

$$= \frac{8}{5a}\int_0^{a/2} \left[\frac{1}{2}\left(1 - \cos\frac{2\pi x}{a}\right) + \frac{1}{8}\left(1 - \cos\frac{4\pi x}{a}\right) + \frac{\cos\omega t}{2}\left(\cos\frac{\pi x}{a} - \cos\frac{3\pi x}{a}\right)\right] dx$$

$$= \frac{8}{5a}\left[\frac{a}{4} + \frac{a}{16} + \frac{\cos\omega t}{2}\left(\frac{a}{\pi} + \frac{a}{3\pi}\right)\right] = \frac{8}{5}\left(\frac{5}{16} + \frac{2}{3\pi}\cos\omega t\right)$$

Q.2 Time independent wave function of a free particle in a box is

$$\Psi(x) = A\,x(a-x) \qquad 0 \le x \le a$$

a) Calculate A.
b) Calculate average energy of the particle.
c) Calculate the corresponding momentum wave function.
d) What is the probability of finding the particle at energy $E_1 = \frac{\pi^2\hbar^2}{2ma^2}$.

Normalized energy eigen states and eigen values are given in the question no. (1)

Ans: a)

$$\int_0^a A^2 x^2 (a-x)^2\,dx = A^2\left[\frac{a^2x^3}{3} - \frac{2ax^4}{4} + \frac{x^5}{5}\right]_0^a$$

$$= A^2 \cdot a^5\left[\frac{1}{3} - \frac{1}{2} + \frac{1}{5}\right] = \frac{A^2a^5}{30} = 1$$

$$\boxed{A = \sqrt{\frac{30}{a^5}}}$$

b)

$$\langle H\rangle = \int_{-\infty}^{\infty} \psi^* \hat{H}\Psi\,dx = \int_{-\infty}^{\infty} \psi^*\left(\frac{\hat{p}^2}{2m}\right)\Psi\,dx$$

$$= \int_0^a A^2 x(a-x)\left(-\frac{\hbar^2}{2m}\right)\frac{d^2}{dx^2}(xa-x^2)\,dx$$

$$= +\frac{A^2\hbar^2}{2m}\int_0^a x(a-x)\cdot 2\,dx$$

$$= \frac{2A^2\hbar^2}{2m}\left[\frac{ax^2}{2} - \frac{x^3}{3}\right]_0^a = \frac{A^2\hbar^2a^3}{m}\frac{1}{6}$$

Average energy of the particle is

$$\langle E\rangle = \frac{\hbar^2a^3}{6m} \times \frac{30}{a^5} = \frac{5\hbar^2}{ma^2}$$

c) Momentum wave function of the particle

$$\Phi(p) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} \Psi(x)\, e^{-\frac{i}{\hbar}px}\, dx$$

$$= \frac{1}{\sqrt{2\pi\hbar}} \int_{0}^{a} Ax(a-x)\, e^{-\frac{i}{\hbar}px}\, dx$$

$$= \frac{A}{\sqrt{2\pi\hbar}} \left[\frac{x(a-x)\, e^{-\frac{i}{\hbar}px}}{\left(-\frac{i}{\hbar}p\right)} - \frac{((a-x) - \cancel{x})\, e^{-\frac{i}{\hbar}px}}{\left(-\frac{i}{\hbar}p\right)^2} + \frac{-2x\, e^{-\frac{i}{\hbar}px}}{\left(-\frac{i}{\hbar}p\right)^3} \right]\Bigg|_0^a$$

$$= \frac{A}{\sqrt{2\pi\hbar}} \left[\frac{a\, e^{-\frac{i}{\hbar}pa}}{\left(-\frac{i}{\hbar}p\right)^2} + \frac{a}{\left(-\frac{i}{\hbar}p\right)^2} - \frac{2e^{-\frac{i}{\hbar}pa}}{\left(-\frac{i}{\hbar}p\right)^3} + \frac{2}{\left(-\frac{i}{\hbar}p\right)^3} \right]$$

$$= \frac{2A}{\sqrt{2\pi\hbar}} \left[-\frac{a\hbar^2 e^{-\frac{i}{\hbar}pa}}{p^2} - \frac{a\hbar^2}{p^2} - \frac{\hbar^3 e^{-\frac{i}{\hbar}pa}}{p^3} + \frac{\hbar^3}{p^3} \right].$$

d) Any general wave function (time independent) can be written as

$$\Psi = \sum A_n \chi_n \qquad \chi_n = \sqrt{\frac{2}{a}} \sin\frac{n\pi x}{a}$$

