PC3130 W1L2

Wednesday, 24 July 2024 10:16 am

State 'ket' $|\psi\rangle$

'bra' $\langle\psi|$

<u>Given a basis</u> for a Hilbert space $\mathcal{H}$ in which $|\psi\rangle$ lives, we can define vectors to represent the state, and use language of linear algebra.

A basis for $\mathcal{H}$ will span $\mathcal{H}$.

Any $|\psi\rangle \in \mathcal{H}$ can be written as a linear combination of basis states.

Eg. If dimension of $\mathcal{H}$ is N, basis is $\{\underbrace{|0\rangle, |1\rangle, \ldots, |N-1\rangle}_{N \text{ states}}\}$

$|\psi\rangle$ can be written as $|\psi\rangle = \sum_{i=0}^{N-1} c_i |i\rangle$

any $|\psi\rangle \in \mathcal{H}$.

$c_i = \langle i|\psi\rangle$

$\hookrightarrow$ definition of a complete basis.

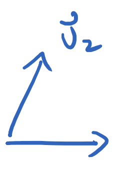
What is the meaning of 'linearly independent'?
(l.i.)

A set of vectors $\{\vec{v}_i\}$ is l.i if :

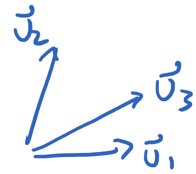
$$\sum_i \lambda_i \vec{v}_i = \vec{0} \quad \underset{\text{if and only if}}{\text{iff}} \quad \lambda_i = 0 \quad \underset{\text{for all}}{\forall} i$$

(ie. we <u>cannot</u> write $\vec{v}_j = \sum_{i \neq j} \frac{-\lambda_i}{\lambda_j} \vec{v}_i$ as a linear combination of the other $\vec{v}_i$'s)

Eg



$\vec{v}_1$ and $\vec{v}_2$ are l.i.



$\{\vec{v}_1, \vec{v}_2, \vec{v}_3\}$ is not l.i.

$\vec{v}_3 = \vec{v}_1 + \frac{1}{2}\vec{v}_2$.

<u>Expectation values</u>

$$\langle \hat{A} \rangle_\psi = \langle\psi|\hat{A}|\psi\rangle$$

$$\frac{d}{dt}\langle \hat{A} \rangle_t = \frac{i}{\hbar}\langle [\hat{H}, \hat{A}] \rangle + \left\langle \frac{\partial \hat{A}}{\partial t} \right\rangle$$

Hamiltonian

States can be $\mathbb{C}$.
But observables are real — eigenvalues of Hermitian operators.

Basis sets — orthonormal

$$\langle m | n \rangle = \delta_{mn} = \begin{cases} 1 & m = n \\ 0 & m \neq n \end{cases}$$

Kronecker delta.

Can always find an orthonormal set of eigenstates.

Continuous variables

Position. $\hat{X}$ position operator

$$\hat{X} |x\rangle = x |x\rangle$$

position eigenstate

(Recall that for a complete basis $\{|n\rangle\}$, $\mathbb{1} = \sum_n |n\rangle\langle n|$)

summed over

"x", "n" are dummy indices/variables

eg $\mathbb{1} = \sum_m |m\rangle\langle m|$

$$\mathbb{1} = \int dx \, |x\rangle\langle x|$$

(integrated over —

$\mathbb{1} = \int dy \, |y\rangle\langle y|$

Apply $\mathbb{1}$ to $|x'\rangle$:

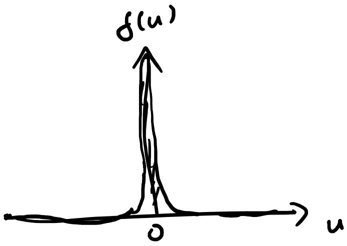
specific

not the same symbol as the dummy variable

$$|x'\rangle \equiv \mathbb{1} |x'\rangle = \int dx \, |x\rangle \boxed{\langle x | x' \rangle}$$

$$\langle x | x' \rangle = \delta(x - x') = \delta(x' - x)$$

Dirac delta distribution



$$\int du \, \delta(u) = 1$$

$$\int dx \, f(x)\, \delta(x - a) = f(a)$$

dummy variable ⇒ RHS should not have this (x)

$$\int dx \, \delta(x - x_1)\, \delta(x - x_0) = \delta(x_1 - x_0) = \delta(x_0 - x_1)$$

