Class 22 Dirac Formalism, continuous eigenvalues

Tuesday, November 13, 2018 8:00 AM

Dirac Formalism (continued)

$$\hat{X}|x\rangle = \underbrace{x}_{\text{Real}}|x\rangle \quad ; \quad \hat{P}|p\rangle = p|p\rangle$$

Since $\hat{X}$ & $\hat{P}$ are Hermitian operators $|x\rangle$ & $|p\rangle$ form a complete basis in the sense that any ket $|\psi\rangle$ corresponding to a quantum state can be expressed in terms of $|x\rangle$ or $|p\rangle$

$$|\psi\rangle = \int dx \; \psi(x)\,|x\rangle \qquad |\psi\rangle = \int dp\; \phi(p)\,|p\rangle$$

$\psi(x)$ ↳ expansion coefficients (labeled by continuous index)

$\phi(p)$ ↳ expansion coefficients

$\psi(x)$ the wavefunction in coordinate space

$\phi(p)$ the wavefunction in momentum space

* $\hat{P}|p\rangle = p|p\rangle \qquad \otimes \langle x| \Rightarrow \langle x|\hat{P}|p\rangle = p\langle x|p\rangle$

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

$$\langle x|\hat{P}\,\mathbb{1}\,|p\rangle = \int \langle x|\hat{P}\int dx'\,|x'\rangle\langle x'|p\rangle$$

$$= \int dx'\,\langle x|\hat{P}|x'\rangle\langle x'|p\rangle$$

$$= p\langle x|p\rangle$$

$\langle x|\hat{P}|x'\rangle = \,?\qquad \langle x|[\hat{X},\hat{P}]|x'\rangle = \langle x|\hat{X}\hat{P}-\hat{P}\hat{X}|x'\rangle$

$$\langle x|[\hat{X},\hat{P}]|x'\rangle = (x-x')\underbrace{\langle x|\hat{P}|x'\rangle}$$

$$i\hbar\langle x|x'\rangle = (x-x')\langle x|\hat{P}|x'\rangle$$

$$i\hbar\,\delta(x-x') = (x-x')\langle x|\hat{P}|x'\rangle \qquad x-x'=\xi$$

$$i\hbar\,\delta(\xi) = \xi\langle x|\hat{P}|x'\rangle$$

claim $\quad \xi \dfrac{d}{d\xi}\delta(\xi) = -\delta(\xi)$ $\quad *$

$$\int d\xi\, f(\xi)\,\delta(\xi) = f(0)$$

$$\int d\xi \left(\xi \frac{d}{d\xi}\delta(\xi)\right) f(\xi) = \;?$$

$$= \int d\xi \frac{d}{d\xi}\cancelto{0}{\left(\xi f(\xi)\delta(\xi)\right)} - \int d\xi\, \delta(\xi) f(\xi) - \cancelto{0}{\int d\xi\, \delta(\xi)\,\xi \frac{d f(\xi)}{d\xi}}$$

$$\int d\xi \left(\xi \frac{d}{d\xi}\delta(\xi)\right) f(\xi) = -\int d\xi\, \delta(\xi) f(\xi) \quad \checkmark$$

$$-i\hbar\, \xi \frac{d}{d\xi}\delta(\xi) = \xi \langle x|p|x'\rangle$$

$$\langle x|p|x'\rangle = -i\hbar \frac{d}{d\xi}\delta(\xi) = -i\hbar \frac{\partial}{\partial x}\delta(x-x')$$

$$= i\hbar \frac{\partial}{\partial x'}\delta(x-x')$$

$$\boxed{\begin{aligned}\langle x|\hat{p}|x'\rangle &= -i\hbar \frac{\partial}{\partial x}\delta(x-x') \\ &= i\hbar \frac{\partial}{\partial x'}\delta(x-x')\end{aligned}}$$

$$\langle p|\hat{x}|p'\rangle = -i\hbar \frac{\partial}{\partial p}\delta(p-p')$$

