Lecture #4 Physics 137A.

Properties of the wave function, probability, normalization, measurement, expectation value, wave packets, & the uncertainty principle.

Interpretation of Ψ —

As the wave function Ψ itself is complex, we can't associate Ψ with any measurements. Instead in the case of Ψ being spread over a range of possible coordinates x, we identify $\Psi\Psi^*$ as a position probability density.

$$P(x,t) = \Psi^*(x,t)\Psi(x,t) = |\Psi(x,t)|^2$$

Therefore,

$$\delta P(x,t) \equiv |\Psi(x,t)|^2 \delta x$$

is the probability of finding a particle in a region δx around x if the measurement is made at time t.

This means that if a large N number of identical experiments w/ the measurement occuring at exactly time t to determine if a particle is in the range $[a,b]$ — sometimes yes, sometimes no, & the results of these N experiments were averaged, the average would converge to

$$P(x\in[a,b]) \equiv \int_a^b |\Psi(x,t)|^2 dx, \quad N \to \infty$$

Normalisation Condition —

The wave function $\psi(x,t)$ in general describes a particle somewhere in a region. As the particle must exist somewhere in that region,

$$\int_D |\psi(x,t)|^2 dx = 1.$$

However, wave functions calculated from Schrödinger's Equation in general have some arbitrary normalisation. We have to fix this.

if $$\int_D |\psi(x,t)|^2 dx = N \Longrightarrow \psi_N(x,t) \equiv \frac{1}{\sqrt{N}} \psi(x,t).$$

Once a wave function at any one t in time, it remains normalised for all time. The proof of this is given next page.

Once a wave function is normalized, it is normalized for all time.

$$\frac{d}{dt}\int_{-\infty}^{\infty} |\psi(x,t)|^2 dx = \int_{-\infty}^{\infty}\left[\psi^*(x,t)\frac{\partial\psi(x,t)}{\partial t} + \frac{\partial\psi^*(x,t)}{\partial t}\psi(x,t)\right] dt$$

$$\left.\begin{aligned}\frac{\partial\psi(x,t)}{\partial t} &= \frac{i\hbar}{2m}\frac{\partial^2\psi(x,t)}{\partial x^2} - \frac{i}{\hbar}V(x)\psi(x,t)\\ \frac{\partial\psi^*(x,t)}{\partial t} &= -\frac{i\hbar}{2m}\frac{\partial^2\psi^*(x,t)}{\partial x^2} + \frac{i}{\hbar}V(x)\psi^*(x,t)\end{aligned}\right\}$$

Therefore,

$$\frac{d}{dt}\int_{-\infty}^{\infty} |\psi(x,t)|^2 dx = \frac{i\hbar}{2m}\int_{-\infty}^{\infty}\left[\psi^*(x,t)\frac{\partial^2\psi(x,t)}{\partial x^2} - \frac{\partial^2\psi^*(x,t)}{\partial x^2}\psi(x,t)\right]dx$$

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

$$= \frac{i\hbar}{2m}\left[\psi^*\frac{\partial\psi(x,t)}{\partial x} - \frac{\partial\psi^*(x,t)}{\partial x}\psi(x,t)\right]\Bigg|_{-\infty}^{\infty} = 0$$

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

A wave function normalized at some t remains normalized for all ~~other~~ t.

Not all problems in quantum mechanics have infinite possible solutions. If we talk about spin we may not care about the location of an electron, but its spin orientation. In this case it's either up, or down.

We can invent something analogous to a wave function in this case. a vector of amplitudes that includes just two possibilities.

$$\vec{\psi} = \begin{pmatrix} c_\uparrow \\ c_\downarrow \end{pmatrix}$$

Then the normalization condition becomes

$$\int_D |\psi(x,t)|^2 dx = 1 \implies |c_\uparrow|^2 + |c_\downarrow|^2 = 1$$

$$\sum_{i \in \{\uparrow, \downarrow\}} |c_i|^2 = 1$$

the domain D in the spin case has only two possibilities.

If we consider an infinite square well of width a, which confines an e^- to reside in the domain $[-\frac{a}{2}, \frac{a}{2}]$

$$\int_{-a/2}^{a/2} |\psi(x,t)|^2 dx = 1$$

Remembering Calculus

$$\int_{-a/2}^{a/2} |\psi(x,t)|^2 dx = \lim_{N \to \infty} \sum_{i=1}^{N} |\psi(x_i,t)|^2 \Delta \qquad \Delta = \frac{a}{N}$$

We have broken the interval $[-a/2, a/2]$ into N equal bins of width Δ, where x_i labels the center-points of the bins.

A continuous probability distribution is just the limiting case of a discrete probability distribution. Comparing to our spin case,

$$\lim_{N\to\infty} \sum_{i=1}^{N} |\Psi(x_i,t)|^2 \Delta \iff \sum_{i\in[\uparrow,\downarrow]} |c_i|^2$$

one sees an analogy between $|c_i|^2$ and $|\Psi(x_i,t)|^2\Delta$ the probability of being in neighborhood of width Δ centered on x_i!

