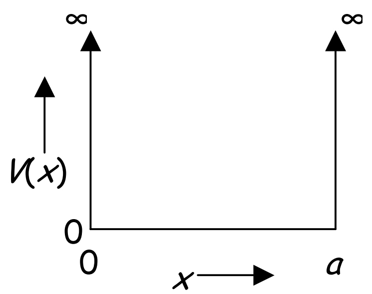
QUANTUM MECHANICAL PARTICLE IN A BOX

Summary so far:



$$V\left(x<0,\ x>a\right)=\infty \qquad \psi\left(x<0,\ x>a\right)=0$$

$$V\left(0\le x\le a\right)=0 \qquad \psi_n\left(0\le x\le a\right)=B\sin\left(\frac{n\pi x}{a}\right)$$

$$E_n=\frac{n^2h^2}{8ma^2} \qquad k=\frac{n\pi}{a} \qquad \lambda=\frac{2a}{n} \qquad n=1,2,3,\ldots$$

What is the "wavefunction" $\psi\left(x\right)$?

Max Born interpretation:

$\left|\psi\left(x\right)\right|^2=\psi^*\left(x\right)\psi\left(x\right)$ is a <u>probability distribution</u> or probability density for the particle

$\therefore$ $\left|\psi\left(x\right)\right|^2 dx$ is the probability of finding the particle in the interval between x and $x+dx$

This is a profound change in the way we view nature!! We can only know the *probability* of the result of a measurement – we can't always know it with certainty! Makes us re-think what is "deterministic" in nature.

Easy implication: <u>Normalization</u> of the wavefunction

$\Rightarrow$ $\int_{x_1}^{x_2}\left|\psi\left(x\right)\right|^2 dx$ = probability of finding particle in interval $x_1\le x\le x_2$

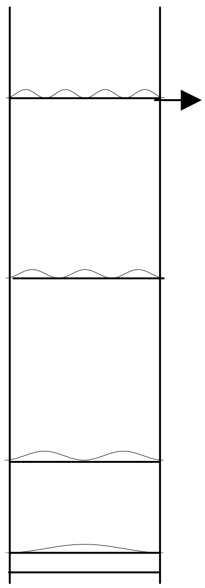
The total probability of finding the particle somewhere must be 1.

For a single particle in a box,

$$\int_{-\infty}^{\infty} |\psi(x)|^2 dx = \int_0^a |\psi(x)|^2 dx = 1$$ Normalization condition

$$\int_0^a B^2 \sin^2\left(\frac{n\pi x}{a}\right) dx = 1 \quad \Rightarrow \quad B = \sqrt{\frac{2}{a}}$$

$$\boxed{\psi_n(x) = \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi x}{a}\right) \qquad n = 1, 2, 3, \ldots}$$ Normalized wavefunction



$$|\psi_4|^2 = (2/a)\sin^2(4\pi x/a)$$

$$|\psi_3|^2 = (2/a)\sin^2(3\pi x/a)$$

$$|\psi_2|^2 = (2/a)\sin^2(2\pi x/a)$$

$$|\psi_1|^2 = (2/a)\sin^2(\pi x/a)$$

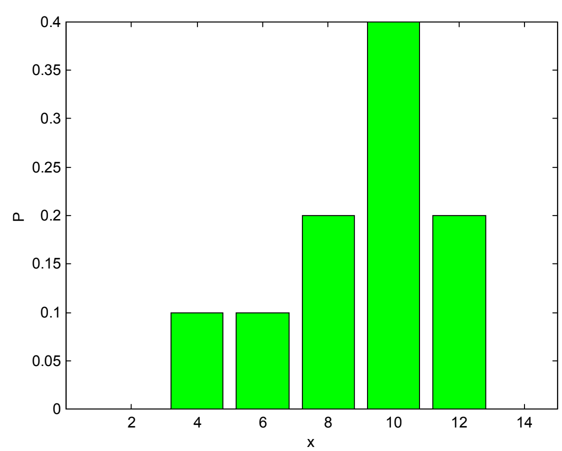
Interpretation of $|\psi(x)|^2$ based on measurement

Each measurement of the position gives one result. Many measurements give a probability distribution of outcomes.

Expectation values or average values

For a discrete probability distribution

e.g.



<*x*> = average value of *x*

= 4(0.1) + 6(0.1) + 8(0.2) + 10(0.4) + 12(0.2)

= $4(P_4) + 6(P_6) + 8(P_8) + 10(P_{10}) + 12(P_{12})$

where P_x is probability that measurement yields value "*x*"

$$\Rightarrow \quad \langle x\rangle = \sum x P_x$$

Now switch to continuous probability distribution

$$P_x \rightarrow |\psi(x)|^2\, dx$$
$$\sum \rightarrow \int$$

$$\Rightarrow \quad \langle x\rangle = \int_{-\infty}^{\infty} x|\psi(x)|^2 dx$$

Similarly

$$\langle x^2\rangle = \int_{-\infty}^{\infty} x^2 |\psi(x)|^2 dx$$

Often written in "sandwich" form

$$\langle x\rangle = \int_{-\infty}^{\infty} \psi^*(x)\, x\, \psi(x)\, dx$$
$$\langle x^2\rangle = \int_{-\infty}^{\infty} \psi^*(x)\, x^2\, \psi(x)\, dx$$

For particle in a box

$$\langle x\rangle = \frac{2}{a}\int_0^a x \sin^2\left(\frac{n\pi x}{a}\right) dx$$

Integrate by parts $\rightarrow$ $\boxed{\langle x \rangle = \frac{a}{2}}$

The average particle position is in the middle of the box.