Wavefunction for a state $|\psi\rangle$ is defined as

$$\langle x|\psi\rangle \equiv \psi(x)$$

$$|\psi\rangle = \int dx\, |x\rangle\langle x|\psi\rangle = \int dx\, \psi(x)\, |x\rangle.$$

$\psi(x)$ is "normalized"

$$\int dx\, |\psi(x)|^2 = 1$$

$$1 = \langle\psi|\psi\rangle = \int dx\, \langle\psi|x\rangle\langle x|\psi\rangle = \int dx\, |\psi(x)|^2$$

$$\langle\psi|\psi\rangle = \langle\psi|\mathbb{1}|\psi\rangle = \int dx\, \langle\psi|x\rangle\langle x|\psi\rangle$$

momentum operator $\hat{p}$ is defined by

$$\hat{p}\,|\psi\rangle = \int dx \left(-i\hbar \frac{d}{dx}\psi(x)\right)|x\rangle$$

ie. $$\langle x'|\hat{p}|\psi\rangle = \int dx \left(-i\hbar \frac{d}{dx}\psi(x)\right)\underbrace{\langle x'|x\rangle}_{\delta(x'-x)}$$

$$= -i\hbar \frac{d}{dx'}\psi(x')$$

OR $$\langle x|\hat{p}|\psi\rangle = -i\hbar \frac{d}{dx}\psi(x)$$

Eg. $\psi(x) = e^{ikx}$ – plane wave – denotes free electrons with kinetic energy $\frac{\hbar^2 k^2}{2m_e}$.

$$-i\hbar \frac{d\psi}{dx} = -i\hbar\,(ik)\,e^{ikx}$$

$$= \hbar k\, e^{ikx}$$

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

$(p = \hbar k)$ – well-defined momentum p.
– but x can go from $-\infty$ to $+\infty$.

$$\boxed{[X, P] = i\hbar\,\mathbb{1}}$$

Eg. $[x, p_x] = i\hbar$

$$x p_x - p_x x$$

$$p_x = -i\hbar \frac{d}{dx}$$

$$[x, p_y] = 0$$

.. p^2

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

We expect from classical physics that momentum $p = mv = m\frac{dx}{dt}$.

Likewise $\langle p \rangle = m\frac{d}{dt}\langle x \rangle$

$$m\frac{d}{dt}\langle x \rangle = m\frac{i}{\hbar}\langle [H, x] \rangle + m\cancel{\left\langle \frac{\partial x}{\partial t} \right\rangle}_{0}$$

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

$$= \left[\frac{p^2}{2m}, x\right]$$

$[V(x), x] = 0$ since $[x, x] = 0$

Commutator relations

In general, operators in QM do not commute, just as matrices do not normally commute.

$$\hat{A}\hat{B}|\psi\rangle = \hat{A}\left((\hat{B}|\psi\rangle)\right)$$

may not be the same

$$\hat{B}\hat{A}|\psi\rangle = \hat{B}\left((\hat{A}|\psi\rangle)\right)$$

Eg. $A = \begin{pmatrix} 1 & 1 \\ 0 & 1 \end{pmatrix}$, $B = \begin{pmatrix} 1 & 0 \\ -1 & 1 \end{pmatrix}$

$AB =$

$BA =$

We define $[\hat{A}, \hat{B}] = \hat{A}\hat{B} - \hat{B}\hat{A}$.

If $[\hat{A}, \hat{B}] = 0$ (i.e. $\hat{A}, \hat{B}$ commute),

it means $\hat{A}\hat{B}|\psi\rangle = \hat{B}\hat{A}|\psi\rangle$ for all $|\psi\rangle$ in the Hilbert space.

