Aug 28, PHYS 3317

announcements:
* MATLAB tutorial: this Thu B30A 6-10 PM
  what is best time
* don't wait with HW/MATLAB, start now!
* office hrs: see the Blackboard

① Action of operators:

linear { Hermitian $\hat{A}$: $|\psi\rangle \to \hat{A}|\psi\rangle$ different norm
linear { Unitary $\hat{U}$: $|\psi\rangle \to \hat{U}|\psi\rangle$ norm preserving (can be another QM state)

Projection operator: $\hat{P} = |\phi\rangle\langle\phi|$ "outer product"

unitary? NO
hermitian? YES $\hat{P}^{+} = |\phi\rangle\langle\phi| = \hat{P}$

another property: $\hat{P}^2 = \hat{P}$

Function of an operator (matrix)?

$f(z) \to f(\hat{A})$

substitute $z \to \hat{A}$ in Taylor series:

$$f(0) + \frac{f'(0)}{1!} z + \frac{f''(0)}{2!} z^2 + \dots$$

Ex: operator $\exp(a \frac{d}{dx})$ acting on $\psi(x)$

$$e^{a\frac{d}{dx}} \psi(x) = \left(1 + a\frac{d}{dx} + \frac{1}{2!} a^2 \frac{d^2}{dx^2} + \dots\right)\psi(x)$$

Taylor expand $\psi(x+a)$ around x:

$$\psi(x) + a\frac{d}{dx}\psi(x) + \frac{1}{2!} a^2 \frac{d^2}{dx^2}\psi(x) + \dots$$

$$\Rightarrow e^{a\frac{d}{dx}} \psi(x) = \psi(x+a)$$ shift operator!

MATLAB functions expm and funm (for general fcn)

* short warmup quiz

② Representation in a complete orthonormal basis $|\varphi_i\rangle$

* state $|\psi\rangle \to$ vector $\psi_i = \langle\varphi_i|\psi\rangle$

$$|\psi\rangle = \sum_i \psi_i |\varphi_i\rangle$$

$$= \sum_i \underbrace{|\varphi_i\rangle\langle\varphi_i|}_{\hat{1}}\psi\rangle$$

$\hat{1}$ "closure relationship"

* operator $\hat{A} \to$ matrix $A_{ij} = \langle \varphi_i | \hat{A} | \varphi_j \rangle$

$$\hat{A} = \sum_{i,j} A_{ij} |\varphi_i\rangle\langle\varphi_j|$$

bilinear expansion of linear operator

Q: how does $\hat{A}$ look in its own eigenbasis?

③ Solving 1D Schrod. eqn. numerically

$\hat{H}|\psi_n\rangle = E_n|\psi_n\rangle$ – time indep. Schrod. eqn.

basis: finite position $x_j = \Delta x \cdot j$ with $j = 0, \dots, N$ $\quad (0 \le x \le L)$

require $V(x<0) = V(x>L) \to \infty$

$\varphi(x_0) = \varphi(x_N) = 0$

How do operators look in this basis?

$$\hat{X} = \begin{pmatrix} x_0 & & & & 0 \\ & x_1 & & & \\ & & x_2 & & \\ & & & \ddots & \\ 0 & & & & x_N \end{pmatrix}$$

$$\hat{p} = \frac{\hbar}{i}\frac{d}{dx} \; ; \qquad \frac{d\psi(x_j)}{dx} \simeq \frac{\psi(x_{j+1}) - \psi(x_{j-1})}{2\Delta x}$$

$$\Rightarrow \quad \hat{p} = \frac{\hbar}{2i\Delta x}\begin{pmatrix} 0 & 1 & 0 & & & 0 \\ -1 & 0 & 1 & & & \\ 0 & -1 & 0 & & & \\ & & & \ddots & & \\ & & & & 0 & 1 \\ 0 & & & & -1 & 0 \end{pmatrix}$$

$\hat{H} =$ HW1; $(N-1)\times(N-1)$ matrix, use Matlab to find $E_n, \psi_n(x_j)$

④ Time evolution of $|\psi(t)\rangle$

All QM states are always time-dependent

* Energy operator $\hat{\mathcal{E}} = i\hbar\frac{\partial}{\partial t}$

$$\hat{\mathcal{H}}|\psi(t)\rangle = \hat{\mathcal{E}}|\psi(t)\rangle$$

$\leftarrow$ $|\psi(t)\rangle$ evolution (like Newton's 2nd law)

$$\boxed{\hat{\mathcal{H}}|\psi(t)\rangle = i\hbar\frac{\partial}{\partial t}|\psi(t)\rangle}$$

Schrod. time dep. eqn.

