Lecture 3: Basis Transformations - I

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Recap

In some orthonormal basis $\mathbb{B} = \{|e_1\rangle, |e_2\rangle, \ldots |e_N\rangle\}$, we write some

$$|a\rangle \equiv \begin{bmatrix} a_1 \\ a_2 \\ \vdots \end{bmatrix} \text{ and } \boldsymbol{X} \equiv \begin{bmatrix} \boldsymbol{X}_{11} & \boldsymbol{X}_{12} & \ldots \\ \boldsymbol{X}_{21} & \boldsymbol{X}_{22} & \ldots \\ \vdots & \vdots & \ddots \end{bmatrix},$$

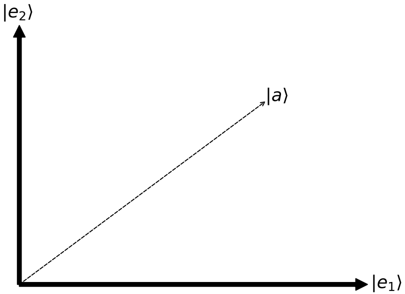
$$a_k = \langle e_k | a \rangle \text{ and } \boldsymbol{X}_{ij} = \langle e_i | \boldsymbol{X} | e_j \rangle .$$

Inner product, $\langle a|a\rangle = \underbrace{\begin{bmatrix} a_1^* & a_2^* & \ldots \end{bmatrix}}_{\langle a|} \underbrace{\begin{bmatrix} a_1 \\ a_2 \\ \vdots \end{bmatrix}}_{|a\rangle} = \sum_i |a_i|^2 \geq 0.$

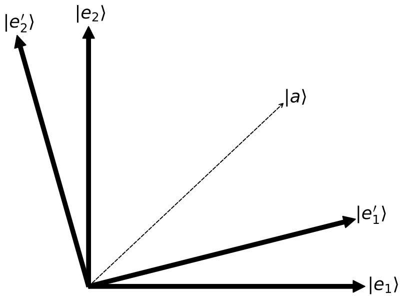
Dual correspondence, $\underbrace{\boldsymbol{X}|a\rangle}_{\text{ket}} \xrightarrow{\text{unique}} \underbrace{\langle a| \boldsymbol{X}^\dagger}_{\text{bra}}$ yields,

$\boxed{\langle a|\boldsymbol{X}|b\rangle = \langle b|\boldsymbol{X}^\dagger|a\rangle^*}$, where $\boldsymbol{X}^\dagger \equiv$ conjugate transpose $\boldsymbol{X}$

Basis Transformation in 2D



Some arbitrary $|a\rangle$ in $\mathbb{B}$



$\mathbb{B}$ rotated to $\mathbb{B}'$

How do the components of $|a\rangle$ transform?

$$\underbrace{\begin{bmatrix} a_1 \\ a_2 \end{bmatrix}}_{\mathbb{B}} \xrightarrow{?} \underbrace{\begin{bmatrix} a'_1 \\ a'_2 \end{bmatrix}}_{\mathbb{B}'}$$

General Ortho-normal Bases

Consider,

$$\mathbb{B} = \{|e_1\rangle, |e_2\rangle, \ldots |e_N\rangle\} \quad \text{and} \quad \mathbb{B}' = \{|e'_1\rangle, |e'_2\rangle, \ldots |e'_N\rangle\}$$

$$\langle e_i|e_j\rangle = \langle e'_i|e'_j\rangle = \delta_{ij}$$

Since both $\mathbb{B}$ and $\mathbb{B}'$ are complete,

$$|e'_i\rangle = \sum_j |e_j\rangle \boldsymbol{U}_{ji} \quad \text{with } \boldsymbol{U}_{ki} = \langle e_k|e'_i\rangle$$

Turns out that the operator $\boldsymbol{U}$ is unitary, i.e, $\boldsymbol{U}^\dagger = \boldsymbol{U}^{-1}$

$$\delta_{ij} = \langle e_i|e_j\rangle = \langle e_i| \underbrace{\left(\sum_k |e'_k\rangle \langle e'_k|\right)}_{\boldsymbol{I}} |e_j\rangle = \sum_k \boldsymbol{U}_{ik} \boldsymbol{U}^\dagger_{kj} = (\boldsymbol{U}\boldsymbol{U}^\dagger)_{ij}$$

How do vectors transform?

Typical component of $|a\rangle$ in $\mathbb{B}'$,

$$a'_k = \langle e'_k | a \rangle = \sum_i \langle e'_k | e_i \rangle \langle e_i | a \rangle = \sum_i \boldsymbol{U}^\dagger_{ki} a_i$$

Looks like a rule,

$$\underbrace{\begin{bmatrix} a'_1 \\ a'_2 \\ \vdots \end{bmatrix}}_{\text{new}} = \underbrace{\begin{bmatrix} \boldsymbol{U}^\dagger_{11} & \boldsymbol{U}^\dagger_{12} & \dots \\ \boldsymbol{U}^\dagger_{21} & \boldsymbol{U}^\dagger_{22} & \dots \\ \vdots & \vdots & \ddots \end{bmatrix}}_{\boldsymbol{U}^\dagger} \underbrace{\begin{bmatrix} a_1 \\ a_2 \\ \vdots \end{bmatrix}}_{\text{old}}$$

