PHYS 262 - PARTICLE IN A BOX, CHAPTER 40

IN QUANTUM MECHANICS THE PROBABILITY DISTRIBUTION FUNCTION IS given BY $|\psi|^2 = \psi\psi^*$

FOR A stationary state, $\psi = \Phi e^{-iEt/\hbar}$

$$\psi\psi^* = \Phi e^{-iEt/\hbar}\Phi^* e^{iEt/\hbar} = |\Phi|^2$$

AVERAGES ARE FOUND BY INTEGRATING THE DISTRIBUTION FUNCTION:

$$\boxed{\bar{x} = \int x|\psi|^2 dx = \int x|\Phi|^2 dx}$$

IN QUANTUM MECHANICS, WE CAN ALSO FIND THE AVERAGE MOMENTUM, $\bar{p}$.

CONSIDER THE FREE PARTICLE, $U = 0 \Rightarrow \Phi = Ae^{ikx} + Be^{-ikx}$

WHERE $p = \hbar k$.

NOTICE THAT $\frac{\partial\Phi}{\partial x} = ikAe^{ikx} - ikBe^{-ikx} = \frac{ip}{\hbar}Ae^{ikx} + \frac{ip}{\hbar}Be^{-ikx}$

$$= \frac{ip}{\hbar}\Phi$$

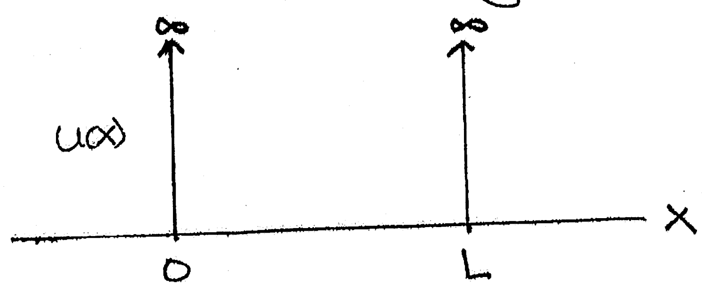
THE NEGATIVE SIGN GOES AWAY BECAUSE e^{-ikx} IS A PLANE WAVE PROPAGATING TO THE LEFT, i.e., WITH momentum $p = -\hbar k$. WE'LL ASSUME THIS IS TRUE IN GENERAL

$$\frac{\partial\Phi}{\partial x} = \frac{ip}{\hbar}\Phi \Rightarrow p\Phi = \frac{\hbar}{i}\frac{\partial\Phi}{\partial x} = \frac{i}{i}\frac{\hbar}{i}\frac{\partial\Phi}{\partial x} = \frac{i\hbar}{i^2}\frac{\partial\Phi}{\partial x} = -i\hbar\frac{\partial\Phi}{\partial x}$$

$$\bar{p} = \int p|\psi|^2 dx = \int p|\Phi|^2 dx = \int p\Phi\Phi^* dx = \int \Phi^* p\Phi\, dx$$

$$\Rightarrow \boxed{\bar{p} = \int \Phi^* (-i\hbar) \frac{\partial \Phi}{\partial x}\, dx}$$

PARTICLE IN A BOX — BOX $\Rightarrow$ REGION OF LENGTH L WHOSE SIDES ARE INFINITELY STRONG.



$U(0) = U(L) = \infty$

$\Rightarrow$ PROBABILITY TO BE OUTSIDE THE BOX IS ZERO $\Rightarrow \Phi(0) = \Phi(L) = 0$.

INSIDE THE BOX, $U(x) = 0 \Rightarrow \Phi = Ae^{ikx} + Be^{-ikx}$

NEED TO MATCH THE BOUNDARY CONDITIONS TO FIND A AND B

BC'S ARE $\Phi(0) = 0$, $\Phi(L) = 0$

$$\Phi(0) = Ae^{ik\phi} + Be^{-ik\phi} = A + B \Rightarrow A + B = 0 \Rightarrow A = -B$$

$$\Rightarrow \Phi = Ae^{ikx} - Ae^{-ikx} = A(e^{ikx} - e^{-ikx}) = A(2i\sin kx) = 2iA\sin(kx)$$

$$\Rightarrow \Phi = C\sin(kx)$$

$$\Phi(L) = C\sin(kL) = 0 \Rightarrow kL = n\pi \quad n = 1, 2, 3, \ldots$$

(CAN'T DO $n = 0$ BECAUSE $L \neq 0$ NOR DOES $k = 0$)

$p = \hbar k$. $U = 0$, $E = K + U \Rightarrow E = K = p^2/2M$

$$\Rightarrow E = \frac{(\hbar k)^2}{2M} = \frac{\hbar^2}{2M}\left(\frac{n\pi}{L}\right)^2 \Rightarrow \boxed{E = \frac{\pi^2\hbar^2}{2ML^2} n^2}$$

