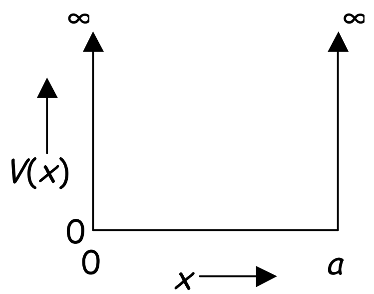
QUANTUM MECHANICAL PARTICLE IN A BOX

Summary so far:



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

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

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

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

Max Born interpretation:

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

$\therefore$ $|\psi(x)|^2\,dx$ 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

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

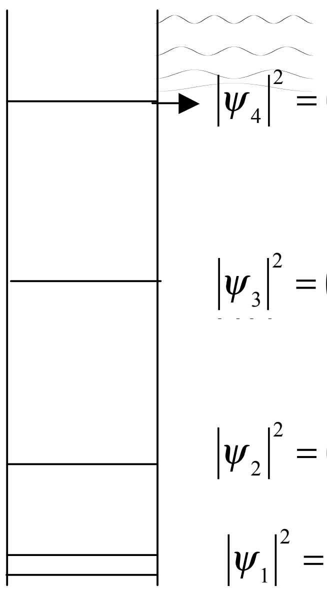
The total probability of finding the particle somewhere must be 1.

For a single particle in a box,

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



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

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

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

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

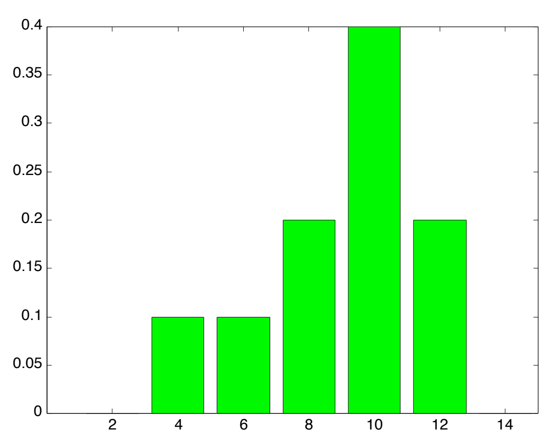
Interpretation of $\left|\psi(x)\right|^2$ based on measurement

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*"

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

Now switch to continuous probability distribution

$$P_x \quad \rightarrow \quad \left|\psi(x)\right|^2 dx$$
$$\sum \quad \rightarrow \quad \int$$

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

Similarly

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

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.