WEEK 4 LECT1

MATRIX MECHANICS: CONTINUED

$$\chi(x) = \hat{A}\,\psi(x)$$

$$\left.\begin{aligned}\chi(x) &= \sum_{m=1}^{N} b_m \psi_m(x)\\ \psi(x) &= \sum_{n=1}^{N} c_n \psi_n(x)\end{aligned}\right\}\ \text{EXPANSION THEOREM}$$

$$b_m = \sum_{n=1}^{N} A_{mn} c_n$$

$$\underset{(N\times 1)}{B} = \underset{(N\times N)}{A}\ \underset{(N\times 1)}{C}$$

MATRIX MULTIPLICATION!

WHAT ABOUT PRODUCTS OF OPERATORS

$$\chi(x) = \hat{A}\hat{B}\psi(x) = \hat{A}\big(\underbrace{\hat{B}\psi(x)}\big)$$

NEW STATE $\phi(x) = \hat{B}\psi(x)$

$$\phi(x) = \sum_{k=1}^{N} d_k \psi_k$$

$$d_k = \sum_{n=1}^{N} B_{kn} c_n$$

MATRIX MECH.

$$b_m = \sum_{k=1}^{N} A_{mk} d_k = \sum_{k=1}^{N}\sum_{n=1}^{N} A_{mk} B_{kn} c_n$$

OPERATOR MULTIPLICATION

$$\hat{A}\hat{B} \Rightarrow \sum_{k=1}^{N} A_{mk} B_{kn} = (\underset{N\times N}{A}\ \underset{N\times N}{B})_{mn}$$

N×N MATRICES

MATRIX MULTIPLICATION

RECALL MATRICES DON'T COMMUTE IN GENERAL.

COMMUTATORS

$$\hat{C} = [\hat{A},\hat{B}] \Longleftrightarrow AB - BA = C$$

ALSO RECALL FROM MT2 (.. OTHER COURSES)

HERMITIAN ADJOINT OF MATRIX

$$A^{\dagger} = (A^*)^T \qquad \text{e.g.} \begin{pmatrix} i & 1-i \\ 1+2i & 3 \end{pmatrix} = A \Rightarrow A^{\dagger} = \begin{pmatrix} -i & 1-2i \\ 1+i & 3 \end{pmatrix}$$

ALSO $\underset{\substack{\uparrow \\ \text{number}}}{(cA)^{\dagger}} = c^* A^{\dagger}$

$$(A+B)^{\dagger} = A^{\dagger} + B^{\dagger}$$

$$(AB)^{\dagger} = B^{\dagger} A^{\dagger}$$

MOREOVER IF $\boxed{A = A^{\dagger}}$ MATRIX A IS HERMITIAN (SELF-ADJOINT)?

$\Rightarrow$ EIGENVALUES REAL
EIGENVECTORS ORTHOGONAL $\quad A\, \underset{\substack{\downarrow \\ \text{EIGENVECTORS}}}{U_{(i)}} = \underset{\text{EIGENVALUE}}{\lambda_i}\, U_{(i)}$

SAME PROPERTY AS $\hat{H}$ (HAMILTONIAN OPERATOR)

- REAL EIGENVALUES
- ORTHOGONAL EIGENSTATES

Q: CAN WE TRANSLATE THE OPERATION OF TAKING HERMITIAN ADJOINT ~~[illegible]~~ FROM MATRICES TO OPERATORS

RECALL $\hat{H}$ IS HERMITIAN (SELF-ADJOINT)

DEF.: $\int \psi^* \hat{H} \psi \, dx = \int (\hat{H}\psi)^* \psi \, dx$

EXAMPLE SPIN ANGULAR MOMENTUM

E.G. ELECTRONS, QUARKS, .. SPIN $= \frac{1}{2}$

$\vec{S}$ SPIN A.M. OPERATORS

$$S_x = \frac{\hbar}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad S_y = \frac{\hbar}{2}\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad S_z = \frac{\hbar}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

