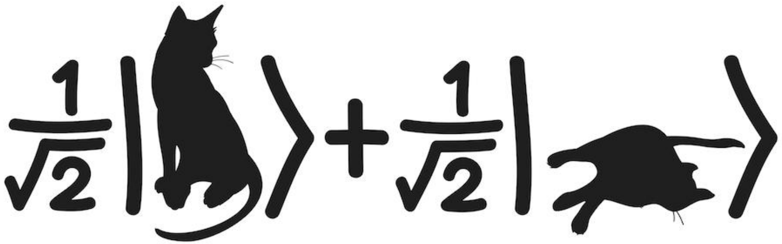
Quantum Mechanics & Quantum Computation



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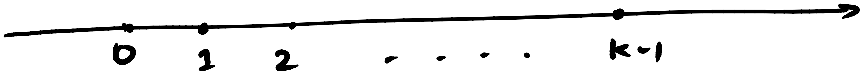
Lecture 10: Observables, Schrödinger's equation, Particle in a box

Position & Momentum Observables



$$|\psi\rangle = \sum_{j=0}^{k-1} \alpha_j |j\rangle$$

Position observable M : $M = M^{\dagger}$

$$M = \begin{bmatrix} 0 & & & & 0 \\ & 1 & & & \\ & & 2 & & \\ & & & \ddots & \\ 0 & & & & k-1 \end{bmatrix}$$

$$M|j\rangle = j\,|j\rangle$$

$$\underbrace{\frac{1}{\sqrt{3}}|0\rangle + \sqrt{\frac{2}{3}}\,|1\rangle}$$

$$|\psi\rangle \begin{pmatrix} \alpha_0 \\ \vdots \\ \alpha_{k-1} \end{pmatrix}$$

wavefunction $\psi(x)$

$$\psi(x) : \mathbb{R} \longrightarrow \mathbb{C}$$

$$\int_{-\infty}^{\infty} |\psi(x)|^2\, dx = 0$$

Inner product: $\psi(x)$ & $\phi(x)$

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

$$\alpha = a + ib$$

$$\alpha^* = a - ib = \bar{\alpha}$$

M Hermitian
self-adjoint

$$M = M^\dagger \iff \langle i|M|j\rangle = \overline{\langle j|M|i\rangle}$$

$$\langle \phi|M|\psi\rangle = \overline{\langle \psi|M|\phi\rangle}$$

Observable: self-adjoint M that maps wavefunctions to wavefunctions.

Position observable $\hat{x}$

$$\hat{x}\,\psi(x) = \phi(x) \quad \text{where} \quad \phi(x) = x\,\psi(x)$$

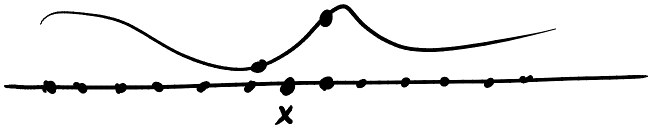
$|j\rangle$

$$\begin{bmatrix} 0 & & & \\ & 1 & & 0 \\ & & \ddots & \\ 0 & & & k-1 \end{bmatrix} \begin{bmatrix} \alpha_0 \\ \vdots \\ \vdots \\ \vdots \\ \alpha_{k-1} \end{bmatrix} = \begin{bmatrix} 0\cdot\alpha_0 \\ 1\cdot\alpha_1 \\ \vdots \\ \vdots \\ (k-1)\alpha_{k-1} \end{bmatrix}$$

Momentum Operator :

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

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



$$\begin{pmatrix} 0 & i & & \\ -i & \ddots & \ddots & \\ & \ddots & \ddots & i \\ & & -i & 0 \end{pmatrix} \begin{pmatrix}\alpha_0\\ \alpha_1\\ \alpha_{j-1}\\ \alpha_j\\ \alpha_{j+1}\\ \alpha_{k-1}\end{pmatrix} = \begin{pmatrix} \alpha_{j+1}-\alpha_{j-1}\end{pmatrix}$$

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

Free particle

$$i\hbar \frac{\partial |\psi\rangle}{\partial t} = H|\psi\rangle$$

H Hamiltonian

energy operator.

Classically: $\cancel{\text{P.E.}}^{=0} + \text{K.E.}$

$\frac{p^2}{2m}$ ← momentum

mass

$$i\hbar \frac{\partial \psi}{\partial t} = \frac{\hat{p}^2}{2m} |\psi\rangle$$

$$= -i\hbar \frac{\partial}{\partial x}\left(-i\hbar \frac{\partial}{\partial x}\right) \cdot \frac{1}{2m} |\psi\rangle$$

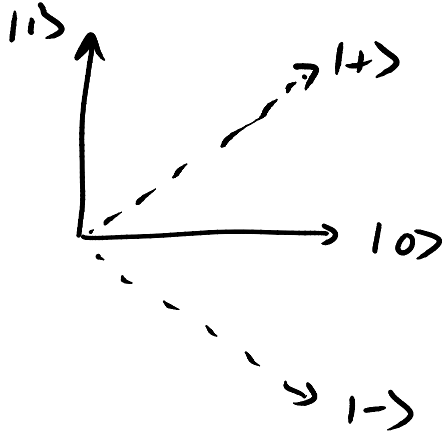
$$= -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} |\psi\rangle$$

bit & sign

$Z = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$ $\qquad$ $X = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$

$|0\rangle$ & $|1\rangle$ $\qquad$ $|+\rangle$ $\quad$ $|-\rangle$

1 $\quad$ -1 $\qquad$ 1 $\quad$ -1.



$$XZ \neq ZX$$

$$\begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}\begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} = \begin{bmatrix} 0 & -1 \\ 1 & 0 \end{bmatrix}$$

$$ZX = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}\begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} = \begin{bmatrix} 0 & 1 \\ -1 & 0 \end{bmatrix}$$

$$[X, Z] = XZ - ZX = \begin{bmatrix} 0 & -2 \\ 2 & 0 \end{bmatrix}$$

Position-momentum Uncertainty:

$$[\hat{x},\hat{p}] = \hat{x}\hat{p} - \hat{p}\hat{x} = i\hbar$$

Thm $\quad \Delta\hat{x}\,\Delta\hat{p} \geq \frac{|[\hat{x},\hat{p}]|}{2} \geq \frac{\hbar}{2}.$ $\qquad (\Delta A)^2 = |\langle\psi|A^2|\psi\rangle|$

Thm $\quad \Delta A\,\Delta B \geq \frac{|[A,B]|}{2}$

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

$$= x\frac{-i\hbar\partial\psi(x)}{\partial x} - \left(\frac{-i\hbar\partial}{\partial x}x\,\psi(x)\right)$$

$$= -i\hbar\left[\cancel{x\frac{\partial\psi}{\partial x}} - \underbrace{\frac{\partial}{\partial x}x\psi(x)}_{\psi(x) + \cancel{x\frac{\partial}{\partial x}\psi(x)}}\right]$$

$$= i\hbar\,\psi(x)$$