Lecture 3 **Momentum**

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

Note: the expectation value is the average of repeated measurements on an ensemble of identically prepared systems, not the average of repeated measurements on the same system.

How to find $\langle p \rangle = m \dfrac{d\langle x \rangle}{dt}$?

$$\frac{d\langle x \rangle}{dt} = \frac{d}{dt} \int x |\psi|^2 dx = \int x \underbrace{\frac{\partial}{\partial t} |\psi|^2}_{\text{We found it in Lecture 2}} dx$$

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

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

Before proceeding further, let's review integration by parts:

$$\frac{d}{dx}(fg) = f \frac{dg}{dx} + \frac{df}{dx} g \quad \Rightarrow$$

$$\int_a^b \frac{d}{dx}(fg)\, dx = \int_a^b f \frac{dg}{dx} dx + \int_a^b \frac{df}{dx} g \, dx \quad \Rightarrow$$

$$fg \Big|_a^b = \int_a^b f \frac{dg}{dx} dx + \int_a^b \frac{df}{dx} g \, dx$$

$$\int_a^b f \frac{dg}{dx} dx = - \int_a^b \frac{df}{dx} g \, dx + fg \Big|_a^b$$

Now, we continue with our derivation:

$$\frac{d\langle x\rangle}{dt} = \underbrace{\frac{i\hbar}{2m}\int_{-\infty}^{\infty} x \, \frac{\partial}{\partial x}\left[\psi^* \frac{\partial \psi}{\partial x} - \frac{\partial \psi^*}{\partial x}\psi\right] dx}_{\text{integrate by parts}}$$

$$= -\frac{i\hbar}{2m}\int_{-\infty}^{\infty} \cancelto{=1}{\frac{\partial x}{\partial x}} \left(\psi^* \frac{\partial \psi}{\partial x} - \frac{\partial \psi^*}{\partial x}\psi\right) dx$$

$$+ \frac{i\hbar}{2m} \, \underbrace{x\left(\psi^* \frac{\partial \psi}{\partial x} - \frac{\partial \psi^*}{\partial x}\right)\Bigg|_{-\infty}^{\infty}}_{=0 \text{ since } \psi \to 0 \text{ if } x \to \pm\infty}$$

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

now we integrate this term by parts

$$\int_{-\infty}^{\infty} \frac{\partial \psi^*}{\partial x}\psi \, dx = -\int_{-\infty}^{\infty} \psi^* \frac{\partial \psi}{\partial x} dx + \cancelto{0}{\psi^*\psi}\Big|_{-\infty}^{\infty}$$

$$= -\frac{i\hbar}{m}\int_{-\infty}^{\infty} \psi^* \frac{\partial \psi}{\partial x} dx$$

Our final result: $\quad \langle p\rangle = m\frac{d\langle x\rangle}{dt} = -i\hbar\int_{-\infty}^{\infty} \psi^* \frac{\partial \psi}{\partial x} dx$

$$\boxed{\langle x \rangle = \int \psi^*(x)\,\psi\,dx}$$ { x- operator that represents position }

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

Operator that represents momentum.

An "operator" is an instruction to do something to the wave function that follows it.

Other operators?

Express in terms of position and momentum.
For example,

$$T = \frac{1}{2}mv^2 = \frac{p^2}{2m}$$ Kinetic energy

$$\vec{L} = \vec{r} \times m\vec{v} = \vec{r} \times \vec{p}$$ Angular momentum

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

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

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

Exercise 2

Problem 1.17. A particle is represented (at time t = 0) by the wave function

$$\Psi(x,0) = \begin{cases} A(a^2 - x^2), & \text{if } -a \le x \le a \\ 0, & \text{otherwise} \end{cases} \qquad A = \sqrt{\frac{15}{16a^5}}$$

(1) What is the expectation value of p at time t=0?
(2) Find the expectation value of p^2.