Important remarks :

1) STDE $\neq$ eigenvalue eqn (any spatial fcn. is a solution)

2) Stationary states are time-dependent too

when $\hat{\mathcal{H}} \neq \hat{\mathcal{H}}(t)$ (or $V \neq V(t)$)

Given eigenstates of $\hat{\mathcal{H}}$: $\hat{\mathcal{H}}|\psi_n\rangle = E_n|\psi_n\rangle$

what's time-dep. of $|\psi_n(t)\rangle$?

$$\hat{\mathcal{H}}|\psi_n(t)\rangle = i\hbar\frac{\partial}{\partial t}|\psi_n(t)\rangle = E_n|\psi_n(t)\rangle$$

or $$|\psi_n(t)\rangle = \underbrace{e^{-iE_nt/\hbar}}_{\text{phase factor : does not enter into probabilities}}|\psi_n(t=0)\rangle$$ evolution of $|\psi_n\rangle$

3) E.g. given arbitrary $|\psi(t=0)\rangle$, decompose in stationary eigenbasis

$$|\psi(t=0)\rangle = \sum_n c_n|\psi_n\rangle , \qquad c_n = \langle\psi_n|\psi(t=0)\rangle$$

$$|\psi(t)\rangle = \sum_n c_n \exp(-iE_nt/\hbar)|\psi_n\rangle$$

$\psi_n = \psi_n(\vec{r})$ only

Matlab example + HW

* spatial form of $|\psi(t=0)\rangle$ defines how $|\psi\rangle$ evolves in time (plus stationary eigenstates $|\psi_n\rangle$)
* superposition of stationary states $\neq$ stationary state

4) time evolution operator :

$$\hat{\mathcal{H}}|\psi(t)\rangle = i\hbar\frac{\partial}{\partial t}|\psi(t)\rangle , \qquad \frac{d|\psi\rangle}{|\psi\rangle} = \frac{1}{i\hbar}\hat{\mathcal{H}}\,dt$$

$$\int_{|\psi(0)\rangle}^{|\psi(t)\rangle}\frac{d|\psi\rangle}{|\psi\rangle} = \int_0^t \frac{1}{i\hbar}\hat{\mathcal{H}}\,dt ; \quad \ln|\psi(t)\rangle - \ln|\psi(0)\rangle = -\frac{i}{\hbar}\hat{\mathcal{H}}t$$

$$|\psi(t)\rangle = \underbrace{e^{-\frac{i\hat{\mathcal{H}}t}{\hbar}}}_{\text{unitary}}|\psi(0)\rangle ;$$

5) Commutators : $[\hat{A},\hat{B}] \equiv \hat{A}\hat{B} - \hat{B}\hat{A}$

$\underbrace{[\hat{A},\hat{B}] = 0}_{\text{commute}} \leftrightarrow$ joint basis of eigenstates $|\psi_n\rangle$ (but not the same eigenvalues !)

$\neq 0 \leftrightarrow$ no joint eigenbasis

e.g. for a free particle in 1D :

$$\hat{p}_x = \frac{\hbar}{i}\frac{d}{dx} , \quad \hat{\mathcal{H}} = \frac{\hat{p}_x^2}{2m} = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} . \quad [\hat{p}_x, \hat{\mathcal{H}}] = 0$$

eigenfcns: $\psi(x) \propto \exp(ip_x x/\hbar)$ for $\hat{p}_x$ & $\hat{\mathcal{H}}$ with cont. spectrum p_x and $\frac{p_x^2}{2m}$

Dispersion (or r.m.s.) $\Delta A = \sqrt{\overline{A^2} - \overline{A}^2} = \sqrt{\langle(\hat{A} - \overline{A})^2\rangle}$

* if $[\hat{A}, \hat{B}] = 0$, $\rightarrow$ can be in a state with $\Delta A = 0$ and $\Delta B = 0$

* if $[\hat{A}, \hat{B}] = i\hat{C}$, $\Delta A \cdot \Delta B \geq \frac{|\overline{C}|}{2}$ (see Griffith)

Example : $[\hat{x}, \hat{p}_x] = x \frac{\hbar}{i} \frac{d}{dx} - \frac{\hbar}{i} \frac{d}{dx} x = x \frac{\hbar}{i} \frac{d}{dx} - x \frac{\hbar}{i} \frac{d}{dx} - \frac{\hbar}{i} = i\hbar$

$\Delta x \cdot \Delta p \geq \frac{\hbar}{2}$