PAULI MATRICES $\sigma_x, \sigma_y, \sigma_z$

- DO NOT COMMUTE E.G. $[S_x, S_y] = i\hbar S_z$
- S_x, S_y, S_z ARE HERMITIAN MATRICES!
- WAVE FUNCT. $\chi = \begin{pmatrix} \alpha \\ \beta \end{pmatrix}$, $\chi^+ = (\alpha^* \ \beta^*)$

NORMALISATION $|\alpha|^2 + |\beta|^2 = 1$

- EIGENSTATES OF $S_z = \frac{\hbar}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$

$$S_z \chi_+ = \frac{\hbar}{2}\chi_+, \quad s_z = +\frac{\hbar}{2}, \quad \chi_+ = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$$

$$S_z \chi_- = -\frac{\hbar}{2}\chi_-, \quad s_z = -\frac{\hbar}{2}, \quad \chi_- = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

$$\chi_+^\dagger \chi_- = (1 \ 0)\begin{pmatrix} 0 \\ 1 \end{pmatrix} = 0 \leftarrow \text{ORTHOGONAL}$$

ASSUME SYSTEM IS IN STATE χ_+: FIND $\Delta S_x, \Delta S_y$, $\boxed{\text{UNCERTAINTY RELATION}}$

$\underline{\psi = \chi_+}$: $\langle S_x \rangle = \chi_+^\dagger \frac{\hbar}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}\chi_+ = \frac{\hbar}{2}(1 \ 0)\begin{pmatrix} 0 \\ 1 \end{pmatrix} = 0$

$$\langle S_x^2 \rangle = \frac{\hbar^2}{4}\chi_+^\dagger \underbrace{\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}}_{=\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}}\chi_+ = \frac{\hbar^2}{4}, \Rightarrow \Delta S_x = \frac{\hbar}{2}$$

ALSO FOR S_y: $\Delta S_y = \frac{\hbar}{2}$

UNCERTAINTY: $[S_x, S_y] = i\hbar S_z$

$$\langle i\hbar S_z \rangle = i\hbar \frac{\hbar}{2}$$

$$\Delta S_x \Delta S_y = \frac{\hbar^2}{4} \geq \frac{1}{2}\underbrace{|\langle [S_x, S_y] \rangle|}_{=\hbar^2/2} = \frac{\hbar^2}{4} \ \checkmark$$

DIRAC NOTATION

UNIFIES THESE REPRESENTATIONS

$$\int_{-\infty}^{+\infty} \chi^*(x)\,\psi(x)\,dx \equiv \langle \chi | \psi \rangle \equiv \sum_{m=1}^{N} b_m^* c_m = B^\dagger C$$

BRA: $\langle \chi | \Leftrightarrow \chi^*(x) \Leftrightarrow B^\dagger$

RECALL $\chi(x) = \sum_{m=1}^{N} b_m \phi_m(x)$ $\quad B = \begin{pmatrix} b_1 \\ b_2 \\ b_3 \\ \vdots \\ b_N \end{pmatrix}$

KET: $|\psi\rangle \Leftrightarrow \psi(x) \Leftrightarrow C$

RECALL: $\psi(x) = \sum_m c_m \phi_m(x)$ $\quad C = \begin{pmatrix} c_1 \\ c_2 \\ \vdots \\ c_N \end{pmatrix}$

$\langle \chi |$, $|\psi\rangle$ $\longrightarrow$ BRA-KET $\langle \chi | \psi \rangle$

integration / summation understood

SIMILARLY

$$\int_{-\infty}^{+\infty} \chi^*(x) \underbrace{\left(\hat{A}\,\psi(x)\right)}_{\rho(x)} dx \equiv \langle \chi | \rho \rangle = \langle \chi | \hat{A}\psi \rangle$$

$$\equiv \langle \chi | \hat{A} | \psi \rangle = B^\dagger \underset{\substack{\uparrow \\ N\times N \text{ MATRIX}}}{A}\, C$$

DIRAC: $\langle \chi | \psi \rangle$ IS "DOT PRODUCT OF STATE-VECTORS"

"HOW MUCH OF χ IS IN ψ"?