$$\therefore \int dx' \left(i\hbar \frac{\partial}{\partial x'}\delta(x-x')\right)\langle x'|p\rangle = p\langle x|p\rangle$$

$$i\hbar \int dx' \left(\frac{\partial}{\partial x'}\left(\delta(x-x')\langle x'|p\rangle\right) - \delta(x-x')\frac{\partial}{\partial x'}\langle x'|p\rangle\right) = p\langle x|p\rangle$$

$$\lim_{L\to\infty}\left(\cancelto{0}{i\hbar\, \delta(x-x')\langle x'|p\rangle\Big|_{-L}^{L}}\right) - i\hbar \frac{\partial}{\partial x}\langle x|p\rangle = p\langle x|p\rangle$$

0 for x : finite.

$$-i\hbar \frac{\partial}{\partial x}\langle x|p\rangle = p\langle x|p\rangle \implies \langle x|p\rangle = A\, e^{i/\hbar\, px}$$

$\langle x|p\rangle$ is the transformation matrix for the x-basis to the p-basis

$$|x\rangle = \int dp\, |p\rangle\langle p|x\rangle = A\int dp\, e^{-i/\hbar\, px}\, |p\rangle$$

$$\langle x| = A\int dp\, e^{i/\hbar\, px}\, \langle p|$$

$$\Rightarrow \langle x|\psi\rangle = \psi(x) = A\int dp\, e^{i/\hbar\, px}\, \phi(p)$$

$$\phi(p) = \langle p|\psi\rangle$$

Likewise you will show for Homework that

$$\hat{H}|E\rangle = E|E\rangle \rightarrow \langle x|\hat{H}|E\rangle = E\langle x|E\rangle$$

$$\int dx' \langle x|H|x'\rangle\langle x'|E\rangle = E\langle x|E\rangle$$

$$\left\{ -\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi_E(x) + V(x)\psi_E(x) = E\,\psi_E(x) \quad \cancel{\#} \right\}$$

$$\psi_E(x) = \langle x|E\rangle$$

Q. S. $\leftrightarrow |\psi\rangle$, Hermitian Operator $\leftrightarrow$ Observables $\oplus$ $\left[\hat{x}, \hat{p}\right] = i\hbar$ }

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Any Operator : $|\phi\rangle\langle\psi|$

Examples: $|x\rangle\langle x| \equiv P_x$ $\qquad \mathbb{P}_i = |e_i\rangle\langle e_i|$

$$\int dx\, P_x = \int dx\, |x\rangle\langle x| = \mathbb{1} \quad ; \quad \sum_i \mathbb{P}_i = \sum_i |e_i\rangle\langle e_i| = \mathbb{1}$$

Note that operators written in their own eigenbasis are diagonal.

$$\hat{Q}|q_n\rangle = q_n|q_n\rangle \qquad \langle q_n|\hat{Q}|q_m\rangle = (\underset{\sim}{Q})_{nm}$$

$\langle x|\hat{q}|x'\rangle$ "the matrix elements of $\hat{q}$ in the x-basis"

$$(\hat{Q})_{nm} = q_m\langle q_n|q_m\rangle$$
$$= q_m\,\delta_{nm}$$

$$\boxed{\hat{Q} = \sum_n q_n\, |q_n\rangle\langle q_n|}$$

$$\underset{\sim}{\hat{Q}} = \begin{pmatrix} q_1 & & \phi \\ & q_2 & \\ \phi & & \ddots \\ & & & q_N \end{pmatrix}$$

$$\cdots q_N$$

$$|q_1\rangle \,\text{"="}\, \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \\ \vdots \end{pmatrix} \qquad |q_2\rangle \,\text{"="}\, \begin{pmatrix} 0 \\ 1 \\ 0 \\ \vdots \end{pmatrix} \qquad |q_3\rangle \,\text{"="}\, \begin{pmatrix} 0 \\ 0 \\ 1 \\ 0 \end{pmatrix}$$