Consider the midterm scores of a large class w/ N_T students, in the range 0 to 10.

$$P[j] \equiv \frac{N(j)}{N_T} \text{ (fraction of students w/ score } j)$$

$$\sum_{j=0}^{10} P(j) = 1.$$

Properties of a probability distribution —

0^{th} moment.

$$\langle 1 \rangle \equiv \sum_{j=0}^{10} 1 P(j) = 1 \qquad \langle 1 \rangle \equiv \int_D 1 |\Psi(x,t)|^2 dx = 1.$$

1^{st} moment — "mean"

$$\langle j \rangle = \sum_{j=0}^{10} j P(j) \qquad \langle x \rangle \equiv \int_D x |\Psi(x,t)|^2 dx$$

2^{nd} moment - "variance"

$$\langle (j - \langle j \rangle)^2 \rangle \equiv \sum_{j=0}^{10} (j - \langle j \rangle)^2 P(j) \qquad \langle (x - \langle x \rangle)^2 \rangle \equiv \int_D (x - \langle x \rangle)^2 |\Psi(x,t)|^2 dx$$

As $\langle j \rangle$ & $\langle x \rangle$ are just #s,

$$\langle (j - \langle j \rangle)^2 \rangle = \langle j^2 - 2j\langle j \rangle + \langle j \rangle^2 \rangle = \langle j^2 \rangle - \langle j \rangle^2 \geq 0$$

$$\langle (x - \langle x \rangle)^2 \rangle = \langle x^2 \rangle - \langle x \rangle^2 \geq 0$$

$$\left.\langle j^2 \rangle \equiv \sum_{j=0}^{10} j^2 P(j) \qquad \langle x^2 \rangle = \int x^2 |\Psi(x,t)|^2 dx \right\}$$

allows one to calculate the variance. The standard deviation

$$\sigma \equiv \sqrt{\langle (j - \langle j \rangle)^2 \rangle} \quad \text{or} \quad \sqrt{\langle (x - \langle x \rangle)^2 \rangle}$$

For Gaussian distributions outcomes within 1σ of $\langle x \rangle$ constitute $2/3$.
The skewness of a distribution how asymmetrical data is about the mean

$$\frac{1}{\sigma^{3/2}} \langle (j - \langle j \rangle)^3 \rangle, \quad \frac{1}{\sigma^{3/2}} \langle (x - \langle x \rangle)^3 \rangle$$

Measurement impacts the wave function. If at t one finds a particle at x, then at $t + \delta t$ one will find the particle at some $x_2 \sim x$ (within some small δx). The first measurement collapses the wave function — greatly narrowing the possibilities

initial: $|\Psi(x,t)|^2$

final: $|\Psi(x, t+\delta t)|^2$

Since x became more precise after measurement, p becomes more spread.

Expectation values of operators —

if the outcome of an experiment is a particle's position & we repeat the experiment 1000 times the mean becomes

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

More accurately,

$$\langle \hat{x} \rangle \equiv \int_{-\infty}^{\infty} \Psi^*(x,t)\, \hat{x}\, \Psi(x,t) dx = \int_{-\infty}^{\infty} \Psi^*(x,t)\, x\, \Psi(x,t) dx$$

$$= \int_{-\infty}^{\infty} x |\Psi(x,t)|^2 dx$$

$\hat{x}$ is an operator that interrogates Ψ, and x is the outcome of the interrogation.

$$\langle \hat{p} \rangle = \int_{-\infty}^{\infty} \Psi^*(x,t)\, \hat{p}\, \Psi(x,t)\, dx = \int_{-\infty}^{\infty} \Psi^*(x,t) \left(\frac{\hbar}{i}\frac{\partial}{\partial x}\right) \Psi(x,t)\, dx$$

if Ψ is a normalized plane wave to a 1D "volume" of length L,

$$\Psi(x,t) = \frac{1}{\sqrt{L}} e^{i(p_0 x - \mathcal{E}_0 t)/\hbar}, \quad \mathcal{E}_0 = \mathcal{E}(p) = p_0^2/2m$$

$$\int_{-L/2}^{L/2} \Psi^*(x,t)\left(\frac{\hbar}{i}\frac{\partial}{\partial x}\right)\Psi(x,t)\, dx = \int_{-L/2}^{L/2} \Psi^*(x,t)\, p_0\, \Psi(x,t)\, dx$$

$$= p_0 \int_{-L/2}^{L/2} |\Psi(x,t)|^2 dx = p_0$$

Time evolution of operator expectation values ——

for $\langle \hat{x} \rangle$,

$$\frac{d\langle \hat{x} \rangle}{dt} = \frac{i\hbar}{2m}\int_{-\infty}^{\infty} x \frac{\partial}{\partial x}\left[\Psi^*(x,t)\frac{\partial \Psi}{\partial x} - \frac{\partial \Psi^*}{\partial x}\Psi\right] dx$$

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

$$= \frac{i\hbar}{m}\int_{-\infty}^{\infty}\Psi^*\frac{\partial}{\partial x}\Psi\, dx = \frac{1}{m}\int_{-\infty}^{\infty}\Psi^*\left(\frac{\hbar}{i}\frac{\partial}{\partial x}\right)\Psi\, dx$$

Classical Mechanics $\Longrightarrow \dfrac{d\langle \hat{x} \rangle}{dt} = \dfrac{\langle \hat{p} \rangle}{m} = \langle \hat{v} \rangle \Longrightarrow \dfrac{d\langle \hat{p} \rangle}{dt} = \left\langle -\dfrac{dV}{dx} \right\rangle$