TISE $\hat{H}|\psi_i\rangle = E_i|\psi_i\rangle$

EXAMPLES:

$$\langle \psi_i | \psi_j \rangle = \delta_{ij} \quad \text{ORTHONORMALITY}$$

$$H_{ij} = \langle \psi_i | \hat{H} | \psi_j \rangle, \quad c_m = \langle \psi_m | \Psi(x,0) \rangle, \ldots$$

PROPERTIES

$$\langle \psi | c\chi \rangle = c \langle \psi | \chi \rangle$$

c.. complex number

$$\langle c\psi | \chi \rangle = c^* \langle \psi | \chi \rangle$$

LINEARITY $\langle \psi | c_1 \chi_1 + c_2 \chi_2 \rangle = c_1 \langle \psi | \chi_1 \rangle + c_2 \langle \psi | \chi_2 \rangle$

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

$$\left(\int \psi^* \chi \, dx \right)^* = \int \psi \chi^* dx = \int \chi^* \psi \, dx$$

SAME PROPERTIES AS DOT PRODUCT OF COMPLEX VECTORS B, C

$$B \updownarrow |\psi\rangle \qquad C \updownarrow |\chi\rangle$$

$$\langle \psi | \chi \rangle \equiv \underline{\underline{B^\dagger C}}$$

$$\langle \hat{H} \rangle = \langle \psi | \hat{H} | \psi \rangle = C^\dagger H C$$

SOME BONUS MATERIAL (NOT DONE IN LECTURES)

$$\langle \phi | A | \psi \rangle^* = \langle \psi | A^\dagger | \phi \rangle$$

integrals: $\left(\int \phi^* \hat{A} \psi \, dx \right)^* = \int (\hat{A}\psi)^* \phi \, dx = \int \psi^* \hat{A}^\dagger \phi \, dx$ ✓

matrices $\left(\underbrace{\vec{u}^\dagger A \vec{v}}_{\text{scalar quantity} \equiv \text{number}} \right)^* = (\vec{u}^\dagger A \vec{v})^\dagger = \vec{v}^\dagger A^\dagger (\vec{u}^\dagger)^\dagger$

$\vec{u}^\dagger$: ROW vector; A: matrix; $\vec{v}$: column vector

$$= \vec{v}^\dagger A^\dagger \vec{u}$$

$$= \langle v | A | u \rangle$$

unit operator

EXPANSION THEOREM

$$\Psi = \sum c_m \psi_m$$

$$c_m = \int \psi_m^* \Psi \, dx = \langle \psi_m | \Psi \rangle$$

$$|\Psi\rangle = \sum c_m |\psi_m\rangle = \sum_m |\psi_m\rangle\langle\psi_m| \Psi\rangle = \hat{I}|\Psi\rangle$$

$$= |\Psi\rangle$$

IDENTITY OPERATOR $\hat{I}$

integrals $\Psi(x) = \sum_m \psi_m(x) \int \psi_m^*(x') \Psi(x') \, dx'$

$$= \int dx' \Big(\underbrace{\sum_m \psi_m(x) \psi_m^*(x')}_{\delta(x-x')} \Big) \Psi(x') = \Psi(x)$$

vectors: $\vec{c} = \sum c_m \hat{e}_m = \sum \hat{e}_m \langle \hat{e}_m | \vec{c} \rangle$

$$= \sum \hat{e}_m (\hat{e}_m^\dagger \cdot \vec{c})$$

HERMITIAN ADJOINT OF OPERATORS/MATRICES

AND SELF-ADJOINT OPERATORS (= HERMITIAN OPERATORS)

MATRIX: $A^\dagger = (A^*)^T \qquad A_{mn} \rightarrow A^*_{nm}$

DEF.: ADJOINT OPERATOR $\hat{A}^\dagger$

$$\boxed{\int_{-\infty}^{+\infty} \chi^*(x)\, \hat{A}\, \psi(x)\, dx = \int_{-\infty}^{+\infty} (\hat{A}^\dagger \chi(x))^*\, \psi(x)\, dx}$$