$$\langle q_n | q_m \rangle = \delta_{mn}$$

$$|q_1\rangle\langle q_1| \,\text{"="}\, \begin{pmatrix} 1 \\ 0 \\ 0 \\ \vdots \end{pmatrix} \otimes \begin{pmatrix} 1 \\ 0 \\ 0 \\ \vdots \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 & \cdots \\ 0 & 0 & & \\ \vdots & & \ddots & \\ \vdots & & & 0 \end{pmatrix}_{N\times N}$$

$$\mathrm{tr}\left(|q_1\rangle\langle q_1|\right) = \langle q_1 | q_1 \rangle = 1$$

$$|q_1\rangle\langle q_2| = \begin{pmatrix} 1 \\ 0 \\ 0 \\ \vdots \end{pmatrix} \otimes \begin{pmatrix} 0 \\ 1 \\ 0 \\ \vdots \end{pmatrix} = \begin{pmatrix} 0 & 1 & 0 & \cdots \\ 0 & & & \\ 0 & & \phi & \\ 0 & & & \end{pmatrix}_{N\times N}$$

$$\mathrm{tr}\left(|q_1\rangle\langle q_2|\right) = \langle q_1 | q_2 \rangle = 0 \checkmark$$

$$\hat{Q} = \sum_n q_n |q_n\rangle\langle q_n| = \begin{pmatrix} q_1 & & & \phi \\ & q_2 & & \\ & \phi & q_3 & \\ & & & \ddots & q_N \end{pmatrix}$$

$$\mathrm{tr}(\hat{Q}) = \sum_n q_n \, \mathrm{tr}\left(|q_n\rangle\langle q_n|\right)$$

$$= \sum_n q_n \langle q_n | q_n \rangle = \sum_n q_n$$

$$\hat{X} = \int dx \; x |x\rangle\langle x|$$

Continue with the discrete case (easy to generalize to continuous case)

$$\langle e_i | \hat{Q} | e_j \rangle = \hat{Q}_{ij}$$ In this basis $\hat{Q}$ is not necessarily diagonal

$$\uparrow \;\; \uparrow$$
$$\mathbb{1} \;\; \mathbb{1}$$

$$\langle e_i | \hat{Q} | e_j \rangle = \sum_{m,n} \langle e_i | q_n \rangle \langle q_n | \hat{Q} | q_m \rangle \langle q_m | e_j \rangle$$

$$= \sum_{m,n} \langle e_i | q_n \rangle \, \delta_{nm} \, q_n \langle q_m | e_j \rangle$$

m, n

$$\langle q_n | \hat{Q} | q_m \rangle = \sum_{i,j} \langle q_n | e_i \rangle \overbrace{\langle e_i | \hat{Q} | e_j \rangle} \langle e_j | q_m \rangle$$

$$\begin{pmatrix} q_1 & & & \\ & q_2 & & \\ & & \ddots & \\ & & & q_n \end{pmatrix} = \begin{pmatrix} \langle q_1|e_1\rangle & \langle q_1|e_2\rangle & \cdots \\ & \langle q_2|e_2\rangle & \\ & & \ddots \end{pmatrix} \begin{pmatrix} Q_{11} & Q_{12} & \cdots \\ Q_{21} & Q_{22} & \\ & & \ddots \end{pmatrix} \begin{pmatrix} \langle e_1|q_1\rangle & \cdots \\ & \ddots \end{pmatrix}$$

$\langle e_j | q_m \rangle$ = transf. matrix from $|\hat{e}_1\rangle$ basis to basis where $\hat{Q}$ is diagonal.

$*$ $\hat{Q} = \sum_n q_n |q_n\rangle\langle q_n|$ $\quad \mathbb{P}_n = |q_n\rangle\langle q_n|$ "In the $\hat{Q}$ eigenbasis"

$*$ $\hat{Q} = \sum_{i,j} Q_{ij} \, |e_i\rangle\langle e_j| \implies \langle e_l | \hat{Q} | e_m \rangle = \hat{Q}_{lm}$