Here $\Psi^* = \Psi$

Solution:

$$(1) \quad \langle p \rangle = \int_{-\infty}^{\infty} \Psi^* \left(-i\hbar \frac{d}{dx}\right) \Psi \, dx$$

$$= A^2(-i\hbar) \int_{-a}^{a} (a^2 - x^2) \underbrace{\left[\frac{d}{dx}(a^2 - x^2)\right]}_{= -2x} dx = -i\hbar A^2 \int_{-a}^{a} \underbrace{x(a^2 - x^2)}_{\text{odd integrand again}} dx = 0$$

$$\langle p \rangle = 0$$

$$(2) \quad \langle p^2 \rangle = \int_{-\infty}^{\infty} \Psi^* \left((-i\hbar)^2 \frac{d^2}{dx^2}\right) \Psi \, dx =$$

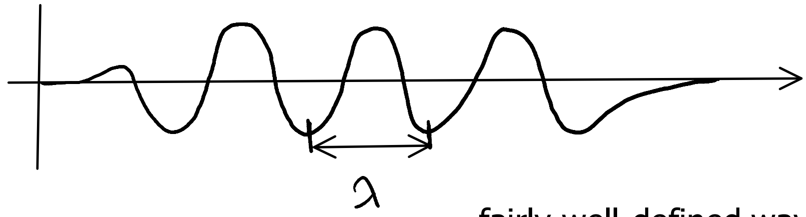
$$= -\hbar^2 A^2 \int_{-a}^{a} (a^2 - x^2) \underbrace{\frac{d^2}{dx^2}(a^2 - x^2)}_{= -2} dx$$

even integrand

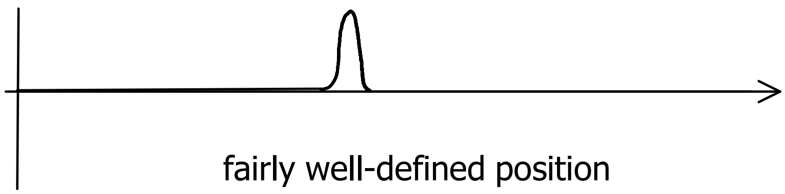
$$= 4\hbar^2 \frac{15}{16a^5} \int_0^a (a^2 - x^2)\, dx = \frac{15\hbar^2}{4a^5}\left(a^2 x - \frac{x^3}{3}\right)\Big|_0^a = \frac{15\hbar^2}{4a^5}\left(a^3 - \frac{a^3}{3}\right)$$

$$= \frac{\cancel{15}^{\,5}\hbar^2}{\cancel{4}_{\,2}\, a^{\cancel{5}\,2}} \frac{\cancel{2}}{\cancel{3}} a^{\cancel{3}} = \frac{5}{2}\frac{\hbar^2}{a^2} \qquad \boxed{\langle p^2 \rangle = \frac{5}{2}\frac{\hbar^2}{a^2}}$$

The uncertainty principle



fairly well-defined wavelength



fairly well-defined position

Wavelength of Ψ is related to the momentum of the particle by the de Broglie formula:

$$\boxed{p = \frac{h}{\lambda} = \frac{2\pi\hbar}{\lambda}}$$

A spread in wavelength corresponds to a spread in momentum. The more precise is particle's position the less precise is its momentum. The "spread" refers to the fact that measurements on identically prepared systems do not yield identical results.

$$\boxed{\sigma_x \sigma_p \geq \frac{\hbar}{2}}$$ $\leftarrow$ **Heisenberg uncertainty principle**

CHAPTER 2

Time-independent Schrödinger equation

How does one solve Schrödinger equation?

Stationary states

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

We assume that the potential V is independent of time. In this case, Schrödinger equation can be solved by the method of separation of variables. We will look for the solutions that are simple products:

$$\Psi(x,t) = \psi(x)\,\varphi(t)$$

ψ (lower-case) is a function of x alone

φ is a function of t alone.

For such separable solutions $\frac{\partial \Psi}{\partial t} = \psi \frac{d\varphi}{dt}$; $\frac{\partial^2 \Psi}{\partial x^2} = \frac{d^2 \psi}{dx^2}\varphi$

ordinary derivatives now

Therefore,

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

$$i\hbar\psi \frac{d\varphi}{dt} = -\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2}\varphi + V\psi\varphi$$

Let's divide by $\psi\varphi$:

$$\underbrace{i\hbar \frac{1}{\varphi}\frac{d\varphi}{dt}}_{\text{function of } t \text{ only}} = \underbrace{-\frac{\hbar^2}{2m}\frac{1}{\psi}\frac{d^2\psi}{dx^2} + V}_{\text{function of } x \text{ only}}$$

This can only be true if both sides are constant.