"DERIVATION" OR RATHER MOTIVATION OF THIS COMES FROM MATRICES

IN BRA-KET FORM: $\langle \chi | \hat{A} | \psi \rangle = \langle \hat{A}^\dagger \chi | \psi \rangle$

MATRIX FORM $\qquad B^\dagger A\, C \stackrel{?}{=} (A^\dagger B)^\dagger\, C$

$$= B^\dagger (A^\dagger)^\dagger C = B^\dagger A C \checkmark$$

RULES (AS FOR MATRICES)

$$(c\hat{A})^\dagger = c^*\hat{A}^\dagger, \quad (\hat{A}\hat{B})^\dagger = \hat{B}^\dagger \hat{A}^\dagger, \ldots$$

EX PROOF $\qquad$ USE BRA-KET

$$\langle \chi | \hat{A}\, \hat{B} | \psi \rangle = \langle \chi | \hat{A} | (\hat{B}\psi) \rangle = \langle (\hat{A}^\dagger \chi) | (\hat{B}\psi) \rangle$$

$$= \langle \hat{B}^\dagger (\hat{A}^\dagger \chi) | \psi \rangle = \langle \hat{B}^\dagger \hat{A}^\dagger \chi | \psi \rangle$$

HERMITIAN (SELF-ADJOINT) OPERATORS

$$\hat{A}^\dagger = \hat{A} \qquad\qquad A^\dagger = A \text{ (MATRIX OP.)}$$

MOST IMPORTANT CLASS OF LINEAR OPERATORS IN Q.M.

POSTULATE ALL PHYSICAL OBSERVABLES ARE HERMITIAN OPERATORS!

WHY? MAIN PROPERTY → REAL EIGEN VALUES

→ ORTHONORMAL EIGENSTATES/VECTORS

LECT3

EX1: $\hat{x}^\dagger = x^\dagger = x^* = x = \hat{x}$ ✓ (REAL)

EX2: $\hat{p}_x = -i\hbar\,\partial_x$

$$\int \chi^* \hat{p}_x \psi \, dx = -i\hbar \int \chi^* \frac{\partial}{\partial x} \psi \, dx$$

$$= -i\hbar \underbrace{\cancel{\left[\chi^* \psi\right]_{-\infty}^{+\infty}}}_{0 \text{ NORMALISABILITY}} + i\hbar \int \left(\frac{\partial \chi}{\partial x}\right)^* \psi \, dx$$

$$= \int \left(-i\hbar \frac{\partial \chi}{\partial x}\right)^* \psi \, dx = \int (\hat{p}_x \chi)^* \psi \, dx$$

$$\Rightarrow \hat{p}_x^\dagger = \hat{p}_x$$

NOTE i in $\hat{p}_x$ was crucial!

OPERATOR $\frac{\partial}{\partial x}$ IS NOT HERMITIAN!

$$\left(\frac{\partial}{\partial x}\right)^\dagger = -\frac{\partial}{\partial x}$$

EX3 $\hat{H}$ SEE EARLIER INTEGRATION BY PARTS (ALSO DONE IN EXERCISE CLASS)

$$\hat{H} = \underbrace{\frac{1}{2m}}_{\text{real}} (\hat{p}_x)^2 + \underbrace{V(x)}_{\text{real, hermitian}}$$

$$(\hat{p}_x^2)^\dagger = (\hat{p}_x \hat{p}_x)^\dagger = \hat{p}_x^\dagger \hat{p}_x^\dagger = \hat{p}_x \hat{p}_x = (\hat{p}_x)^2$$

$(V(x))^\dagger = V(x^\dagger) = V(x)$ ✓

EX4 $(\hat{x}\hat{p}_x)^\dagger = \hat{p}_x^\dagger \hat{x}^\dagger = \hat{p}_x \hat{x}$ NOT HERMITIAN!
SINCE $\hat{p}_x \hat{x} \neq \hat{x}\hat{p}_x$

BUT $\frac{1}{2}(\hat{x}\hat{p}_x + \hat{p}_x\hat{x})$ IS!