Properties of commutators

$$[A, B] = -[B, A]$$

$$[A, aB] = a[A, B] = [aA, B]$$

$$[A, A] = 0$$

$$[A, f(A)] = 0$$

$$[A+B, C] = [A, C] + [B, C]$$

$$[AB, C] = [A, C]B + A[B, C]$$

1 2

$$[A, BC] = [A,B]C + B[A,C]$$

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

$$[A,[B,C]] + [B,[C,A]] + [C,[A,B]] = 0$$

$$m\frac{d}{dt}\langle x\rangle = m\frac{i}{\hbar}\langle [H,x]\rangle$$

$$= m\frac{i}{\hbar}\left\langle \left[\frac{p^2}{2m}, x\right]\right\rangle$$

$$= m\frac{i}{\hbar}\left(\left\langle \frac{1}{2m}\left([p,x]p + p[p,x]\right)\right\rangle\right)$$

$[x,p] = i\hbar\mathbb{1}$

$[p,x] = -i\hbar\mathbb{1}$

$$= \frac{\cancel{m}\, i}{\hbar}\cdot\frac{1}{2\cancel{m}}\left(\left\langle (-i\hbar)p + p(-i\hbar)\right\rangle\right)$$

$$= \langle p\rangle \quad ✓$$

Commutator relations — uncertainty principle (Ch 3 Griffiths)

Compatible observables — course reading (Liboff)

(next lecture) Complete set of compatible/commuting observables.

— course reading (Liboff)

Uncertainty principle

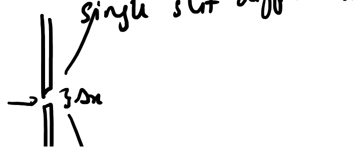
Two operators $\hat{A}, \hat{B}$:

$$(\Delta\hat{A})(\Delta\hat{B}) \geq \frac{1}{2}\left|\langle[\hat{A},\hat{B}]\rangle\right|$$

where $\Delta\hat{A} = \sqrt{\langle\hat{A}^2\rangle - \langle\hat{A}\rangle^2}$ expectation value.

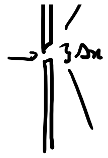
Eg $[\hat{x},\hat{p}] = i\hbar$

$$(\Delta x)(\Delta p) \geq \frac{1}{2}|i\hbar| = \frac{\hbar}{2}$$



$$(\Delta x)(\Delta p) \geq \frac{1}{2}|i\hbar| = \frac{\hbar}{2}$$

x and p cannot be measured simultaneously.



$\Delta x \downarrow \quad \Delta p \uparrow$

- wave properties.

Commuting observables can actually be measured simultaneously.

We call them compatible observables.

Commutator theorem

If $[\hat{A}, \hat{B}] = 0$, then $\hat{A}$ and $\hat{B}$ have a set of common eigenstates.; ie. there exists a set of common eigenstates.

Proof

Suppose $\hat{A}|\psi_a\rangle = \underset{\text{eigenvalue}}{a}|\psi_a\rangle$

Then $\hat{B}\hat{A}|\psi_a\rangle = \hat{B}(\underset{\text{scalar}}{a}|\psi_a\rangle) = a\hat{B}|\psi_a\rangle$. —(1)

But $[\hat{A}, \hat{B}] = 0$

$\Rightarrow \hat{A}(\hat{B}|\psi_a\rangle) = \hat{B}\hat{A}|\psi_a\rangle = \underset{\text{eigenvalue}}{a}(\hat{B}|\psi_a\rangle)$ from (1)

$\Rightarrow \hat{B}|\psi_a\rangle$ is an eigenstate of $\hat{A}$ with eigenvalue a.

Case 1 If $|\psi_a\rangle$ is the only linearly independent eigenstate of $\hat{A}$ with eigenvalue a,

Then $\hat{B}|\psi_a\rangle$ must just be $\mu|\psi_a\rangle$ for some μ,

ie they represent the same state up to a global phase.

(if $\hat{B}$ is Hermitian, μ must be real:)

So $|\psi_a\rangle$ is also an eigenstate of $\hat{B}$.

$$\hat{B}|\psi_a\rangle = \mu|\psi_a\rangle$$

μ: eigenvalue of $\hat{B}$.

