# Hermitian operators

Definition: $$\hat{O} = \hat{O}^\dagger$$

$$\int_{-\infty}^{\infty} \phi^*(x)\hat{O}\psi(x)dx$$

$$= \int_{-\infty}^{\infty} \psi(x)\hat{O}^*\phi^*(x)dx$$

$$(AB)^\dagger = B^\dagger A^\dagger$$

# Momentum operator p is Hermitian

Proof: $$\int_{-\infty}^{\infty} \phi^*(x)\hat{p_x}\psi(x)dx$$

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

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

$$= -i\hbar\phi^*(x)\psi(x)\;\Big|_{-\infty}^{\infty}$$

$$+\; i\hbar\int_{-\infty}^{\infty}\frac{\partial\phi^*(x)}{\partial x}\psi(x)dx$$

$$\psi(\pm\infty)\rightarrow 0, \qquad \phi(\pm\infty)\rightarrow 0$$

Well behaved functions

$$= \; i\hbar \int_{-\infty}^{\infty} \psi(x) \frac{\partial \phi^*(x)}{\partial x} dx$$

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

$$= \; \int_{-\infty}^{\infty} \psi(x) (\hat{p}_x)^* \phi^*(x) dx$$

# Hermitian operators have real eigenvalues

Proof: $$\psi(x) = \phi(x) = \chi(x)$$

$$\hat{O}\chi(x) = \lambda\chi(x)$$

*LHS* = $\int_{-\infty}^{\infty} \phi^*(x)\hat{O}\psi(x)dx$

$$= \int_{-\infty}^{\infty} \chi^*(x)\hat{O}\chi(x)dx$$

$$= \int_{-\infty}^{\infty} \chi^*(x)\lambda\chi(x)dx$$

$$= \lambda \int_{-\infty}^{\infty} \chi^*(x)\chi(x)dx$$

$$RHS = \int_{-\infty}^{\infty} \psi(x)\hat{O}^* \phi^*(x)dx$$

$$= \int_{-\infty}^{\infty} \chi(x)\hat{O}^* \chi^*(x)dx$$

$$= \int_{-\infty}^{\infty} \chi(x)\lambda^* \chi^*(x)dx$$

$$= \lambda^* \int_{-\infty}^{\infty} \chi(x)\chi^*(x)dx$$

$$= \lambda^* \int_{-\infty}^{\infty} \chi^*(x)\chi(x)dx$$

$$(\lambda - \lambda^*) \int_{-\infty}^{\infty} \chi^*(x)\chi(x)dx = 0$$

$$\Longrightarrow \lambda = \lambda^*$$

$\lambda$ Real

# Eigenfunctions with different eigenvaules are orthogonal

$$H\psi_0 = E_0\psi_0\,,\; H\psi_1 = E_1\psi_1,\;\; H\psi_2 = E_2\psi_2,$$

etc.

If $$E_i \neq E_j$$

$$\int_{-\infty}^{\infty} \psi_i^*(x)\psi_j(x)dx$$

$$= \int_{-\infty}^{\infty} \psi_j^*(x)\psi_i(x)dx = 0$$

Proof:

$$\psi(x) = \chi(x)$$

$$\phi(x) = \xi(x)$$

$$\hat{O}\chi(x) = \lambda\chi(x)$$

$$\hat{O}\xi(x) = \eta\xi(x)$$

$$LHS = \int_{-\infty}^{\infty} \xi^*(x)\hat{O}\chi(x)dx$$

$$= \int_{-\infty}^{\infty} \xi^*(x)\lambda\chi(x)dx$$

$$= \lambda \int_{-\infty}^{\infty} \xi^*(x)\chi(x)dx$$

$$RHS = \int_{-\infty}^{\infty} \chi(x) \hat{O}^* \xi^*(x) dx$$

$$= \int_{-\infty}^{\infty} \chi(x) \eta^* \xi^*(x) dx$$

$$= \eta^* \int_{-\infty}^{\infty} \chi(x) \xi^*(x) dx$$

$$= \eta \int_{-\infty}^{\infty} \xi^*(x) \chi(x) dx$$

$$(\lambda - \eta)\int_{-\infty}^{\infty} \xi^*(x)\chi(x)dx = 0$$

If $\lambda \neq \eta$

$$\Longrightarrow \int_{-\infty}^{\infty} \xi^*(x)\chi(x)dx = 0$$

# Shrödinger Equation

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

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

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

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

$$i\hbar\frac{1}{f(t)}\frac{\partial f(t)}{\partial t} = -\frac{\hbar^2}{2m}\frac{1}{\psi(x)}\frac{\partial^2\psi(x)}{\partial x^2}+V(x) = E$$