EX5 ANGULAR MOM.: $\hat{L}_z = x\hat{p}_y - y\hat{p}_x = \hat{L}_z^\dagger$ since $[x, \hat{p}_y] = [y, \hat{p}_x] = 0$

PROOF OF MAIN PROPERTIES OF HERMITIAN OPERATORS
IDENTICAL TO PROOF FOR $\hat{H}$, USE BRA-KET NOTATION FOR ALTERNATIVE PROOF

GENERAL $\hat{A} = \hat{A}^\dagger$ HERMITIAN

CONSIDER $A_{ij} = \overset{①}{\langle \phi_i | \hat{A} | \phi_j \rangle} = \overset{②}{\langle \hat{A}\phi_i | \phi_j \rangle}$

$$\hat{A}|\phi_i\rangle = \lambda_i |\phi_i\rangle$$

eigenvalues λ_i, eigenstate $\phi_i(x)$

① $\langle \phi_i | \hat{A} | \phi_j \rangle = \lambda_j \langle \phi_i | \phi_j \rangle$

② $\langle \hat{A}\phi_i | \phi_j \rangle = \underbrace{\langle \lambda_i \phi_i}_{\sim(\lambda_i\phi_i)^*} | \phi_j \rangle = \lambda_i^* \langle \phi_i | \phi_j \rangle$

① = ② $\Rightarrow$ $\boxed{(\lambda_j - \lambda_i^*) \langle \phi_i | \phi_j \rangle = 0}$

$i = j \Rightarrow \lambda_j = \lambda_j^* \Rightarrow \lambda_j$ real

$i \neq j \Rightarrow \underbrace{(\lambda_j - \lambda_i)}_{\neq 0} \langle \phi_i | \phi_j \rangle = 0$

(ASSUMING EIGENVALUES ARE NOT DEGENERATE)

SO: λ_i REAL

AND $\langle \phi_i | \phi_j \rangle = \int_{-\infty}^{+\infty} \phi_i^*(x)\, \phi_j(x)\, dx = \delta_{ij}$

ORTHONORMAL

IF $\hat{A} = \hat{A}^\dagger$

- EXPANSION THEOREM AND MEASUREMENT THEOREM CAN BE GENERALISED IMMEDIATELY TO ALL HERMITIAN OPERATOR $\hat{A} = \hat{A}^\dagger$.

- $\Psi(x) = \sum_{i=1}^{N} c_i \, \phi_i(x)$ $\quad c_i = \int_{-\infty}^{+\infty} dx\, \phi_i^*(x)\, \Psi(x) = \langle \phi_i | \Psi \rangle$

  IN GENERAL DIFFERENT FROM EIGENSTATES $\phi_i(x)$ OF $\hat{H}$

NORMALISATION: $\sum |c_i|^2 = 1$

$|c_i|^2$ .. PROBABILITY TO FIND RESULT λ_i IN MEASUREMENT OF $\hat{A}$

$\langle \hat{A} \rangle = \langle \Psi | \hat{A} | \Psi \rangle = \sum |c_i|^2 \lambda_i$

(PROOF AS FOR $\hat{H}$)

- MEASUREMENT OF $\hat{A}$ YIELDS ONE OF THE EIGENVALUES λ_i WITH PROBABILITY $|c_i|^2$.
- AFTER MEASUREMENT SYSTEM IS IN EIGENSTATE ϕ_i, SUBSEQUENT MEASUREMENTS OF $\hat{A}$ WILL GIVE λ_i (IF SYSTEM IS UNDISTURBED)

<u>ALSO</u> ALL EXPECTATION VALUES OF

HERMITIAN OPERATORS ARE REAL!

$$\langle \hat{A} \rangle = \langle \hat{A} \rangle^*$$

NOTE: $\langle \chi | \psi \rangle^* = \langle \psi | \chi \rangle$

$$\langle \hat{A} \rangle^* = \langle \Psi | \hat{A} \Psi \rangle^* \overset{\Downarrow}{=} \langle \hat{A} \Psi | \Psi \rangle$$

$$= \underset{\text{HERMITICITY}}{\langle \Psi | \hat{A} \Psi \rangle} = \langle \hat{A} \rangle \quad \checkmark$$