Matrix repre of $\hat{A}$, $\hat{B}$, ... 2022-UKM-T3.1.

Eigenstates & states $i\frac{d}{d\phi}$ $i\sin\phi$; ~~what's~~ $\hat{H}$ for rotor ~~str~~?

Basis transformation

Other ops & examples, $\hat{H}_0$, $\hat{H}'$

We still have $\hat{A} = i\frac{d}{d\phi}$; $\hat{B} = \sin\phi$ (operators)

Functions: $\psi_0 = \frac{1}{\sqrt{2\pi}}$; $\psi_{sn} = \frac{1}{\sqrt{\pi}}\sin(n\phi)$; $\psi_{cn} = \frac{1}{\sqrt{\pi}}\cos(n\phi)$

- we know • ψ_i is a ON basis on $(0, 2\pi) \ni \phi$.
- Let's start calling ψ_s states & using $|\ \rangle$: $|0\rangle$; $|s_n\rangle$; $|c_n\rangle$

we know
$$\hat{A}|0\rangle = 0$$
$$\hat{A}|s_n\rangle = in|c_n\rangle$$
$$\hat{A}|c_n\rangle = -in|s_n\rangle$$

$$\hat{B}|0\rangle = \frac{1}{\sqrt{2}}|s_1\rangle$$
$$\hat{B}|s_n\rangle = -\frac{1}{2}\left[|c_{n+1}\rangle - |c_{n-1}\rangle\right]$$
(but $\hat{B}|s_1\rangle = \frac{1}{\sqrt{2}}|0\rangle - \frac{1}{2}|c_2\rangle$)
$$\hat{B}|c_1\rangle = \frac{1}{2}|s_2\rangle$$
$$\hat{B}|c_n\rangle = \frac{1}{2}\left[|s_{n+1}\rangle - |s_{n-1}\rangle\right]$$

also $\langle i|j\rangle = \delta_{ij}$ (ON basis)

We can do $\hat{A}(\sum_i |i\rangle) = \sum_i \hat{A}|i\rangle$ (linear operators)

- Example: $\hat{A}$ ~~&~~ $\frac{1}{\sqrt{2\pi}}e^{3i\phi}$ → normaliz: $\int_0^{2\pi}\frac{1}{2\pi}e^{-3i\phi}e^{3i\phi}d\phi = \frac{1}{2\pi}\int_0^{2\pi}1 = \underline{\underline{1}}$ OK

$$|\psi\rangle = \frac{1}{\sqrt{2\pi}}e^{3i\phi} = \frac{1}{\sqrt{2\pi}}\left[\cos(3\phi) + i\sin(3\phi)\right] = \frac{1}{\sqrt{2}}\left[|c_3\rangle + i|s_3\rangle\right] = |\psi\rangle$$

→ Normaliz:

$$\langle\psi| = \frac{1}{\sqrt{2}}\left[\langle c_3| - i\langle s_3|\right]$$
$$\langle\psi|\psi\rangle = \frac{1}{2}\left[\langle c_3| - i\langle s_3|\right]\left[|c_3\rangle + i|s_3\rangle\right] =$$
$$= \frac{1}{2}\Big[\underbrace{\langle c_3|c_3\rangle}_{=1} + i\underbrace{\langle c_3|s_3\rangle}_{=0} - i\underbrace{\langle s_3|c_3\rangle}_{=0} + \underbrace{\langle s_3|s_3\rangle}_{=1}\Big] = \frac{1}{2}[1+1] = \underline{\underline{1}}$$ OK

$$\hat{A}|\psi\rangle = \hat{A}\frac{1}{\sqrt{2}}\left[|c_3\rangle + i|s_3\rangle\right] = i\frac{1}{\sqrt{2}}\left[-i3|s_3\rangle + i\,i\,3|c_3\rangle\right]$$
$$= \frac{i}{\sqrt{2}}\left[-3|c_3\rangle - i3|s_3\rangle\right] = -\frac{3i}{\sqrt{2}}\left[|c_3\rangle + i|s_3\rangle\right]$$
$$= -3|\psi\rangle \quad \text{(eigenstate)}$$

$$\hat{A}|\psi\rangle = i\frac{d}{d\phi}\frac{1}{\sqrt{2\pi}}\left[\cos(3\phi) + i\sin(3\phi)\right] = \frac{i}{\sqrt{2\pi}}\left[-3\sin(3\phi) + i3\cos(3\phi)\right]$$
$$= \frac{-3}{\sqrt{2\pi}}\left[\cos(3\phi) + i\sin(3\phi)\right] = -\frac{3}{\sqrt{2}}\left[|c_3\rangle + i|s_3\rangle\right] \quad \text{OK}$$

