1_16_08

Note Title 1/15/2008

The wavefunction is a

$\boxed{\text{probability amplitude}}$

i.e $|\psi(\vec{r},t)|^2$ is a probability density function (PDF)

Generically speaking a PDF $\rho(x)$ has the following properties

1) $\rho(x) \geq 0 \quad \forall x$

2) $\int_{-\infty}^{\infty} \rho(x)\, dx = 1$

3) The probability that $x \in [a, b]$ is:

$$\int_a^b \rho(x)\, dx$$

Examples

$P[x \geq 0] = \int_0^{\infty} \rho(x)\, dx$

i.e. probability

$P[x \leq 0] = \int_{-\infty}^{0} \rho(x)\, dx$

mean value of x = Expectation of x

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

other notations you will see

$$\langle x \rangle = E[x] = \bar{x}$$

Ex. $\rho(x) = \frac{1}{\sqrt{2\pi}} e^{-(x-2)^2/2}$

$$\frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{-(x-2)^2/2}\,dx = 2$$

By inspection: $\langle x \rangle = 2$

$\langle x^2 \rangle - \langle x \rangle^2 = 1$ (i.e. $\sigma = 1$)

in fact $\frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} x\, e^{-(x-2)^2/2}$

$$x - 2 = u$$

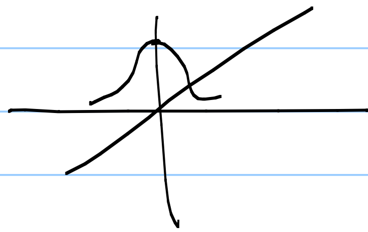
$$\frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} (u+2)\, e^{-u^2/2}\,du$$

$$u^2/2 = y^2$$
$$u = \sqrt{2}\,y$$
$$du = \sqrt{2}\,dy$$

$$\downarrow \quad \frac{\sqrt{2}}{\sqrt{2\pi}}\int_{-\infty}^{\infty}(\sqrt{2}\,y+2)\,e^{-y^2}\,dy$$

$$= \underbrace{\frac{1}{\sqrt{\pi}}\int_{-\infty}^{\infty} y\,e^{-y^2}\,dy}_{0} + \frac{2}{\sqrt{\pi}}\underbrace{\int_{-\infty}^{\infty} e^{-y^2}\,dy}_{\sqrt{\pi}}$$

$$\int_{-\infty}^{\infty} y\,e^{-y^2}\,dy = 0 \qquad\qquad = 2$$



$$\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} x\,e^{-(x-2)^2/2} = 2$$

As expected

Similarly $\displaystyle \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} x^2\,e^{-(x-2)^2/2}\,dx = 5$

So $\langle (x-\langle x\rangle)^2\rangle = \langle x^2\rangle - \langle x\rangle^2 = \underline{5-2^2=1}$

You can verify (e.g. with Mathematica)

$$\frac{1}{\sqrt{2\pi}}\int (x-2)^2\,e^{-(x-2)^2/2}\,dx = \underline{1}$$

Normalization:

Physically realizable states are normalizable.

Plane waves are not normalizable

$$\psi(\vec{r},t) = \psi_0 \, e^{i(\vec{p}\cdot\vec{r} - Et)/\hbar}$$

$$\Rightarrow \quad |\psi(\vec{r},t)|^2 = \underbrace{|\psi_0|^2}_{\text{a positive number}}$$

$$\iiint_{-\infty}^{\infty} |\psi(\vec{r},t)|^2 d^3r = |\psi_0|^2 \iiint_{-\infty}^{\infty} d^3r = \infty$$

If a state is normalized initially it is normalized forever!

$$\frac{d}{dt}\int_{-\infty}^{\infty} |\psi(x,t)|^2 dx = \int_{-\infty}^{\infty} \frac{\partial}{\partial t}|\psi(x,t)|^2 dx$$

$$= \int_{-\infty}^{\infty} \frac{\partial}{\partial t}\psi^*\psi \, dt = \int_{-\infty}^{\infty} \left(\frac{\partial}{\partial t}\psi^*\right)\psi + \psi^*\frac{\partial \psi}{\partial t} \, dx$$

