Operators, Expection and The Schrodinger Equation.

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

$$\Psi(x,t) = \underbrace{\psi(x)\,\phi(t)}_{\text{Seperable Solutions possible when } V=V(x)}$$

Seperable Solutions possible when $V = V(x)$ ~ no time dependence

$$-\frac{\hbar^2}{2m}\phi(t)\frac{d^2}{dx^2}\psi(x) + V(x)\,\phi(t)\,\psi(x) = i\hbar\,\psi(x)\frac{d}{dt}\phi(t)$$

TDSE

$$-\frac{\hbar^2}{2m}\frac{1}{\psi(x)}\frac{d^2}{dx^2}\psi(x) + V(x) = \frac{i\hbar}{\phi(t)}\frac{d}{dt}\phi(t) = E \rightsquigarrow \phi(t) = e^{-i\omega t}$$

$$\omega = \frac{E}{\hbar}$$

$$\Rightarrow \left[\frac{\hat{p}^2}{2m} + V(x)\right]\psi(x) = E\,\psi(x)$$

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

and $\frac{\hat{p}^2}{2m} + V(x) = \hat{H}(x)$ → Hamiltonian

$\hat{E} = i\hbar\frac{\partial}{\partial t}$ → Energy Operator

$\psi(x) \equiv$ Stationary States : Constant Energy Values due to variable seperation → EIGENSTATES OF $\hat{H}$

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

$\Psi(x,t) = \psi(x)\,e^{-i\omega t}$ → Total Solution.

$\hat{O}\psi = \lambda\psi$ is called the Eigenvalue eq^n. λ is the eigenvalue of operator $\hat{O}$ associated with the eigenfunction ψ.

Wave function $\Psi(x,t)$ gives all properties of the concerned particle

Probablity density : Probabity of finding the particle in an interval x and $x+dx \equiv |\Psi(x,t)|^2 = \Psi^*\Psi$

Ψ^* → complex conjugate

$$\Psi^* = (\psi(x)\,\phi(t))^* = \phi^*(t)\,\psi^*(x)$$

$$\Psi = \psi(x)\,\phi(t) \longrightarrow \Rightarrow \Psi^*\Psi = |\Psi|^2 = \psi^*(x)\,\psi(x)\,\cancel{e^{-i\omega t}}\,\cancel{e^{i\omega t}}$$

$$\Rightarrow \boxed{\Psi^*\Psi = \psi^*\psi}$$

$$\Rightarrow \boxed{\Psi^* \Psi = \psi^* \psi}$$

$$P(a < x < b) = \int_a^b \psi^* \psi \, dx$$

$$\Rightarrow P(-\infty < x < \infty) = \int_{-\infty}^{\infty} \psi^* \psi \, dx = 1 \longrightarrow \text{Normalizable}$$

Square integ : $P(-\infty < x < \infty) = \int_{-\infty}^{\infty} \psi^* \psi \, dx = N \rightsquigarrow$ finite

$\Rightarrow \frac{1}{\sqrt{N}} \psi$ is the Normalized function

★ SCHRÖDINGER EQUATION IS LINEAR ⇒ if ψ_1 and ψ_2 are solutions then so is $\psi_1 + \psi_2$ ★

Operators in QM : Correspond to taking measurement.

$$\hat{x}\, \psi(x) = x\, \psi(x)$$

$$\hat{p}\, \psi(x) = i\hbar \frac{\partial}{\partial x} \psi(x)$$

$$\hat{H}\, \psi(x) = \left[\hat{p}^2/2m + V(x) \right] \psi(x)$$

$$\hat{T}\, \psi(x) = \hat{p}^2/2m \; \psi(x)$$

Note : Operators that correspond to measurement of "real" observables are Hermitian

Ex $\langle v \rangle = \frac{d\langle x \rangle}{dt}$

$\boxed{\text{Ehrenfest's Theorem : Expectation value obey classical Laws.}}$ $\rightsquigarrow$ Ex $\frac{d\langle p \rangle}{dt} = \left\langle -\frac{\partial V}{\partial x} \right\rangle$

General Solution : $\Psi(x,t) = \sum_{n=1}^{\infty} c_n \psi_n(x) e^{-iEt/\hbar} = \sum_{n=1}^{\infty} c_n \Psi_n(x,t)$

The seperable solutions themselves ($\Psi_n(x,t) = \psi_n(x) e^{-iEt/\hbar}$) are stationary states but this property is not shared by the General sol.

⟶ exp values of observables are time indep - due to sep sol^{n}s.