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-T3.2

- $\hat{A}|i\rangle = \sum_j a_{ij}|j\rangle$ ← general thing

$\langle k|\hat{A}|i\rangle = \sum_j {}^{*}\langle k|\sum_j a_{ji}|j\rangle = \sum_j a_{ji}\langle k|j\rangle = \cancel{\sum_j a_{ki}} = \sum_j a_{ji}\,\delta_{kj} = a_{ki}$ ← some number

$\langle i|\hat{A}|i\rangle = \langle i|\sum_j a_{ij}|j\rangle = \sum a_{ij}\langle i|j\rangle$

$\langle\ \rangle = \sum_j a_{ij}\delta_{ij} = a_{ii}$

- order basis elements $\ldots, |s_2\rangle, |s_1\rangle, |0\rangle, |c_1\rangle, |c_2\rangle, \ldots$
- Each $|\psi\rangle = \sum_i c_i|i\rangle$, ordered → list of numbers - vector

$\langle k|\hat{A}|i\rangle = a_{ki}$ ← matrix element

$$\mathbb{A} = \begin{pmatrix} \ddots & & & & \\ & a_{s_1s_1} & a_{s_10} & a_{s_1c_1} & \\ \cdots & a_{0s_1} & a_{00} & a_{0c_1} & \cdots \\ & a_{c_1s_1} & a_{c_10} & a_{c_1c_1} & \\ & & \vdots & & \ddots \end{pmatrix}$$

matrix

- matrix of $\hat{A}$

$$\begin{array}{c|ccccc} & a_{s_2} & a_{s_1} & 0 & a_{c_1} & a_{c_2} \\ \hline a_{s_2} & 0 & 0 & 0 & 0 & -2i \\ a_{s_1} & 0 & 0 & 0 & -i & 0 \\ a_0 & 0 & 0 & 0 & 0 & 0 \\ a_{c_1} & 0 & i & 0 & 0 & 0 \\ a_{c_2} & 2i & 0 & 0 & 0 & 0 \end{array}$$

$\hat{A}|0\rangle = 0$

$\Downarrow$

$\langle i|\hat{A}|0\rangle = 0$

$a_{i0} = 0$

$\hat{A}|s_n\rangle = in|c_n\rangle$

$\langle j|\hat{A}|s_n\rangle = in\,\delta_{c_n,s_n}$

$\langle j|\hat{A}|c_n\rangle = \langle j|-in|s_n\rangle$

$= -in\langle a_j|s_n\rangle = -in\,\delta_{js_n}$

$\langle j|\hat{A}|c_n\rangle = \begin{cases} 0 \\ -in & \text{if } j = s_n \end{cases}$

- diagonalize 3x3 sub of $\mathbb{A}$

$$\begin{pmatrix} 0 & 0 & -i \\ 0 & 0 & 0 \\ i & 0 & 0 \end{pmatrix} \to \begin{vmatrix} -\lambda & 0 & -i \\ 0 & -\lambda & 0 \\ i & 0 & -\lambda \end{vmatrix} = -\lambda^3 - i(-i)(-\lambda) = -\lambda(\lambda^2-1) = -\lambda(\lambda-1)(\lambda+1) = 0$$

$\lambda = 0 \quad \lambda = 1 \quad \lambda = -1$

eigenvectors

$\lambda = 0$: $\begin{pmatrix} 0 & 0 & -i \\ 0 & 0 & 0 \\ i & 0 & 0 \end{pmatrix}\begin{pmatrix} a \\ b \\ c \end{pmatrix} = 0 \Rightarrow \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}$

$\lambda = 1$: $\begin{vmatrix} -1 & 0 & -i \\ 0 & -1 & 0 \\ i & 0 & 0 \end{vmatrix}\begin{vmatrix} a \\ b \\ c \end{vmatrix} = 0$

$-a - ic = 0$

$a = 1$

$-1 - ic = 0 \to c = i \quad \to \begin{pmatrix} 1 \\ 0 \\ i \end{pmatrix}$

Normalize

$v^{\dagger}\cdot v = (1\ \ 0\ \ -i)\cdot\begin{pmatrix} 1 \\ 0 \\ i \end{pmatrix} = 1 + 0 - i\cdot i = 2 = N^2 \to N = \frac{1}{\sqrt{2}} \qquad v_{\lambda=1} = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 0 \\ i \end{pmatrix}$