<u>Pause</u> we need

$$\frac{\partial \psi^*}{\partial t} \quad \text{and} \quad \frac{\partial \psi}{\partial t}$$

$$i\hbar \frac{\partial \psi}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2 \psi}{\partial x^2} + V\psi \qquad 1.1$$

$$\boxed{\frac{\partial \psi}{\partial t} = i\frac{\hbar}{2m}\frac{\partial^2 \psi}{\partial x^2} - i\frac{V}{\hbar}\psi}$$

$$\Rightarrow -i\hbar \frac{\partial \psi^*}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2 \psi^*}{\partial x^2} + V\psi^*$$

$$\boxed{\frac{\partial \psi^*}{\partial t} = -\frac{i\hbar}{2m}\frac{\partial^2 \psi^*}{\partial x^2} + i\frac{V}{\hbar}\psi^*}$$

$$\left(\frac{\partial}{\partial t}\psi^*\right)\psi + \psi^*\frac{\partial \psi}{\partial t} \Rightarrow$$

$$-\frac{i\hbar}{2m}\frac{\partial^2 \psi^*}{\partial x^2}\psi + \boxed{i\frac{V}{\hbar}\psi^*\psi}$$

$$+ \psi^*\frac{i\hbar}{2m}\frac{\partial^2 \psi}{\partial x^2} - \boxed{i\frac{V}{\hbar}\psi^*\psi}$$

cancel

$$= \frac{i\hbar}{2m}\left[\psi^*\frac{\partial^2 \psi}{\partial x^2} - \frac{\partial^2 \psi^*}{\partial x^2}\psi\right]$$

$$= \frac{i\hbar}{2m}\frac{\partial}{\partial x}\left[\psi^*\frac{\partial \psi}{\partial x} - \frac{\partial \psi^*}{\partial x}\psi\right]$$

which is $\frac{d}{dt}\int_{-\infty}^{\infty} |\psi|^2 dx$

becomes

$$\int_{-\infty}^{\infty} \frac{\partial}{\partial x}\left[\frac{i\hbar}{2m}\left(\psi^* \frac{\partial \psi}{\partial x} - \frac{\partial \psi^*}{\partial x}\psi\right)\right] dx$$;

$$= \frac{i\hbar}{2m}\left[\psi^* \frac{\partial \psi}{\partial x} - \frac{\partial \psi^*}{\partial x}\psi\right]\Bigg|_{-\infty}^{\infty}$$

$\lim_{x\to\infty} \psi(x,t) = 0$ or else not normalizable.

So $$\boxed{\frac{d}{dt}\int_{-\infty}^{\infty} |\psi(x,t)|^2 dx = 0}$$

conservation of probability

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interpretation of $\langle x \rangle$

It is not the result of repeatedly measuring the position of a particle in initially in state $\psi(\vec{r},t)$.

As we will see, measurement changes the state of a particle.

$\langle x \rangle$. Suppose you had a large number of particles, all in state Ψ. (i.e., "identically prepared") measure x for each one of these particles independently: $\{x_i\}_{i=1}^{N}$.

then $\langle x \rangle = \frac{1}{N}\sum_{i=1}^{N} x_i$

Ensemble average. A collection of identically prepared particles is called an Ensemble.

in general $\langle x \rangle$ changes with time;

$$\langle x \rangle = \int x \, |\Psi(x,t)|^2 dx$$

time dependence.

so $\frac{d}{dt}\langle x \rangle = ?$

$$= \int x \frac{\partial}{\partial t} \Psi^* \Psi \, dx$$

$$= \int x \left[\frac{\partial \psi^*}{\partial t} \psi + \psi^* \frac{\partial \psi}{\partial t} \right] dx$$

$$\boxed{\frac{\partial \psi}{\partial t} = i \frac{\hbar}{2m} \frac{\partial^2 \psi}{\partial x^2} - i \frac{V}{\hbar} \psi}$$

$$\boxed{\frac{\partial \psi^*}{\partial t} = -\frac{i\hbar}{2m} \frac{\partial^2 \psi^*}{\partial x^2} + i \frac{V}{\hbar} \psi^*}$$

