1) Introduction — see slides, material on Canvas (General information).

2) Revision

Postulates of QM (Ch 3 Griffiths)

A set of assumptions put forth to explain experimental mysteries that cannot be explained classically.

(I) The state of the quantum system is completely specified by $|\psi\rangle$, which propagates in space and time according to Schrödinger's equation.

$\uparrow$ quantum state

(defined up to a global phase)

$|\psi\rangle \longrightarrow e^{i\theta}|\psi\rangle$

(II) All observables of a quantum system can be described by Hermitian operators; one measures only the eigenvalues of these operators.

(Eg eigenvalue λ; label eigenstate as $|\lambda\rangle$)

(III) The probability of measuring λ for a system in state $|\psi\rangle$ is $|\langle\lambda|\psi\rangle|^2$.

(I) States $|\psi\rangle$ 'ket'

$\langle\psi|$ 'bra'

Inner product $\langle\phi|\psi\rangle$

Basis $\underbrace{\{|\phi_1\rangle, |\phi_2\rangle, \ldots, |\phi_N\rangle\}}_{N\text{ = dimension of the Hilbert space for } |\psi\rangle}$

member of

Any $|\psi\rangle \in$ Hilbert space can be written as

$|\psi\rangle = \sum_i c_i|\phi_i\rangle$ and c_i is unique.

$c_i = \langle\phi_i|\psi\rangle$

With a basis, we can use the language of linear algebra.

$|\phi_1\rangle \longrightarrow \begin{pmatrix} 1 \\ 0 \\ 0 \\ \vdots \\ 0 \end{pmatrix}$ N dimensional

ket

$|\phi_2\rangle \longrightarrow \begin{pmatrix} 0 \\ 1 \\ 0 \\ \vdots \\ 0 \end{pmatrix}$

$\vdots$

$|\phi_N\rangle \longrightarrow \begin{pmatrix} 0 \\ 0 \\ \vdots \\ 0 \\ 1 \end{pmatrix}$

$|\psi\rangle = \sum_i c_i|\phi_i\rangle \longrightarrow \begin{pmatrix} c_1 \\ c_2 \\ \vdots \\ c_N \end{pmatrix}$

ket

column vectors

$\langle\psi| \longrightarrow (c_1^* \; c_2^* \; \ldots \; c_N^*)$

'bra'

row vectors

Inner product $\langle\phi|\psi\rangle$ $\quad (\; \cdots \;)\begin{pmatrix} \vdots \end{pmatrix} \longrightarrow 1\times1$ scalar $\in \mathbb{C}$.

We can always choose a basis that is orthonormal.

$$\langle \phi_m | \phi_n \rangle = \begin{cases} 0 & m \neq n \quad \leftarrow \text{'ortho'} \\ 1 & m = n \quad \leftarrow \text{'normal'} \end{cases}$$

$$= \delta_{mn} \quad \text{Kronecker delta}$$

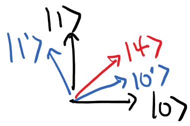
A basis set obeys

$$\sum_{i=1}^{N} |\phi_i\rangle\langle\phi_i| = \mathbb{1} \quad \text{identity} \text{ — Completeness}$$

$$|\psi\rangle = \mathbb{1}|\psi\rangle = \sum_{i=1} |\phi_i\rangle \underbrace{\langle\phi_i|\psi\rangle}_{c_i}$$

$\in$ Hilbert space

Hilbert space – dimension 2



in basis $\{|0\rangle, |1\rangle\}$

$$|\psi\rangle \longrightarrow \begin{pmatrix} \langle 0|\psi\rangle \\ \langle 1|\psi\rangle \end{pmatrix}$$

in basis $\{|0'\rangle, |1'\rangle\}$,

$$|\psi\rangle \longrightarrow \begin{pmatrix} \langle 0'|\psi\rangle \\ \langle 1'|\psi\rangle \end{pmatrix}$$

$|\psi\rangle \longrightarrow \underbrace{e^{i\theta}}_{\mathbb{C} \text{ number, magnitude } 1.} |\psi\rangle$ represent the same quantum state.

$$i\hbar \frac{\partial|\psi\rangle}{\partial t} = H|\psi\rangle \quad \text{— time-dependent Schrodinger's equation}$$

$$H|\psi_n\rangle = E_n|\psi_n\rangle \quad \text{— time-independent — '' —}$$

$|\psi\rangle$, $e^{i\theta}|\psi\rangle$ does not change relation to Schrodinger's equation.