$\lambda = -1$: $\begin{vmatrix} 1 & 0 & -i \\ 0 & 1 & 0 \\ i & 0 & 1 \end{vmatrix}\begin{vmatrix} a \\ b \\ c \end{vmatrix} = 0 \Rightarrow$

$a - ic = 0$

$a = 1$

$1 - ic = 0 \Rightarrow c = -i \quad \to N\begin{pmatrix} 1 \\ 0 \\ -i \end{pmatrix}$

Normalizeee $N^*(1\ 0\ i)N\begin{pmatrix} 1 \\ 0 \\ -i \end{pmatrix} = N^2[1 + 0 + 1] = N^2\cdot 2 = 1 \to v_{\lambda=-1} = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 0 \\ -i \end{pmatrix}$

$\Rightarrow N = \frac{1}{\sqrt{2}}$

Basis rotation of 2x2 ~~subset~~matrix $\{s_1, c_1\}$ 2022-UKM-T3.3

$$\underset{2\times 2}{A} = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \quad U = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 1 \\ i & -i \end{pmatrix} \quad U^+ = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & -i \\ 1 & i \end{pmatrix}$$

(?)

$$AU = \frac{1}{\sqrt{2}}\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}\begin{pmatrix} 1 & 1 \\ i & -i \end{pmatrix} = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & -1 \\ i & i \end{pmatrix}$$

$$U^+AU = \frac{1}{2}\begin{pmatrix} 1 & -i \\ 1 & i \end{pmatrix}\begin{pmatrix} 1 & -1 \\ i & i \end{pmatrix} = \frac{1}{2}\begin{pmatrix} 2 & 0 \\ 0 & -2 \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} = A'$$

- What's actually $V_{\lambda=1} = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 0 \\ i \end{pmatrix}$ c_{s_1}, $? c_0$, c_{c_1} coeffs. of expansion in basis

$$\frac{1}{\sqrt{2}}\,1\cdot|s_1\rangle + \frac{1}{\sqrt{2}}\,i\,|c_1\rangle = \frac{1}{\sqrt{2}}\left(\frac{1}{\sqrt{\pi}}\sin\phi + \frac{1}{\sqrt{\pi}}\,i\cos\phi\right) = \frac{i}{\sqrt{2\pi}}\left[\cos\phi - i\sin\phi\right]$$
$$= \frac{i}{\sqrt{2\pi}}e^{-i\phi}$$

$V_{\lambda=-1}$ $\Rightarrow$

$$\frac{1}{\sqrt{2}}|s_1\rangle - \frac{1}{\sqrt{2}}\,i\,|c_1\rangle = -\frac{i}{\sqrt{2\pi}}(\cos\phi + i\sin\phi) = -\frac{i}{\sqrt{2\pi}}e^{i\phi}$$

Normalized: Yes $V_{\lambda=-1}$
$$\int_0^{2\pi}\frac{i}{\sqrt{2\pi}}e^{-i\phi}\left(-\frac{i}{\sqrt{2\pi}}e^{i\phi}\right)d\phi = \frac{1}{2\pi}\int_0^{2\pi}1\,d\phi = \underline{\underline{1}}$$

Orthonormal: Yes
$$\langle V_{\lambda=1}|V_{\lambda=-1}\rangle = \int_0^{2\pi} -\frac{i}{\sqrt{2\pi}}e^{i\phi}\left(-\frac{i}{\sqrt{2\pi}}e^{i\phi}\right)d\phi = \frac{1}{2\pi}\int_0^{2\pi}e^{2i\phi}d\phi = 0$$

$$\int_0^{2\pi}e^{iN\phi}d\phi = 0 \quad \forall N\neq 0$$

Eigenstates:

$$\hat{A}|V_{\lambda=1}\rangle = \frac{i\,d}{d\phi}\frac{i}{\sqrt{2\pi}}e^{-i\phi} = \frac{-1(-i)}{\sqrt{2\pi}}e^{-i\phi} = i\,|V_{\lambda=1}\rangle$$

what about $|0\rangle$ -> eigenvector $\begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}$ $\rightarrow$ $|0\rangle$ keeps being $|0\rangle$

what about higher states

-> $\begin{pmatrix} 0 & -2i \\ +2i & 0 \end{pmatrix}$ -> same story -> $\frac{i}{\sqrt{2\pi}}e^{-i\phi n}$ & $-\frac{i}{\sqrt{2\pi}}e^{i\phi n}$ states