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

By using orthogonality property, the probability amplitude A_n of finding the particle at energy E_n is

$$A_n = \int_{-\infty}^{\infty} \chi_n^* \Psi\, dx$$

Hence

$$A_1 = \int_0^a X_1^* \Psi \, dx$$

$$= \int_0^a \sqrt{\frac{2}{a}} \sin\frac{\pi x}{a} \, A x(a-x) \, dx$$

$$= A\sqrt{\frac{2}{a}} \int_0^a x(a-x) \sin\frac{\pi x}{a} \, dx$$

$$= A\sqrt{\frac{2}{a}} \left[\frac{x(a-x)\left(-\cos\frac{\pi x}{a}\right)}{(\pi/a)} - \frac{-2x\left(-\sin\frac{\pi x}{a}\right)}{(\pi/a)^2} + \frac{-2\cos\frac{\pi x}{a}}{(\pi/a)^3} \right]_0^a$$

$$= A\sqrt{\frac{2}{a}} \left[-\frac{2a\sin\frac{\pi a}{a}}{(\pi/a)^2} - \frac{2\cos\pi}{(\pi/a)^3} + \frac{2\cos 0^\circ}{(\pi/a)^3} \right]$$

$$= A\sqrt{\frac{2}{a}} \left[\frac{4}{(\pi/a)^3} \right]$$

Therefore the probability is

$$|A_1|^2 = A^2 \frac{2}{a} \frac{16a^6}{\pi^6} = \frac{30}{a^5} \frac{2}{a} \frac{16a^6}{\pi^6} = \frac{60 \times 16}{\pi^6}$$

$$= 0.998$$

Q3. For a free particle the momentum space wave function at $t=0$ is given by

$$\phi(P,0) = A e^{-\alpha p^2}$$

a) Find A.

b) Find $\Psi(x,t)$.

Ans:

a) $$\int_{-\infty}^{\infty} A^2 e^{-2\alpha p^2} dp = A^2 \sqrt{\frac{\pi}{2\alpha}} = 1$$

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

b) $$\Psi(x,t) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} \Phi(P)\, e^{\frac{i}{\hbar}(PX - Et)} dp$$

Now for free particle $E = \frac{p^2}{2m}$

Therefore: $$\Psi(x,t) = \frac{A}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} e^{-\alpha p^2} e^{\frac{i}{\hbar}\left(PX - \frac{p^2 t}{2m}\right)} dp$$

$$\boxed{\beta = \alpha + \frac{it}{2m}}$$

$$= \frac{A}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} e^{-\left(\alpha + \frac{it}{2m}\right)p^2 + \frac{ipx}{\hbar}} dp$$

$$= \frac{A}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} e^{-\left(\alpha + \frac{it}{2m}\right)\left[p^2 + \frac{ix\, p}{\hbar\left(\alpha + \frac{it}{2m}\right)}\right]} dp$$

$$\Psi(x,t) = \frac{A}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} e^{-\beta\left(P + \frac{ix}{2\hbar\beta}\right)^2 + \beta\left(\frac{ix}{2\hbar\beta}\right)^2} dp$$

$$\Psi(x,t) = \frac{A e^{-\frac{\beta x^2}{4\hbar^2\beta^2}}}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} e^{-\beta\left(p + \frac{ix}{2\beta\hbar}\right)^2} dp$$

$$= \frac{A}{\sqrt{2\pi\hbar}} \sqrt{\frac{\pi}{\beta}}\, e^{-\frac{\beta x^2}{4\hbar^2\beta}} = \frac{A}{\sqrt{2\pi\hbar}} \sqrt{\frac{\pi}{\beta}}\, e^{-\frac{x^2}{4\hbar^2\beta}}$$

$$\boxed{\Psi(x,t) = \frac{A}{\sqrt{2\pi\hbar}} \sqrt{\frac{\pi}{\alpha + \frac{it}{2m}}}\, e^{-\frac{x^2}{4\hbar^2\left(\alpha + \frac{it}{2m}\right)}}}$$

Q.4 In quantum mechanics two operators $(\hat{a}, \hat{b})$ may (6)
not commute i.e. $\hat{a}\hat{b} - \hat{b}\hat{a} \neq 0$. We use $[\hat{a}, \hat{b}] = \hat{a}\hat{b} - \hat{b}\hat{a}$.
Show that

a) $[\hat{x}^2, \hat{p}] = 2i\hbar\, \hat{x}$

b) By process of induction show $[\hat{x}^n, \hat{p}] = (+n) i\hbar\, \hat{x}^{n-1}$

Use fundamental commutation relation $[\hat{x}, \hat{p}] = i\hbar$

It can be shown that
$[AB, C] = A[B,C] + [A,C]B$

Ans: a) $[x^2, p] = xxp - pxx$

$= xxp - xpx + xpx - pxx$

$= x[x,p] + [x,p]x$

$= x\, i\hbar + i\hbar\, x = 2i\hbar\, x$

b) $[x^n, p] = ?$

take $n = 3$: $[x^3, p] = x[x^2, p] + [x, p]x^2$

$= 2x . i\hbar x + i\hbar\, x x$

$= 3 i\hbar x^2 = 3 i\hbar\, x^2$

Hence : $\boxed{[x^n, p] = n i\hbar\, x^{n-1}}$

Anothe method   Since $\hat{x}, \hat{p}$ are operator, they must
act on a state :

$[\hat{x}^n, \hat{p}]\Psi = (x^n \hat{p} - \hat{p}\, x^n)\Psi = x^n\left(-i\hbar \frac{\partial \psi}{\partial x}\right) - \left(-i\hbar \frac{\partial}{\partial x} x^n \Psi\right)$

$= x^n\left(-i\hbar \frac{\partial \psi}{\partial x}\right) + i\hbar\, n\, x^{n-1}\Psi - x^n\left(-i\hbar \frac{\partial \psi}{\partial x}\right)$

$= n i\hbar\, x^{n-1}\, \Psi$

Therefore, as an operator, we can identify $[\hat{x}^n, \hat{p}] = n i\hbar\, \hat{x}^{n-1}$