H: Hamiltonian — operator for the total energy.

$$\langle\psi|\psi\rangle = 1$$

(II) Observables — Hermitian operators

have eigenstates, eigenvalues.

$$\text{operator} \rightarrow \hat{A}\underbrace{|\alpha\rangle}_{\text{eigenstate}} = \underbrace{\alpha}_{\text{eigenvalue}}|\alpha\rangle$$

Hermitian operators have real eigenvalues.

Dyadic form of an operator – depends on choice of basis – $\{|0\rangle, |1\rangle, |2\rangle \ldots, |N\rangle\}$

$$\hat{A} = \mathbb{1}\hat{A}\mathbb{1} = \Big(\underbrace{\sum_{m=0}^{N}}_{\text{dummy variable}} |m\rangle\langle m|\Big)\hat{A}\Big(\underbrace{\sum_{n=0}^{N}}_{\text{dummy variable}} |n\rangle\langle n|\Big)$$

$$= \sum_{m,n} |m\rangle \underbrace{\langle m|\hat{A}|n\rangle}_{\text{matrix element}} \langle n|$$

matrix element $A_{mn} = \langle m|\hat{A}|n\rangle$ scalar $\in \mathbb{C}$.

mth row, nth column

$$\underset{1\times N}{(\cdot \; \cdots \;)} \underset{N\times N}{\begin{pmatrix} & \\ & \end{pmatrix}} \underset{N\times 1}{\begin{pmatrix} \vdots \end{pmatrix}}$$

Hermitian conjugate / adjoint

Eg $\hat{A} = \begin{pmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{pmatrix}$

$$\hat{A}^{\dagger} = (A^*)^T = \begin{pmatrix} a_{11}^* & a_{12}^* \\ a_{21}^* & a_{22}^* \end{pmatrix}^T = \begin{pmatrix} a_{11}^* & a_{21}^* \\ a_{12}^* & a_{22}^* \end{pmatrix}$$

$\hat{A}$ is Hermitian $\equiv$ $\hat{A} = \hat{A}^{\dagger}$

Eg $\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}^{\dagger} = \begin{pmatrix} 0 & i \\ -i & 0 \end{pmatrix}^T = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$ — Hermitian

$\begin{pmatrix} 1 & i \\ i & 0 \end{pmatrix}^{\dagger} = \begin{pmatrix} 1 & -i \\ -i & 0 \end{pmatrix}$ — not Hermitian

$$\langle \phi_m | \hat{A} | \phi_N \rangle = \langle \phi_m | (\hat{A}\phi_N) \rangle$$

RHS

$$\langle \phi_m | \hat{A} | \phi_N \rangle = \langle (\hat{A}^{\dagger}\phi_m) | \phi_N \rangle$$

LHS

$$|\phi\rangle \longrightarrow e^{i\theta}|\phi\rangle = |\tilde{\phi}\rangle$$

$$\langle \phi | \phi \rangle = 1$$

$$\langle \tilde{\phi} | \tilde{\phi} \rangle = (\langle \phi | e^{-i\theta})(e^{i\theta}|\phi\rangle) = \langle \phi | \phi \rangle = 1$$

Theorem 1 All eigenvalues of a Hermitian operator are real.