WE FIND THE C CONSTANT FROM NORMALIZATION

$\int_{-\infty}^{\infty} |\Phi|^2 dx = 1$. THE PROBABILITY TO BE OUTSIDE THE BOX $(x<0, x>L)$ IS $\phi \Rightarrow \Phi = 0$ FOR $x<0$ AND $x>L \Rightarrow$

$$\int_{-\infty}^{\infty} |\Phi|^2 dx = \int_0^L |\Phi|^2 dx = \int_0^L C^2 \sin^2 kx \, dx = C^2 \int_0^L \sin^2 kx \, dx$$

$$K = \frac{n\pi}{L} \Rightarrow C^2 \int_0^L \sin^2\left(\frac{n\pi x}{L}\right) dx = C^2 \int_0^L \frac{1}{2}\left(1 - \cos\left(\frac{2\pi n x}{L}\right)\right) dx$$

$$= \frac{C^2}{2}\left(L - \frac{L}{2\pi n} \sin\left(\frac{2\pi n x}{L}\right)\Big|_0^L\right) = \frac{C^2}{2}(L - 0) = \frac{C^2 L}{2} \Rightarrow \frac{C^2 L}{2} = 1$$

$$\Rightarrow C^2 = \frac{2}{L} \Rightarrow C = \sqrt{\frac{2}{L}}$$

$$\boxed{\Phi_n = \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi x}{L}\right)} \text{ WITH } \boxed{E_n = \frac{\pi^2 \hbar^2}{2ML^2} n^2}$$

STATIONARY STATES / ENERGIES FOR PARTICLE IN A BOX.

<u>EXAMPLE</u> AN ELECTRON IS CONFINED TO A BOX OF LENGTH 10^{-10}m. WHAT ARE THE POSSIBLE ELECTRON ENERGIES?

$$E_n = \frac{\pi^2 \hbar^2}{2ML^2} n^2 = \frac{\pi^2 (1.06 \times 10^{-34} \text{J}\cdot\text{s})^2}{2(9.11 \times 10^{-31} \text{kg})(1 \times 10^{-10} \text{m})^2} n^2 = 6.09 \times 10^{-18} \text{J}\, n^2 = 38 \text{eV}\, n^2$$

$$\text{UNIT: } \frac{J^2 s^2}{\text{kg m}^2} = J\left(\frac{J s^2}{\text{kg m}^2}\right) = J\left(\frac{\text{kg m}^2/s^2 \cdot s^2}{\text{kg m}^2}\right) = J$$

$\rightarrow$ NOTE: YOU HAVE TO USE $\hbar = 1.06 \times 10^{-34}$ J·s WHEN USING kg AND meters.

FOR $n=1$, WHAT IS THE AVERAGE VALUE OF POSITION AND MOMENTUM?

$$\Phi_1 = \sqrt{\frac{2}{L}}\sin\left(\frac{\pi x}{L}\right) \qquad (\text{for } 0<x<L)$$

$$\bar{X} = \int_0^L x\,|\Phi_1|^2\,dx = \int_0^L x\left(\frac{2}{L}\right)\sin^2\left(\frac{\pi x}{L}\right)dx = \frac{2}{L}\int_0^L x\sin^2\left(\frac{\pi x}{L}\right)dx$$

$$= \frac{2}{L}\int_0^L x\cdot\frac{1}{2}\left(1-\cos\frac{2\pi x}{L}\right)dx = \frac{2}{L}\cdot\frac{1}{2}\int_0^L x\left(1-\cos\frac{2\pi x}{L}\right)dx$$

$$= \frac{1}{L}\int_0^L x\,dx - \underbrace{x\cos\frac{2\pi x}{L}\,dx}_{\text{INTEGRATION BY PARTS}} = \frac{1}{L}\left(\frac{1}{2}x^2\Big|_0^L - \underbrace{\phi}_{\text{I'll let you verify}}\right) = \frac{1}{L}\cdot\frac{1}{2}L^2 = \frac{1}{2}L$$

$$\bar{p} = \int_0^L \Phi^*(-i\hbar)\frac{\partial\Phi}{\partial x} = \int_0^L \Phi^*(-i\hbar)\frac{\partial}{\partial x}\left(\sqrt{\frac{2}{L}}\sin\left(\frac{\pi x}{L}\right)\right)dx$$

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

$$= \frac{2}{L}(-i\hbar)\frac{\pi}{L}\int_0^L \sin\left(\frac{\pi x}{L}\right)\cos\left(\frac{\pi x}{L}\right)dx = \frac{2}{L}(-i\hbar)\,\frac{1}{2}\sin^2\left(\frac{\pi x}{L}\right)\Big|_0^L = \phi$$

SO ON AVERAGE THE PARTICLE IS AT THE MIDDLE OF THE BOX AND HAS ZERO MOMENTUM.