

Hermitian operators in quantum mechanics

they allow us to define physical observables, and their eigenvalues are real numbers. and the eigenstate of a Hermitian operator form a basis in the state space.

$\hat{A} = \hat{A}^\dagger$ an operator which is equal to its adjoint.

$$\hat{A}|\psi\rangle = |\psi'\rangle \quad \longleftrightarrow \quad \langle\psi|\hat{A}^\dagger = \langle\psi'|$$
$$\quad \quad \quad \longleftrightarrow \quad \langle\psi|\hat{A} = \langle\psi'|$$

① Eigenvalues of a Hermitian operator are real numbers since they represent physical observables and hence should have real eigenvalues.

② Eigenstates of an Hermitian operator can be chosen to form an orthonormal set

we can always write an arbitrary quantum state in the representation given by the eigenstate of a physical observable.

$$\hat{A}|\psi\rangle = \lambda|\psi\rangle \quad \sim \quad \text{Eigenvalue Equation}$$

$$\hat{A}|\psi\rangle = \lambda|\psi\rangle \implies \langle\psi|\hat{A}|\psi\rangle = \lambda \underbrace{\langle\psi|\psi\rangle}$$

$$\langle\psi|\hat{A}^\dagger = \lambda^* \langle\psi|$$

$$\langle\psi|\hat{A} = \lambda^* \langle\psi|$$

we just need to show that

$\lambda^* = \lambda$ and hence eigenvalues are $\mathbb{R}$.

$$\langle \psi | \hat{A} | \psi \rangle = \underbrace{\lambda^* \langle \psi | \psi \rangle}_{\lambda = \lambda^*} \quad \lambda \in \mathbb{R}$$

$$\lambda \langle \psi | \psi \rangle = \lambda^* \langle \psi | \psi \rangle$$

$$\lambda \geq 0$$

$$\neq 0 \iff \langle \psi | \psi \rangle = 0$$

Eigenstates

$$\hat{A} |\psi\rangle = \lambda |\psi\rangle \quad \hat{A} |\varphi\rangle = \mu |\varphi\rangle$$

$$\lambda \neq \mu$$

$$\hat{A} |\psi\rangle = \lambda |\psi\rangle \quad \langle \varphi | \in \Rightarrow \boxed{\langle \varphi | \hat{A} | \psi \rangle = \lambda \langle \varphi | \psi \rangle}$$

$$\hat{A} |\varphi\rangle = \mu |\varphi\rangle \quad \exists \langle \varphi | \hat{A} = \mu \langle \varphi |$$

$$\hat{A} = \hat{A}^\dagger \quad \mathbb{R}$$

$$\langle \varphi | \hat{A} = \mu \langle \varphi | \quad \xrightarrow{\in |\psi\rangle} \boxed{\langle \varphi | \hat{A} | \psi \rangle = \mu \langle \varphi | \psi \rangle}$$

$$\text{so } \lambda \langle \varphi | \psi \rangle = \mu \langle \varphi | \psi \rangle$$

$$\underbrace{(\lambda - \mu)}_{\neq 0} \underbrace{\langle \varphi | \psi \rangle}_{=0} = 0$$

$$\langle \varphi | \psi \rangle = 0$$

$\therefore$ eigenstate of Hermitian operator, corresponding to different eigenvalues form an orthonormal pair.

Degenerate Eigenvalues

What happens to the eigenstates then?

$$\textcircled{1} \quad \hat{A} |\psi^i\rangle = \lambda |\psi^i\rangle \quad i=1,2,\dots,n$$

the n -eigenstates that share the same eigenvalues λ .

$$|\varphi\rangle = \sum c_i |\psi^i\rangle$$

linear combination of these also have the same eigenvalue

$$\hat{A} |\varphi\rangle = \lambda |\varphi\rangle$$

for an n -fold degenerate eigenvalue, any ket that lives in the n -dim subspace of state space spanned by the eigenkets $|\psi^i\rangle$ is also a valid eigenstate.

② For n -fold degenerate eigenvalues, there are n linearly independent eigenstates.

n -dim state space

↓

n linearly independent eigenstates

(may not be mutually orthogonal)

How to make all of them mutually orthogonal?

Gram-Schmidt orthonormalization

$$\{ |\psi^i\rangle \} \longrightarrow \{ |\varphi^i\rangle \}$$

set of linearly independent but not necessarily orthogonal states $\rightarrow$ mutually orthonormal states

$$\langle \varphi^i | \varphi^j \rangle = \delta_{ij}$$

$$\textcircled{3} \quad |\varphi^i\rangle = \frac{|\psi^i\rangle}{\sqrt{\langle \psi^i | \psi^i \rangle}}$$

normalize even the state ψ^i

$\sqrt{\langle \psi' | \psi' \rangle} \rightarrow$ to make the state normalized.