$$i\hbar\frac{1}{f(t)}\frac{\partial f(t)}{\partial t} = E$$

$$\frac{1}{f(t)}\frac{\partial f(t)}{\partial t} = \frac{-iE}{\hbar}$$

$$\frac{\partial f(t)}{f(t)} = \frac{-iE}{\hbar}\partial t$$

$$f(t) = f_0 \exp(\frac{-iE}{\hbar}t)$$

# Time independent Schrödinger eqn.

$$-\frac{\hbar^2}{2m}\frac{\partial^2\psi(x)}{\partial x^2} + V(x)\psi(x) = E\psi(x)$$

$$\frac{d^2\psi(x)}{dx^2} + \frac{2m}{\hbar^2}(E - V(x))\psi(x) = 0$$

# Solution in constant potential $V(x) = V_0$

$$\frac{d^2\psi(x)}{dx^2} + k^2\psi(x) = 0$$

$$k = \sqrt{\frac{2m}{\hbar^2}(E - V_0)}$$

$$\psi(x) = A\exp(\pm ikx)$$

$$-\frac{\hbar^2}{2m}\frac{\partial^2\psi(x)}{\partial x^2} + V(x)\psi(x) = E\psi(x)$$

$$H\psi = E\psi$$

$$\boxed{\hat{A}\psi = a\psi}$$

Eigenvalue equation

$a$ : Eigenvalue

$\psi$ : Eigenfunction

# Hermitian operators have real eigenvalues

## Eigenfunctions of momentum operator

$$\psi(x) = A\exp(\pm ikx)$$

$$\hat{p}_x\psi = p\psi$$

$$p = \pm\hbar k$$

# Eigenfunctions of Hamiltonian H

$$H\psi_0 = E_0\psi_0$$

$$H\psi_1 = E_1\psi_1$$

$$H\psi_2 = E_2\psi_2$$

Etc.

$$\psi_0(x,t) = \psi_0(x)\exp\left(\frac{-iE_0}{\hbar}t\right)$$

$$\psi_1(x,t) = \psi_1(x)\exp\left(\frac{-iE_1}{\hbar}t\right)$$

Etc.

If $E_i \neq E_j$

$$\int_{-\infty}^{\infty} \psi_i^*(x)\psi_j(x)dx$$ Orthogonality

$$= \int_{-\infty}^{\infty} \psi_j^*(x)\psi_i(x)dx = 0$$

Normalisation

$$\int_{-\infty}^{\infty} \psi_i^*(x)\psi_i(x)dx = 1$$

$$\Psi(x,t) = c_0\psi_0(x)\exp\left(\frac{-iE_0}{\hbar}t\right)$$
$$+c_1\psi_1(x)\exp\left(\frac{-iE_1}{\hbar}t\right)$$
$$+c_2\psi_2(x)\exp\left(\frac{-iE_2}{\hbar}t\right)+\cdots$$

# Assuming orthonormal eigenfunctions

## Expectation or average value of energy

$$< E >= \frac{|c_0|^2 E_0 + |c_1|^2 E_1 + |c_2|^2 E_2 + \cdots}{|c_0|^2 + |c_1|^2 + |c_2|^2 + \cdots}$$

## Probability of obtaining eigenvalue Ei

$$P_i = |c_i|^2 / \sum_i |c_i|^2$$

Example: $\psi_1, \ \psi_2$ Normalised

$$H\psi_1 = 2\psi_1, \qquad H\psi_2 = 6\psi_2$$

$$\psi = \frac{\sqrt{3}}{2}\psi_1 + \frac{i}{2}\psi_2$$

$$< E >= \frac{3}{4} \times 2 + \frac{1}{4} \times 6 = 3$$

$$P_1 = \frac{3}{4}, \qquad P_2 = \frac{1}{4}$$

# Expectation value of an operator for a state $\Psi(x,t)$

$$< \hat{O} >= \frac{\int_{-\infty}^{\infty} \Psi^*(x,t)\hat{O}\Psi(x,t)dx}{\int_{-\infty}^{\infty} \Psi^*(x,t)\Psi(x,t)dx}$$