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

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

$-\infty$

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

$[\hat{x}, \hat{p}]$ ~ commutator of two operators

$$[\hat{x},\hat{p}] = (x\hat{p} - \hat{p}x) \Rightarrow [\hat{x},\hat{p}]f(x) = \left[x(-i\hbar)\frac{d}{dx}(f(x)) - (i\hbar)\frac{d}{dx}(xf)\right]$$

$$= -i\hbar\left[\cancel{x\frac{df}{dx}} - \cancel{x\frac{df}{dx}} - f\right] = \boxed{i\hbar f(x)}$$

Drop the test function: $[\hat{x}, \hat{p}] = i\hbar$

Dirac Notation: Short-hand : $\int_{-\infty} \psi^* \hat{Q}\, \psi\, dx = \langle Q\rangle = \langle \psi | \hat{Q}\psi\rangle$

$$\Rightarrow \int_{-\infty}^{\infty} \psi^* \psi\, dx = \langle \psi|\psi\rangle$$

Eigenvalues are $\mathbb{R}$

Hermitian Operators: outcome of a measurement has to be real

$\langle Q\rangle = \langle Q\rangle^*$

$$\Rightarrow \int_{-\infty}^{\infty} \psi^*(\hat{Q}\psi)\, dx = \int_{-\infty}^{\infty} [\psi^*(\hat{Q}\psi)]^* dx = \int_{-\infty}^{\infty} (\hat{Q}\psi)^* \psi\, dx$$

$\therefore \langle \psi|\hat{Q}\psi\rangle = \langle \hat{Q}\psi|\psi\rangle$ → Real observables are represented by Hermitian operators.

Example $\langle f|\hat{p}g\rangle = \int_{-\infty}^{\infty} f^*(-i\hbar)\frac{dg}{dx}\, dx = \cancel{-i\hbar f^* g\Big|_{-\infty}^{\infty}} + \int_{-\infty}^{\infty}\left(-i\hbar\frac{df}{dx}\right)^* g\, dx = \langle \hat{p}f|g\rangle$

0

↳ coz wave func^ns must die off to 0 @ $\pm\infty$

The Hermitian conjugate of operator $\hat{Q}$ is the operator $\hat{Q}^\dagger$

↳ "Q dagger"

$\langle f|\hat{Q}g\rangle = \langle \hat{Q}^\dagger f|g\rangle$

$\Rightarrow$ for Hermitian operators $\hat{Q} = \hat{Q}^\dagger$

Properties :
1. $(\hat{Q}\hat{R})^\dagger = \hat{R}^\dagger \hat{Q}^\dagger$
2. $(\hat{Q}+\hat{R})^\dagger = \hat{Q}^\dagger + \hat{R}^\dagger$
3. $(c\hat{Q})^\dagger = c^*\hat{Q}^\dagger$

↳ constant complex no.

Ex. Hermitian conjugates of $x, i, d/dx$:

a) $\langle \psi | \hat{x} \psi \rangle = \int_{-\infty}^{\infty} \psi^* x \psi \, dx = \int_{-\infty}^{\infty} (x\psi)^* \psi \, dx = \langle \hat{x} \psi | \psi \rangle$

$\hat{x}$ is Hermitian $\Rightarrow \boxed{\hat{x}^\dagger = \hat{x}}$

b) $\langle \psi | i \psi \rangle = \int_{-\infty}^{\infty} \psi^* i \psi \, dx = \int_{-\infty}^{\infty} (-i\psi)^* \psi \, dx = \langle (-i) \psi | \psi \rangle$

$\hat{i}^\dagger = -\hat{i}$

c) $\langle \psi | \frac{d}{dx} \psi \rangle = \int_{-\infty}^{\infty} \psi^* \frac{d\psi}{dx} dx = \cancel{\psi^* \psi \Big|_{-\infty}^{\infty}} - \int_{-\infty}^{\infty} \frac{d\psi^*}{dx} \psi \, dx = \langle -\frac{d}{dx} \psi | \psi \rangle$

0

$\therefore \frac{d}{dx}^\dagger = -\frac{d}{dx}$: Not Hermitian

★ In QM all useful (Hermitian) Ops are Linear!

d) $\hat{A}\psi = \frac{\partial^2}{\partial x^2} \psi \qquad \langle \hat{A} \rangle = \langle \psi | \hat{A} \psi \rangle$

$\Rightarrow \langle \hat{A} \rangle = \int_{-\infty}^{\infty} \psi^* \frac{\partial^2}{\partial x^2} \psi \, dx = \cancel{\left(\psi^* \frac{\partial \psi}{\partial x} \right)_{-\infty}^{\infty}} - \int_{-\infty}^{\infty} \frac{\partial \psi^*}{\partial x} \frac{\partial \psi}{\partial x} dx$

0

$= \left(-\frac{\partial \psi^*}{\partial x} \psi \right)_{-\infty}^{\infty} + \int_{-\infty}^{\infty} \frac{\partial^2 \psi^*}{\partial x^2} \psi \, dx = \langle \hat{A} \psi | \psi \rangle = \langle \hat{A} \rangle^*$

$\therefore$ Hermitian.

e) $\hat{A}\psi = \int_a^x \psi \, dx \rightarrow$ consider ϕ : the Eigenfunc of A

$\hat{A}\phi = \int_a^x \phi \, dx = \lambda \phi \Rightarrow \lambda \phi' = \phi \Rightarrow \underline{\phi = e^{\lambda x}}$

Let $\hat{A}$ be Hermitian

E-F-s blow up

Not allowed