3/9/2025 Day 16. Matrix representation of Operators (cont.)

Consider the eigenvalue equation for a Hermitian operator:

$$\hat{\alpha}\,|\alpha_i\rangle = \alpha_i\,|\alpha_i\rangle \quad -(14)$$

Representing this in the $\{|\alpha\rangle\}$ basis we get,

$$\langle\alpha_j|\hat{\alpha}|\alpha_i\rangle = \alpha_i\,\langle\alpha_j|\alpha_i\rangle \quad -(15)$$

or $$(\overleftrightarrow{\alpha})_{ji} = \alpha_i\,\delta_{ji} \quad -(16)$$

($\because \langle\alpha_j|\alpha_i\rangle = \delta_{ij}$ for a Hermitian operator eigenkets)

$\therefore$ Any Hermitian operator is represented by a diagonal matrix in its eigenbasis (basis of $\hat{\alpha}$ eigenkets)

This is called a "diagonal representation".

Sum of operators: $\hat{\alpha}+\hat{\beta} \longleftrightarrow \overleftrightarrow{\alpha}+\overleftrightarrow{\beta}$ $\rightarrow$ (16.5)

Product of Operators : $\hat{\alpha}, \hat{\beta} \rightarrow$ observables

$|V\rangle = \hat{\alpha}\hat{\beta}|U\rangle \Rightarrow$ (in $\{\langle\lambda_i|\}$ basis)

$$\langle\lambda_i|V\rangle = \sum_{j=1}^{N} \langle\lambda_i|\hat{\alpha}\hat{\beta}|\lambda_j\rangle\langle\lambda_j|U\rangle$$

$$= \sum_{j=1}^{N}\sum_{k=1}^{N} \langle\lambda_i|\hat{\alpha}|\lambda_k\rangle\langle\lambda_k|\hat{\beta}|\lambda_j\rangle \langle\lambda_j|U\rangle \quad \text{— (17)}$$

or

$$V_i = \sum_j \underbrace{\sum_k \alpha_{ik}\beta_{kj}}_{\text{matrix multiplication}} U_j \quad \text{— (18)}$$

$$(\overleftrightarrow{\alpha}\overleftrightarrow{\beta})_{ij} \equiv \sum_{k=1}^{N} \alpha_{ik}\beta_{kj} \quad \text{— (19)}$$

Thus, $\hat{\alpha}\hat{\beta} \leftrightarrow \overleftrightarrow{\alpha}\overleftrightarrow{\beta}$ defined by (19).

Theorem 8: If an observable $\hat{\alpha}$ is diagonal in a basis, and if another observable $\hat{\beta}$ commutes with it, then $\hat{\beta}$ is also diagonal in that basis

Proof:

$$\text{Let } \langle \lambda_i | \hat{\alpha} | \lambda_j \rangle = \alpha_i \, \delta_{ij} \quad \text{— (20)}$$

$$\text{Given } [\hat{\alpha}, \hat{\beta}] = 0 \quad \text{— (21)}$$

$$\Rightarrow \langle \lambda_i | [\hat{\alpha}, \hat{\beta}] | \lambda_j \rangle = 0 \quad \text{— (22)}$$

$$\text{or } \sum_k \left\{ \langle \lambda_i | \hat{\alpha} | \lambda_k \rangle \langle \lambda_k | \hat{\beta} | \lambda_j \rangle - \langle \lambda_i | \hat{\beta} | \lambda_k \rangle \langle \lambda_k | \hat{\alpha} | \lambda_j \rangle \right\} = 0$$

$$\text{or } \sum_k \left\{ \alpha_i \, \delta_{ik} \, \beta_{kj} - \beta_{ik} \, \alpha_j \, \delta_{kj} \right\} = 0$$

$$\text{or } (\alpha_i \beta_{ij} - \alpha_j \beta_{ij}) = 0$$

or $\beta_{ij}(\alpha_i - \alpha_j) = 0$ — (23)

$\Rightarrow$ if $i \neq j$, $\beta_{ij} = 0$ — (24)

$\Rightarrow \hat{\beta}$ is also diagonal in the $\{\langle x_i|\}$ basis.