② $|\chi^2\rangle = |\psi^2\rangle + \alpha |\psi'\rangle \rightarrow$ we want $|\chi^2\rangle$ to be orthogonal to $|\psi'\rangle$

$$\langle \psi' | \chi^2 \rangle = 0$$

$$\Rightarrow \langle \psi' | \psi^2 \rangle + \alpha \langle \psi' | \psi' \rangle = 0$$

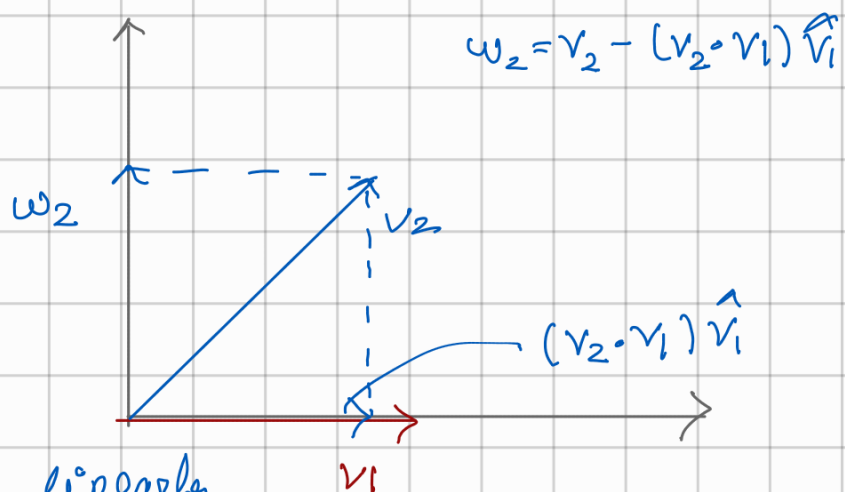
$$\text{if we choose } \alpha = -\langle \psi' | \psi^2 \rangle$$

Replace this in ②

$$|\chi^2\rangle = |\psi^2\rangle - |\psi'\rangle \langle \psi' | \psi^2 \rangle$$

$$|\psi^2\rangle = \frac{|\chi^2\rangle}{\sqrt{\langle \chi^2 | \chi^2 \rangle}}$$

$|\psi^2\rangle$ is parallel to $|\chi^2\rangle$



Suppose v_1 and v_2 are linearly independent, but not orthogonal. So keeping v_1 as reference, we want to make a state which is orthonormal to it.

Repeat the same procedure.

Matrix formulation

$\sim$ transpose conjugate matrix

$$\hat{A} = A_{ij}$$

$$A^\dagger = A_{ji}^*$$

$$A_{ij} = A_{ji}^*$$

$$\begin{pmatrix} A_{11} & A_{12} & A_{13} & \dots \\ A_{21} & A_{22} & A_{23} & \dots \\ A_{31} & A_{32} & A_{33} & \dots \\ \vdots & \vdots & \vdots & \ddots \end{pmatrix}$$

$$i=j \Rightarrow A_{ii} = A_{ii}^* \Rightarrow A_{ii} \in \mathbb{R}$$

$$i \neq j \Rightarrow A_{ij}^* = A_{ji}$$

$$\Downarrow$$

$$\begin{pmatrix} A_{11} & A_{12} & A_{13} & \dots \\ A_{12}^* & A_{22} & A_{23} & \dots \\ A_{13}^* & A_{23}^* & A_{33} & \dots \\ \vdots & \vdots & \vdots & \ddots \end{pmatrix}$$

$$\hat{A} |\varphi_m\rangle = \lambda_m |\varphi_m\rangle, \quad \langle \varphi_m | \varphi_m \rangle = \delta_{mm}$$

$$A_{mmb} = \langle \varphi_m | \hat{A} | \varphi_m \rangle \Rightarrow \lambda_m \langle \varphi_m | \varphi_m \rangle$$

$$\xrightarrow{\quad} \lambda_m |\varphi_m\rangle \Rightarrow \lambda_m \delta_{mm}$$

matrix is diagonal
and the diagonal values are just the
eigenvalues

$$\begin{pmatrix} \lambda_1 & 0 & 0 & \dots \\ 0 & \lambda_2 & 0 & \dots \\ 0 & 0 & \lambda_3 & \dots \\ \vdots & \vdots & \vdots & \ddots \end{pmatrix}$$

$$\lambda_i \in \mathbb{R}$$

$$\begin{pmatrix} 0 & \lambda_2 & 0 & 0 & \dots \\ 0 & 0 & \lambda_3 & 0 & \dots \\ 0 & 0 & \vdots & \lambda_4 & \dots \\ \vdots & \vdots & \vdots & \vdots & \ddots \end{pmatrix}$$

$$\lambda_m \in \mathbb{R}.$$

the matrix associate with an operator $\hat{A}$ is diagonal when written in the basis spanned by the eigenstate of $\hat{A}$, and the diagonal entries are the eigenvalues of the operator.