$$\frac{d}{dt}\langle x \rangle = -\frac{i\hbar}{2m} \int x \left[\frac{\partial^2 \psi^*}{\partial x^2} \psi - \psi^* \frac{\partial^2 \psi}{\partial x^2} \right] dx$$

$$= -\frac{i\hbar}{2m} \int x \frac{\partial}{\partial x} \left[\frac{\partial \psi^*}{\partial x} \psi - \psi^* \frac{\partial \psi}{\partial x} \right] dx$$

integrate by parts $= \underbrace{-\frac{i\hbar}{2m} \Big[x [\quad] \Big]_{-\infty}^{\infty}}_{0} + \frac{i\hbar}{2m} \int_{-\infty}^{\infty} \frac{\partial \psi^*}{\partial x} \psi - \psi^* \frac{\partial \psi}{\partial x} \, dx$

consider the term $\int \frac{\partial \psi^*}{\partial x} \psi \, dx$

$$= \underbrace{\psi^* \psi \Big|_{-\infty}^{\infty}}_{0} - \int \psi^* \frac{\partial \psi}{\partial x} dx$$

So $\boxed{\frac{d}{dt}\langle x \rangle = -\frac{i\hbar}{m} \int \psi^* \frac{\partial \psi}{\partial x} dx}$

$$m \frac{d\langle x \rangle}{dt} = \int \psi^* \left(-i\hbar \frac{\partial}{\partial x}\right) \psi \, dx$$

$$\equiv \langle p \rangle$$

Similarly we can write

$$\langle x \rangle = \int x \, |\psi|^2 dx$$

$$= \int x \, \psi^* \psi \, dx$$

$$\boxed{\begin{aligned} \langle x \rangle &= \int \psi^* \, x \, \psi \, dx \\ \langle p \rangle &= \int \psi^* \left(-i\hbar \frac{\partial}{\partial x}\right) \psi \, dx \end{aligned}}$$

<u>major step</u> we say

the operator $-i\hbar \frac{\partial}{\partial x}$ represents

P.

We can now take classical formulae involving x + p and compute quantum mech expectations.

Eg. Kinetic Energy, $T = \frac{p^2}{2m}$

$$\langle T \rangle = \int \psi^* \left(-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} \right) \psi \, dx$$

$$= \frac{-\hbar^2}{2m} \int \psi^* \frac{\partial^2 \psi}{\partial x^2} dx$$

Eg. deBroglie wave

$$\psi = \psi_0 e^{i(px - Et)/\hbar}$$
$$\psi^* = \psi_0^* e^{-i(px - Et)/\hbar}$$

$$\frac{\partial^2 \psi}{\partial x^2} = \frac{-p^2}{\hbar^2} \psi$$

$$\langle T \rangle = \frac{p^2}{2m} \int \psi^* \psi \, dx = \frac{p^2}{2m}$$

Because the deBroglie wave was constructed to have a precise p.

In general take any function of x, p $\quad Q(x,p)$ then

$$\langle Q(x,p)\rangle = \int \psi^* \, Q\left(x, -i\hbar \frac{\partial}{\partial x}\right) \psi \, dx$$

Ex. $\quad \psi(x,t) = \frac{1}{(2\pi)^{1/4}} e^{-x^2/4}$ $\quad \left\{ \begin{array}{l} \langle x\rangle = 0 \\ \sigma = 1 \end{array} \right.$

Remember: it is $|\psi|^2$ that is normalized not ψ!

$$|\psi|^2 = \frac{1}{\sqrt{2\pi}} e^{-x^2/2} \quad \checkmark$$

$$\frac{\partial \psi}{\partial x} = \frac{1}{(2\pi)^{1/4}} \frac{x}{2} e^{-x^2/4}$$

$$\langle p\rangle = \frac{-i\hbar}{2\sqrt{2\pi}} \int x \, e^{-x^2/2} \, dx = 0$$

$$\langle p^2\rangle = \frac{-\hbar^2}{2\sqrt{2\pi}} \int \left[\frac{x^2}{2} - 1\right] e^{-x^2/2} \, dx$$

$$= \frac{\hbar^2}{2\sqrt{2\pi}} \sqrt{\frac{\pi}{2}} = \frac{\hbar^2}{4}$$