<u>Representation in continuous basis</u>:

If (at least) one real parameter, say ξ, labeling the base states is continuous then we get functions of ξ representing the states.

$$|U\rangle \longleftrightarrow \langle\xi|U\rangle \equiv U(\xi) \quad \text{— (25)}$$

These are called wave function

For operators, we get a function of 2 variables.

$$|v\rangle = \hat{\alpha}|u\rangle$$

$$\Rightarrow \langle \xi | v\rangle = \int d\xi' \langle \xi|\hat{\alpha}|\xi'\rangle\langle\xi'|u\rangle \quad -(26)$$

&

$$v(\xi) = \int d\xi' \underbrace{\alpha(\xi,\xi')}_{} u(\xi'). \quad -(27)$$

Matrix representation of $\hat{\alpha}$.
in $\{\langle \xi |\}$ basis.

The most common such basis is the position basis : $\{|\vec{r}\rangle \equiv |x,y,z\rangle : \hat{\vec{r}}|\vec{r}'\rangle = \vec{r}'|\vec{r}'\rangle\}$

$$\hat{\alpha} \longleftrightarrow \alpha(\vec{r},\vec{r}') \qquad \vec{r} \in \mathbb{R}^3 \quad -(28)$$

<u>Space local Operators</u>: Operators that have a diagonal representation in position basis are called space-local operators.

i.e. $\langle \vec{r} | \hat{\alpha} | \vec{r}' \rangle = \alpha(\vec{r}, \vec{r}')$

$$= \alpha(\vec{r})\, \delta(\vec{r} - \vec{r}') \quad — (29)$$

Note that

$$\delta(\vec{r} - \vec{r}') = \delta(x - x')\, \delta(y - y')\, \delta(z - z') \quad — (30)$$

For such an operator, (27) would become

$$V(\vec{r}) = \int d^3 r'\, \alpha(\vec{r}, \vec{r}')\, U(\vec{r}')$$

$$= \int d^3 r'\, \alpha(\vec{r})\, \delta(\vec{r} - \vec{r}')\, U(\vec{r}')$$

$$= \alpha(\vec{r})\, U(\vec{r}) \quad — (31)$$

so, it seems that the operator acts on $U(\vec{r})$ to yield $V(\vec{r})$ one position at a time. This is why its called local.

In contrast, if $\alpha(\vec{r},\vec{r}')$ cannot be written in terms of a Dirac delta function then it is said to be "non-local".

Eg. Potential energy operator.

$$V(\hat{\vec{r}}) = \frac{1}{2} k \hat{r}^2 \quad \left(\begin{matrix}\text{isotropic} \\ \text{oscillator}\end{matrix}\right)$$

It's a function of $\hat{\vec{r}}$ hence $\{|\vec{r}\rangle\}$ are also its eigenstates. $\therefore$ it is diagonal in position basis, and hence, space-local.

For 1-d systems $\hat{x}$ is the position operator for x position. Correspondingly $\{|x'\rangle\}$ form the basis and $\Psi(x)$ the state representation, $\alpha(x,x')$ the operator representation.

Momentum representation:

$\{\langle \vec{p}'|\}$: $\quad \hat{\vec{p}}\,|\vec{p}'\rangle = \vec{p}'\,|\vec{p}'\rangle$ — (32)

$$\vec{p}' = (p_x', p_y', p_z') \quad — (33)$$

Functions of $\hat{\vec{p}}$ are diagonal in this representation.

e.g. kinetic energy of a particle: $\hat{T} \equiv \dfrac{\hat{p}^2}{2m}$ — (34)

$$\langle \vec{p}''|\hat{T}|\vec{p}'\rangle = \frac{p'^2}{2m}\,\delta(\vec{p}''-\vec{p}') \quad — (35)$$

This representation is otherwise uncommon. It is useful to ask, then, how $\hat{\vec{p}}$ would be represented in position basis.
To show this let us consider a quantum particle moving along x, so that the position kets $\{|x'\rangle\}$ form a complete set.