This is not the same as

$$\cancel{|a'\rangle = \boldsymbol{U}^\dagger |a\rangle} \quad \dots |a\rangle \text{ has not changed!}$$

Transformation of Operators

In $\mathbb{B}$, consider the operation

$$|b\rangle = \boldsymbol{X}\,|a\rangle$$

put simply, $$\begin{bmatrix} b_1 \\ b_2 \\ \vdots \end{bmatrix} = \begin{bmatrix} \boldsymbol{X}_{11} & \boldsymbol{X}_{12} & \dots \\ \boldsymbol{X}_{21} & \boldsymbol{X}_{22} & \dots \\ \vdots & \vdots & \ddots \end{bmatrix} \begin{bmatrix} a_1 \\ a_2 \\ \vdots \end{bmatrix} \quad \text{with } \boldsymbol{X}_{ij} = \underbrace{\langle e_i|\boldsymbol{X}|e_j\rangle}_{\text{known}}$$

In $\mathbb{B}'$, the above operation becomes

$$\begin{bmatrix} b'_1 \\ b'_2 \\ \vdots \end{bmatrix} = \begin{bmatrix} \boldsymbol{X}'_{11} & \boldsymbol{X}'_{12} & \dots \\ \boldsymbol{X}'_{21} & \boldsymbol{X}'_{22} & \dots \\ \vdots & \vdots & \ddots \end{bmatrix} \begin{bmatrix} a'_1 \\ a'_2 \\ \vdots \end{bmatrix} \quad \text{with } \boldsymbol{X}'_{ij} = \underbrace{\langle e'_i|\boldsymbol{X}|e'_j\rangle}_{\textbf{unknown}}$$

Operator Elements in the New Basis

We use the identity operator $\boldsymbol{I}$, tactfully!

$$\boldsymbol{X}'_{ij} = \langle e'_i|\boldsymbol{X}|e'_j\rangle = \langle e'_i| \underbrace{\left(\sum_k |e_k\rangle\langle e_k|\right)}_{\boldsymbol{I}} \boldsymbol{X} \underbrace{\left(\sum_l |e_l\rangle\langle e_l|\right)}_{\boldsymbol{I}} |e'_j\rangle$$

$$= \sum_{kl} \underbrace{\langle e'_i|e_k\rangle}_{\boldsymbol{U}^\dagger_{ik}} \underbrace{\langle e_k|\boldsymbol{X}|e_l\rangle}_{\boldsymbol{X}_{kl}} \underbrace{\langle e_l|e'_j\rangle}_{\boldsymbol{U}_{lj}}$$

$$= (\boldsymbol{U}^\dagger \boldsymbol{X} \boldsymbol{U})_{ij}$$

yielding the unitary transform of the operator

$$\boldsymbol{X}' = \boldsymbol{U}^\dagger \boldsymbol{X} \boldsymbol{U}$$

Observations

- Determinant of a unitary operator is a unit complex number

$$\det(\boldsymbol{U}) = e^{i\phi}, \quad \phi \equiv \text{some phase}$$

Proof: Since $\boldsymbol{U}^\dagger \boldsymbol{U} = \boldsymbol{I}$,

$$\begin{aligned}
1 &= \det(\boldsymbol{I}) \\
&= \det(\boldsymbol{U}^\dagger \boldsymbol{U}) \\
&= \det(\boldsymbol{U}^\dagger) \cdot \det(\boldsymbol{U}) \\
&= \det(\boldsymbol{U}^{*T}) \cdot \det(\boldsymbol{U}) \\
&= \det(\boldsymbol{U}^{*}) \cdot \det(\boldsymbol{U}) \\
&= (\det(\boldsymbol{U}))^{*} \cdot \det(\boldsymbol{U}) \\
&= |\det(\boldsymbol{U})|^2
\end{aligned}$$

Implying, $\det(\boldsymbol{U}) = e^{i\phi}$.

Observations

- Trace & determinant of operators are invariants of the transform

Proof: We first notice that the trace,

$$\begin{aligned}\mathrm{Tr}\,(\boldsymbol{X}') &= \mathrm{Tr}\,(\boldsymbol{U}^\dagger \boldsymbol{X}\boldsymbol{U}) \\ &= \mathrm{Tr}\,(\boldsymbol{X}\boldsymbol{U}\boldsymbol{U}^\dagger) \quad \ldots \mathrm{Tr\ is\ cyclic} \\ &= \mathrm{Tr}\,(\boldsymbol{X}), \quad \text{is unchanged}\end{aligned}$$

and the determinant,
$$\begin{aligned}\det\,(\boldsymbol{X}') &= \det\,(\boldsymbol{U}^\dagger \boldsymbol{X}\boldsymbol{U}) \\ &= \det\,(\boldsymbol{U}^\dagger)\cdot\det\,(\boldsymbol{X})\cdot\det\,(\boldsymbol{U}) \\ &= \det\,(\boldsymbol{X})\cdot\underbrace{|\det\,(\boldsymbol{U})|^2}_{1} \\ &= \det\,(\boldsymbol{X}), \quad \text{is also unchanged}\end{aligned}$$