Modern Physics

Lecture 16

Expectation Values
or average values

Once we solve Schrödinger's equation for Ψ, we know all about the particle that is knowable within the limits imposed by the uncertainty principle.

To get an expectation value the approach is to make a “Ψ*Ψ sandwich”

$$\langle x \rangle = \int_{x_1}^{x_2} \psi^* x \psi dx$$

Expectation value of *x*

Any **measurable quantity** for which **expectation value** can be calculated is called physical **observable**

Position, momentum, energy, kinetic energy, etc. are ***operators***, and the order in which we take them ***is*** important to find the expectation values.

Example, momentum operator is related to ∂/∂x and energy operator is related to ∂/∂t.

This means an operation is require to find the expectation values

In summary, the expectation value of any quantity, including operators, is

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

The operator for a physical observable

Using the operator expression for momentum

$$\langle \hat{p} \rangle = \int_{-\infty}^{\infty} \psi^{*} \hat{p} \psi dx$$

the "hat" tells us momentum is an operator

Expectation value of momentum *p*

Operators

Mathematically operator transforms one function into another

$$\hat{A}f(x) = g(x)$$

Physically every observable has an associated operator
This operator is used to find the corresponding expectation value

Representation

$\hat{A}$ represents operator A

Momentum operator $\hat{p}$

Energy operator $\hat{E}$

Angular momentum operator $\hat{L}$

All are physical observable

How to derive the form of Operators

Wave function is $\psi = Ae^{-(i/\hbar)(Et-px)}$

Differentiating we get, $\dfrac{\partial\psi}{\partial x} = \dfrac{ip}{\hbar} Ae^{-(i/\hbar)(Et-px)}$

$$\frac{\partial\psi}{\partial x} = \frac{ip}{\hbar}\psi$$

$\dfrac{\hbar}{i}\dfrac{\partial\psi}{\partial x} = p\psi$ This implies $p = \dfrac{\hbar}{i}\dfrac{\partial}{\partial x}$

Therefore momentum operator is defined as, $\hat{p} = \dfrac{\hbar}{i}\dfrac{\partial}{\partial x}$

Precisely x component of momentum operator will be, $\hat{p}_x = \dfrac{\hbar}{i}\dfrac{\partial}{\partial x}$

Similarly how can we get energy operator $\hat{E}$

$$\psi = Ae^{-(i/\hbar)(Et-px)}$$

Differentiating w.r.t. time,

$$\frac{\partial \psi}{\partial t} = -\frac{iE}{\hbar} Ae^{-(i/\hbar)(Et-px)}$$

$$\frac{\partial \psi}{\partial t} = -\frac{iE}{\hbar}\psi$$

$$-\frac{\hbar}{i}\frac{\partial \psi}{\partial t} = E\psi$$

This means energy operator is,

$$\hat{E} = -\frac{\hbar}{i}\frac{\partial}{\partial t}$$

What will be kinetic energy operator $\hat{E}_{KE}$

$$E_{KE} = \frac{p^2}{2m}$$

We already know

$$\hat{p} = \frac{\hbar}{i}\frac{\partial}{\partial x}$$

$$E_{KE} = \frac{\hat{p}^2}{2m} = \frac{1}{2m}\left(\frac{\hbar}{i}\frac{\partial}{\partial x}\right)\left(\frac{\hbar}{i}\frac{\partial}{\partial x}\right)$$

$$E_{KE} = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}$$

Total energy,

$$E_T = E_{KE} + E_{PE}$$

$$E_T = \underbrace{-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x)}_{\text{Hamiltonian } \hat{H}}$$

Commutator

Definition of commutator

$$[A, B] \equiv [AB - BA]$$

Where *A* and *B* are two operators

If $[A, B] = 0$ This means A, B are commuting with each other

If $[A, B] \neq 0$ means A, B are non-commuting

Let us consider $\hat{x}\ and\ \hat{p}_x$ are two operators

Commutation of these two operators will be, $[x, p_x] \equiv [xp_x - p_x x]$

$$[x, p_x]\psi \equiv [xp_x - p_x x]\psi$$

$$[xp_x - p_x x]\psi = -i\hbar\left[x\frac{\partial\psi}{\partial x} - \frac{\partial(x\psi)}{\partial x}\right] \qquad \hat{p}_x = \frac{\hbar}{i}\frac{\partial}{\partial x}$$

$$[xp_x - p_x x]\psi = -i\hbar\left[\cancel{x\frac{\partial\psi}{\partial x}} - \cancel{x\frac{\partial\psi}{\partial x}} - \psi\right]$$

$$[xp_x - p_x x]\psi = i\hbar\psi$$

This means, $[xp_x - p_x x] \equiv i\hbar$ $\qquad [x, p_x] \equiv i\hbar$

$$[xp_x - p_x x] \equiv i\hbar$$

$$[yp_y - p_y y] \equiv i\hbar$$

$$[zp_z - p_z z] \equiv i\hbar$$

Non-commuting pair

But,

$$[xp_y - p_y x] \equiv [yp_z - p_z y] \equiv [zp_x - p_x z] \equiv 0$$

Similarly,

$$[xy - yx] \equiv [yz - zy] \equiv [zx - xz] \equiv 0$$

$$[xy] \equiv [yz] \equiv [zx] \equiv 0$$

Commuting pair

Eigen values and Eigen functions in Quantum mechanics

Eigen value equation $$\hat{G}\psi_n = G_n\psi_n$$

$\hat{G}$ is the operator corresponds to observable

G_n is the corresponding eigen value

ψ_n is the corresponding eigen function

Eigen value equation for energy $$\left[-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x)\right]\psi = E\psi$$

$$H\psi = E_n\psi$$

Operation of Hamiltonian on eigen function gives energy eigen values

Problem

An eigen function of the operator $\frac{d^2}{dx^2}$ is $\psi = e^{2x}$. Find the corresponding eigen value.

Solution

Operator $\hat{G} = \frac{d^2}{dx^2}$

$$\hat{G}\psi = \frac{d^2\psi}{dx^2} = \frac{d}{dx}\left[\frac{d}{dx}\left[e^{2x}\right]\right]$$

$$\hat{G}\psi = 4e^{2x}$$

$$\hat{G}\psi = 4\psi$$

This means eigen value of operator G is 4

or

$$G_n = 4$$