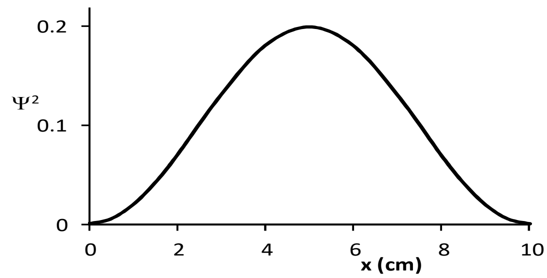
Expectation Values – Particle in a Box

Most Probable Position: Maximum in Ψ^2

$$\Psi(x) = \left(\frac{2}{a}\right)^{1/2} \sin\left(\frac{n\pi x}{a}\right)$$

$$\Psi^2(x) = \left(\frac{2}{a}\right) \sin^2\left(\frac{n\pi x}{a}\right)$$

for n = 1 $\quad \Rightarrow \quad x_{mp} = 0.5\ a$



$$<o> = \frac{\int_{-\infty}^{\infty} \Psi^* \hat{o}\, \Psi\, dx}{\int_{-\infty}^{\infty} \Psi^* \Psi\, dx}$$

if Ψ is real and normalized: $\quad <o> = \int_{-\infty}^{\infty} \Psi\, \hat{o}\, \Psi\, dx$

Average Position: $<x> = \int \Psi^*\, x\, \Psi\, dx$ integral "over all space"

$$<x> = \underbrace{\int_{-\infty}^{\infty}}_{average\ x} \left(\frac{2}{a}\right)^{1/2} \sin\left(\frac{n\pi x}{a}\right) x \left(\frac{2}{a}\right)^{1/2} \sin\left(\frac{n\pi x}{a}\right) dx$$

$$<x> = \underbrace{\int_0^a x}_{average\ x} \underbrace{\left(\frac{2}{a}\right) \sin^2\left(\frac{n\pi x}{a}\right) dx}_{\Psi^2 dx\ =\ probability\ distribution}$$

$$y = \frac{n\pi x}{a} \qquad \frac{dy}{dx} = \frac{n\pi}{a} \qquad x = \frac{a}{n\pi}\, y \qquad dx = \frac{a}{n\pi}\, dy$$

$$<x> = \left(\frac{2}{a}\right)\left(\frac{a}{n\pi}\right)^2 \int_0^{n\pi} y \sin^2(y)\, dx$$

$$\int x \sin^2(x)\, dx = \frac{x^2}{4} - \frac{x \sin 2x}{4} - \frac{\cos 2x}{8}$$

$$<x> = \left(\frac{2}{a}\right)\left(\frac{a}{n\pi}\right)^2 \left[\frac{y^2}{4} - \frac{y \sin 2y}{4} - \frac{\cos 2y}{8}\right|_0^{n\pi}$$

$\sin(0) = \sin(2n\pi) = 0, \ \cos(0) = \cos(2n\pi) = 1$

$$<x> = \left(\frac{2a}{n^2\pi^2}\right)\left(\frac{n^2\pi^2}{4}\right) = \frac{a}{2}$$

Momentum: $\hat{p}\, \Psi = \frac{\hbar}{i} \frac{d\Psi}{dx}$

$$\hat{E}_k = \frac{\hat{p}^2}{2m} = -\frac{\hbar^2}{2m} \frac{d^2}{dx^2}$$

$$<p> = \int_{-\infty}^{\infty} \Psi^*\, \hat{p}\, \Psi\, dx = \int_{-\infty}^{\infty} \Psi^* \left(\frac{\hbar}{i} \frac{d}{dx}\right) \Psi\, dx$$

$$\hat{p}\, \Psi = \frac{\hbar}{i} \frac{d\Psi}{dx} = \frac{\hbar}{i} \left(\frac{2}{a}\right)^{1/2} \frac{d \sin(n\pi x/a)}{dx} = \frac{\hbar}{i} \left(\frac{2}{a}\right)^{1/2} \left(\frac{n\pi}{a}\right) \cos\left(\frac{n\pi x}{a}\right)$$

$$<p> = \frac{\hbar}{i} \left(\frac{2}{a}\right)\left(\frac{n\pi}{a}\right) \int_0^a \sin\left(\frac{n\pi x}{a}\right) \cos\left(\frac{n\pi x}{a}\right) dx$$

$$<p> = \frac{\hbar}{i} \left(\frac{2}{a}\right)\left(\frac{n\pi}{a}\right)\left(\frac{a}{n\pi}\right) \int_0^{n\pi} \sin y\ \cos y\, dy = 0$$

$$\int_0^{n\pi} \sin y \cos y\, dy = [\ \tfrac{1}{2} \sin^2 y \,|_0^{n\pi} = 0$$