Theorem 2 If $\hat{A}$ is a Hermitian operator, $\hat{A}|\varphi_1\rangle = \alpha_1|\varphi_1\rangle$

$\hat{A}|\varphi_2\rangle = \alpha_2|\varphi_2\rangle$

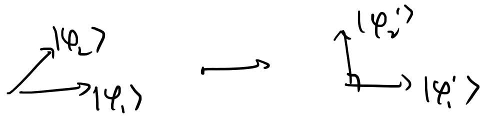
$\alpha_1 \neq \alpha_2$ then $\langle \varphi_1 | \varphi_2 \rangle = 0$

ie eigenstates of a Hermitian operator that correspond to different eigenvalues are orthogonal.

// If $\alpha_1 = \alpha_2$, $|\varphi_1\rangle \neq |\varphi_2\rangle$ we can always find a linear combination that

If $\alpha_1 = \alpha_2$, $|\varphi_1\rangle \neq |\varphi_2\rangle$ we can always find a linear combination that orthogonal

degeneracies



Thus we can always find an orthonormal basis that diagonalises $\hat{A}$.

$$\longrightarrow \quad \hat{A} = \begin{pmatrix} \alpha_1 & & \text{\Large 0} \\ & \alpha_2 & \\ \text{\Large 0} & & \ddots \; \alpha_N \end{pmatrix}$$

$$\hat{A} = \sum_{m,n} |m\rangle\langle m|\hat{A}|n\rangle\langle n|$$

$$= \sum_i \alpha_i |i\rangle\langle i|$$

Choose o.n. basis of eigenvector

Expectation value

For a system in state $|\psi\rangle$,

expectation value of $\hat{A}$ is $\langle \hat{A}\rangle_\psi = \langle\psi|\hat{A}|\psi\rangle$.

To show: Expectation value of Hermitian operator is real-valued

and $\langle \hat{A}\rangle_\psi = \sum_i \alpha_i |c_i|^2$ – probability of finding state $|\psi\rangle$ in $|\varphi_i\rangle$ with eigenvalue α_i.

find c_i — eigenstate

Time evolution of expectation value

$$\frac{d}{dt}\langle \hat{A}\rangle_\psi = \frac{d}{dt}\langle\psi|\hat{A}|\psi\rangle$$

$$= \left\langle \frac{\partial\psi}{\partial t}\right|\hat{A}|\psi\rangle + \langle\psi|\frac{\partial}{\partial t}\left(\hat{A}|\psi\rangle\right)$$

$$= \left\langle \frac{\partial\psi}{\partial t}\right|\hat{A}|\psi\rangle + \langle\psi|\frac{\partial\hat{A}}{\partial t}|\psi\rangle + \langle\psi|\hat{A}\left|\frac{\partial\psi}{\partial t}\right\rangle$$

$$\left(i\hbar\frac{\partial|\psi\rangle}{\partial t} = \hat{H}|\psi\rangle \qquad \frac{\partial|\psi\rangle}{\partial t} = \frac{1}{i\hbar}\hat{H}|\psi\rangle = -\frac{i}{\hbar}\hat{H}|\psi\rangle \right)$$

$$\left(\frac{\partial}{\partial t}\langle\psi| = \frac{i}{\hbar}\langle\psi|\hat{H}^\dagger = \frac{i}{\hbar}\langle\psi|\hat{H} \right)$$

$$= \frac{i}{\hbar}\langle\psi|\hat{H}\hat{A}|\psi\rangle + \langle\psi|\frac{\partial\hat{A}}{\partial t}|\psi\rangle + \langle\psi|\hat{A}\left(-\frac{i}{\hbar}\right)\hat{H}|\psi\rangle$$

$$= \frac{i}{\hbar}\langle\psi|[\hat{H},\hat{A}]|\psi\rangle + \langle\psi|\frac{\partial\hat{A}}{\partial t}|\psi\rangle$$

$$= \frac{i}{\hbar}\langle[\hat{H},\hat{A}]\rangle + \left\langle\frac{\partial\hat{A}}{\partial t}\right\rangle$$

$$\left([\hat{H},\hat{A}] = \hat{H}\hat{A} - \hat{A}\hat{H}\right)$$

Commutator