We will call the separation constant E.

$$i\hbar \frac{1}{\varphi}\frac{d\varphi}{dt} = E \qquad E = -\frac{\hbar^2}{2m}\frac{1}{\psi}\frac{d^2\psi}{dx^2} + V$$

E

$$\boxed{\frac{d\varphi}{dt} = -\frac{iE}{\hbar}\varphi} \qquad \boxed{-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + V\psi = E\psi}$$

Now we have two ordinary differential equations instead of a partial differential equation.

Easy to solve,
multiply by dt and
integrate:

$$\varphi(t) = Ce^{-iEt/\hbar}$$

We will absorb constant C into ψ, so

$$\boxed{\varphi(t) = e^{-iEt/\hbar}}$$

Time-independent Schrödinger equation. Need to know V to proceed any further.

Separable solutions: $$\Psi(x,t) = \psi(x)\, e^{-iEt/\hbar}$$

Why do we want to find these solutions?

1.These are stationary states, i.e. the probability density does not depend on time:

$$|\Psi|^2 = \Psi^*\Psi = \psi^* e^{+iEt/\hbar}\,\psi\, e^{-iEt/\hbar} = |\psi(x)|^2$$

Time-dependence cancels out.

The same thing happens when your calculate the expectation value of any dynamic variable:

$$\langle Q(x,p)\rangle = \int \Psi^*(x,t)\, Q(x, -i\hbar \frac{d}{dx})\, \Psi(x,t)\, dx$$

$$\downarrow$$

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

Every expectation value is constant in time, so we can drop φ and use ψ in place of Ψ.

2. They are the states of definite total energy.

In classical mechanics, the total energy is the Hamiltonian:

$$H(x,p) = \frac{p^2}{2m} + V(x)$$

In quantum mecamics, we replace $p \to i\hbar \frac{\partial}{\partial x}$ to get the Hamiltonian operator

operator label "hat"

$$\hat{H} = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x) \Rightarrow$$

The time-independent Schrödinger equation

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dt^2} + V\psi = E\psi \quad \text{is}$$

$$\boxed{\hat{H}\psi = E\psi}$$

The expectation value of the total energy is

$$\langle H\rangle = \int \psi^* \hat{H}\psi\, dx = E\int |\psi|^2 dx = E\int |\Psi(x,t)|^2 dx = E$$

$$\hat{H}^2\psi = \hat{H}(\hat{H}\psi) = \hat{H}(E\psi) = E(\hat{H}\psi) = E^2\psi$$

$$\langle H^2\rangle = \int \psi^* \hat{H}^2 \psi\, dx = E^2\int |\psi|^2 dx = E^2$$

$$\sigma_H^2 = \langle H^2 \rangle - \langle H \rangle^2 = E^2 - E^2 = 0$$

If $\sigma=0$ $\Rightarrow$ every measurement of the total energy is certain to return the value E for these states.

3.The general solution is a linear combination of separable solutions.

As we will discover later, the time-independent Schrödinger equation yields collection of solutions $(\psi_1(x), \psi_2(x) \ldots)$ each with its value of the separation constant $(E_1, E_2, \ldots)$ $\Rightarrow$ there is different wave function for each allowed energy:

$$\Psi_1(x,t) = \psi_1(x)\, e^{-iE_1 t/\hbar}$$

$$\Psi_2(x,t) = \psi_2(x)\, e^{-iE_2 t/\hbar}$$

$$\vdots$$

Any linear combination of solutions of S.E. is a solution $\Rightarrow$ general solution can be constructed as

$$\Psi(x,t) = \sum_{n=1}^{\infty} c_n \psi_n(x)\, e^{-iE_n t/\hbar}$$

Constants c_n are found to fit the initial conditions.