More clearly, we can write

$$\hat{B}|\psi_a\rangle = b|\psi_a\rangle$$

common eigenstate of $\hat{A}$ & $\hat{B}$ — eigenvalues

More clearly, we can write

$$\hat{B}|\psi_a\rangle = b|\psi_a\rangle$$

and denote $|\psi_a\rangle$ as $|\psi_{a,b}\rangle$ where $\underbrace{\hat{A}|\psi_{a,b}\rangle}_{\text{eigenstate of } \hat{A} \,\&\, \hat{B}} = a|\psi_{a,b}\rangle$, $\hat{B}|\psi_{a,b}\rangle = b|\psi_{a,b}\rangle$ (a, b: eigenvalues)

Case 2 If $|\psi_a\rangle$ is not the only linearly independent eigenstate of $\hat{A}$, we say a is degenerate.

Eg if the degeneracy is 2,

$$\hat{A}|\psi_a^{(1)}\rangle = a|\psi_a^{(1)}\rangle$$

$$\hat{A}|\psi_a^{(2)}\rangle = a|\psi_a^{(2)}\rangle \quad , \quad |\psi_a^{(1)}\rangle \neq |\psi_a^{(2)}\rangle$$

Then any $|\psi_a\rangle = \alpha|\psi_a^{(1)}\rangle + \beta|\psi_a^{(2)}\rangle$ satisfies $\hat{A}|\psi_a\rangle = a|\psi_a\rangle$

Recall $\hat{B}|\psi_a\rangle$ is an eigenstate of $\hat{A}$ with eigenvalue a.

So $\hat{B}|\psi_a\rangle = \tilde{\alpha}|\psi_a^{(1)}\rangle + \tilde{\beta}|\psi_a^{(2)}\rangle$ for some $\tilde{\alpha}$ and $\tilde{\beta}$.

$\hat{B}|\psi_a'\rangle = \gamma|\psi_a'\rangle$ for some γ.

and $|\psi_a'\rangle = \alpha'|\psi_a^{(1)}\rangle + \beta'|\psi_a^{(2)}\rangle$ for some α' and β'.

Such that $\hat{A}|\psi_a'\rangle = a|\psi_a'\rangle$

Then $|\psi_a'\rangle$ is a common eigenstate of $\hat{A}$ and $\hat{B}$.

[If $[\hat{A},\hat{B}]=0$ and a is a degenerate eigenvalue of $\hat{A}$, the corresponding eigenstate of $\hat{A}$ need not be an eigenstate of $\hat{B}$. We can find a linear combination of eigenstates that are eigenstates of both $\hat{A}$ and $\hat{B}$.]

Eg. Free particle Hamiltonian

$$\hat{H} = \frac{\hat{p}^2}{2m}.$$

$$[\hat{p}, \hat{H}] = 0$$

$\Rightarrow$ we can find a set of common eigenstates for $\hat{p}$ and $\hat{H}$.

$\Rightarrow$ We can find a set of common eigenstates for $\hat{p}$ and H.

$\hat{p} = -i\hbar \vec{\nabla}$, $\hat{H} = \frac{p^2}{2m} = -\frac{\hbar^2}{2m}\nabla^2$

$$H\psi(x) = E\psi(x)$$

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

$$\nabla^2\psi(x) = -\frac{2mE}{\hbar^2}\psi(x)$$

Possible $\psi(x)$ are

$\psi_1(x) = \cos kx$,

$\psi_2(x) = \sin kx$.

$k = \sqrt{\frac{2mE}{\hbar^2}}$

Here $\vec{p}\psi_1(x) \propto \psi_2(x)$

$\neq \psi_1(x)$

So $\psi_1(x)$ is <u>not</u> an eigenfunction of $\vec{p}$.

Possible $\psi(x)$ are

$\psi_+(x) = e^{ikx}$

$\psi_-(x) = e^{-ikx}$

$\vec{p}\,\psi_+(x) = \hbar k\,\psi_+(x)$

$\vec{p}\,\psi_-(x) = -\hbar k\,\psi_-(x)$

So $\{\psi_+(x), \psi_-(x)\}$ is a set of common eigenstates for $\hat{p}$ and $\hat{H}$.