• $(\hat{A})^2$

$$\hat{A}\hat{A}\,|s_n\rangle = i\frac{d}{d\phi}\, i\frac{d}{d\phi}\,\frac{1}{\sqrt{\pi}}\sin(n\phi) = -1\left(\frac{d^2}{d\phi^2}\right)\frac{1}{\sqrt{\pi}}\sin(n\phi) = -1\,\frac{1}{\sqrt{\pi}}\,n^2[-\sin(n\phi)]$$

$$= \frac{n^2}{\sqrt{\pi}}\sin(n\phi) = n^2|s_n\rangle$$ ← eigenstate, same for $|c_n\rangle$

Matrix? – need to consider only s_n & c_n for fixed n

$$A_{2\times2} = \begin{pmatrix} 0 & -ni \\ ni & 0 \end{pmatrix} \qquad s_n = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \;\&\; c_n = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

$$A_{2\times2}\vec{s}_n = \begin{pmatrix} 0 & -ni \\ ni & 0 \end{pmatrix}\begin{pmatrix} 1 \\ 0 \end{pmatrix} = ni\begin{pmatrix} 0 \\ 1 \end{pmatrix} \;(= ni\,\vec{c}_n)$$

$$A_{2\times2}\, ni\begin{pmatrix} 0 \\ 1 \end{pmatrix} = \begin{pmatrix} 0 & -ni \\ ni & 0 \end{pmatrix}\begin{pmatrix} 0 \\ 1 \end{pmatrix} ni = ni\begin{pmatrix} -ni \\ 0 \end{pmatrix} = n^2\begin{pmatrix} 1 \\ 0 \end{pmatrix} = n^2\vec{s}_n$$

Can we do $A^2 = A\cdot A$? YES!

$$\begin{pmatrix} 0 & -ni \\ ni & 0 \end{pmatrix}\begin{pmatrix} 0 & -ni \\ ni & 0 \end{pmatrix} = \begin{pmatrix} n^2 & 0 \\ 0 & n^2 \end{pmatrix}$$ → diagonal operator, basis functions are eigenfunctions / e.-vectors / e. states

BTW ~~ka-it~~ Rotor $H = -\frac{\hbar^2}{2I}\frac{d^2}{d\phi^2} = \frac{\hbar^2}{2I}A^2$ $\qquad -i\hbar(-i\hbar) = -\hbar^2$

⇒ we diagonalized S. Eq. for rotor → we found eigenstates !! → we solved it !!

$V = 3\frac{\hbar^2}{I}$ → $\mathbb{V}$?

$$\langle i|V|j\rangle = \langle i|\frac{3\hbar^2}{I}|j\rangle = \frac{3\hbar^2}{I}\langle i|j\rangle = \frac{3\hbar^2}{I}\delta_{ij} \rightarrow \begin{pmatrix} \Delta E & & & & 0 \\ & \Delta E & & & \\ & & \Delta E & & \\ & & & \Delta E & \\ 0 & & & & \Delta E \end{pmatrix}$$

ΔE

only ~~constant~~ adds a number

$A = \sum_i d_i\, |i\rangle\langle i|$

only ± 1: $A = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ i \end{pmatrix}$ $\quad d-1 = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ -i \end{pmatrix}$

$\uparrow |1\rangle \qquad \uparrow |-1\rangle$

$A = 1\cdot|1\rangle\langle 1| - 1|-1\rangle\langle -1| = 1\cdot\frac{1}{2}\cancel{(1\;\; -i)\begin{pmatrix} 1 \\ i \end{pmatrix}} - \frac{1}{2}(1\;\; i)\begin{pmatrix} 1 \\ -i \end{pmatrix}$

$= \frac{1}{2}\begin{pmatrix} 1 & -i \\ i & 1 \end{pmatrix} \cancel{- \frac{1}{2}\begin{pmatrix} 1 & i \\ -i & +1 \end{pmatrix}}$

$= 1\,\frac{1}{2}\begin{pmatrix} 1 \\ i \end{pmatrix}(1\;\; -i) - 1\frac{1}{2}\begin{pmatrix} 1 \\ -i \end{pmatrix}(1\;\; -i) = \frac{1}{2}\begin{pmatrix} 1 & -i \\ i & 1 \end{pmatrix} - \frac{1}{2}\begin{pmatrix} 1 & i \\ -i & 1 \end{pmatrix} = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$

OK