Dr Mohammad Abdur Rashid

Schrödinger Equation

$$i\hbar \frac{\partial}{\partial t} \Psi(x,t) = \hat{H} \Psi(x,t)$$

For a particle quantum mechanical of mass m moving in a potential V(x,t) the Hamiltonian operator is

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

Hermitian operator

An operator $\hat{\Omega}$, which corresponds to a physical observable Ω , is said to be Hermitian if

$$\int \Phi^* \hat{\Omega} \Psi \, \mathrm{d}x = \int (\hat{\Omega} \Phi)^* \Psi \, \mathrm{d}x$$

Examples: position operator \hat{x} , momentum operator \hat{p} , Hamiltonian operator \hat{H} , etc.

Expectation value

The expectation value $\langle \Omega \rangle$ of any operator $\hat{\Omega}$:

$$\langle \Omega \rangle = \int_{-\infty}^{\infty} \Psi^*(x,t) \, \hat{\Omega} \Psi(x,t) \, \mathrm{d}x$$

The physical meaning of this would be if we consider many copies of the identical system, and measure Ω at a time t in all of them, then the average value recorded will converge to $\langle \Omega \rangle$ as the number of systems and measurements approaches infinity.

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

$$\left|i\hbar\frac{\partial\Psi}{\partial t}=\hat{H}\Psi
ight|$$

$$\left| -i\hbar \frac{\partial \Psi^*}{\partial t} = (\hat{H}\Psi)^* \right|$$

$$i\hbar \frac{\mathrm{d}}{\mathrm{d}t} \langle \Omega \rangle = \int_{-\infty}^{\infty} \left\{ -(\hat{H}\Psi)^* \hat{\Omega}\Psi + \Psi^* \hat{\Omega}(\hat{H}\Psi) \right\} \mathrm{d}x$$
$$= \int_{-\infty}^{\infty} \left\{ \Psi^* \hat{\Omega}(\hat{H}\Psi) - (\hat{H}\Psi)^* \hat{\Omega}\Psi \right\} \mathrm{d}x$$

Hermitian operator:
$$\int \Phi^* \hat{\Omega} \Psi \, \mathrm{d}x = \int (\hat{\Omega} \Phi)^* \Psi \, \mathrm{d}x$$

$$i\hbar \frac{\mathrm{d}}{\mathrm{d}t} \langle \Omega \rangle = \int_{-\infty}^{\infty} (\Psi^* \hat{\Omega} \hat{H} \Psi - \Psi^* \hat{H} \hat{\Omega} \Psi) \, \mathrm{d}x$$
$$= \int_{-\infty}^{\infty} \Psi^* (\hat{\Omega} \hat{H} - \hat{H} \hat{\Omega}) \Psi \, \mathrm{d}x$$
$$= \int_{-\infty}^{\infty} \Psi^* [\hat{\Omega}, \hat{H}] \Psi \, \mathrm{d}x$$

Commutator of two operators: $[\hat{A}, \hat{B}] \equiv \hat{A}\hat{B} - \hat{B}\hat{A}$

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We have proven that for operators $\hat{\Omega}$ that do not explicitly depend on time,

$$i\hbar \frac{\mathrm{d}}{\mathrm{d}t} \langle \Omega \rangle = \left\langle [\hat{\Omega}, \, \hat{H}] \right\rangle$$

Therefore, for an operation which commute with the Hamiltonian operator \hat{H} the expectation value will not change over time.

Example: Consider the momentum operator \hat{p} for a free particle.

For a free particle the Hamiltonian operator: $\hat{H} = \frac{\hat{p}^2}{2m}$

Hence the momentum operator \hat{p} commute with \hat{H} :

$$[\hat{p}, \, \hat{H}] = [\hat{p}, \, \frac{\hat{p}^2}{2m}] = \frac{1}{2m} [\hat{p}, \, \hat{p}^2]$$
$$= \frac{1}{2m} \Big([\hat{p}, \, \hat{p}] \hat{p} + \hat{p} [\hat{p}, \, \hat{p}] \Big) = 0$$

$$[\hat{A}, \hat{B}\hat{C}] = [\hat{A}, \hat{B}]\hat{C} + \hat{B}[\hat{A}, \hat{C}]$$

$$i\hbar \frac{\mathrm{d}}{\mathrm{d}t} \langle p \rangle = \left\langle [\hat{p}, \, \hat{H}] \right\rangle = 0$$

For a free particle the expectation value of momentum does not change over time.

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