PHYS 621 Lecture Notes 2

Today: • More about vector spaces
- change of basis
- Unitary, Hermitian operators

• Hilbert Space

N1.2

Matrix representation

$$|v\rangle = \sum_i v_i \underset{\uparrow}{|i\rangle} = \sum_i |i\rangle \underbrace{\langle i|v\rangle}_{v_i}$$

Basis vector

(orthonormal basis: $\langle i|j\rangle = \delta_{ij}$)

Basis vectors in matrix representation:

$$|i\rangle = \begin{pmatrix} 0 \\ \vdots \\ 1 \\ \vdots \\ 0 \end{pmatrix} \leftarrow 1 \text{ in } i^{th} \text{ component}$$

Matrix element of operator $\hat{A}$ in $\{|i\rangle\}$ basis:

$$A_{ij} = \langle i|\hat{A}|j\rangle$$

row column

$$(\hat{A}\hat{B})_{ij} = \sum_k \langle i|\hat{A}|k\rangle\langle k|\hat{B}|j\rangle$$

$$= \sum_k A_{ik} B_{kj}$$

$$= (\underline{A}\,\underline{B})_{ij}$$ — like matrix multiplication

$\underline{A}$ = matrix with elements A_{ij}.

<u>Operator Inverse</u>: $\hat{A}^{-1}$ defined s.t.

$$\hat{A}\hat{A}^{-1} = \hat{A}^{-1}\hat{A} = \underline{\mathbb{1}}$$

N1.3 <u>Dual Space</u>

† Adjoint operation: transpose and complex conjugate

$$(|v\rangle)^\dagger = (v_1^*, v_2^*, \ldots, v_n^*)$$

$$\langle v|u\rangle = \sum_i v_i^* u_i = (v_1^*, \ldots, v_n^*)\begin{pmatrix} u_1 \\ \vdots \\ u_n \end{pmatrix}$$

$$\Rightarrow \langle v| = (|v\rangle)^\dagger$$

$|u\rangle \in$ vector space $\mathbb{V}$ ket vector

$\langle v| \in$ dual space $\mathbb{V}^*$ bra vectors

$$\langle \alpha v| = (|\alpha v\rangle)^\dagger = \alpha^* \langle v|$$

Scalar vector

$$|v\rangle = \sum_i v_i |i\rangle$$

$$\langle v| = \sum_i v_i^* \langle i|$$

Adjoint operation on operators

$$(\hat{A}^\dagger)_{ij} = \langle j|\hat{A}|i\rangle^* = A_{ji}^*$$

writing $\hat{A}|v\rangle = |\hat{A}v\rangle$,

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

Transpose of product reverses order:

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

Change of basis:

Orthonormal basis $\{|i\rangle\}$

Different orthonormal basis $\{|i'\rangle\}$.

Question: How can $\{|i\rangle\}$ and $\{|i'\rangle\}$ be related.

(Compare with rotation of spatial basis vectors $\hat{x}, \hat{y}, \hat{z}$.)

Suppose $|i'\rangle = \sum_j U_{ji} |j\rangle$ (linear transformation)

The power of the bra-ket notation:

$$\langle k|i'\rangle = \sum_j \langle k| \underbrace{U_{ji}}_{\text{numbers}} |j\rangle$$

$$= \sum_j U_{ji} \langle k|j\rangle$$

$$= \sum_j U_{ji} \underbrace{\delta_{kj}}_{\substack{1 \text{ if } k=j \\ 0 \text{ if } k\neq j}}$$

$$= U_{ki}$$

Define operator $\hat{U}$ s.t. $\langle k | \hat{U} | i \rangle = U_{ki}$

$= \langle k | \hat{U} i \rangle$

$= \langle k | i' \rangle$

$\Rightarrow \hat{U} | i \rangle = | i' \rangle$

Suppose $| i \rangle = \sum_j V_{ji} | j' \rangle$ (inverse relation)

$\langle k' | i \rangle = \sum_j V_{ji} \langle k' | i' \rangle$

$= V_{ki}$

$= (\langle i | k' \rangle^*) = U_{ik}^*$

$= \hat{U}^\dagger_{ki}$

$\rightarrow \boxed{\hat{V} = \hat{U}^\dagger}$

$| i \rangle \xrightarrow{\hat{U}} | i' \rangle \xrightarrow{\hat{U}^\dagger} | i \rangle .$

$\hat{U}^\dagger \hat{U} | i \rangle = | i \rangle$

$\rightarrow \boxed{\hat{U}^\dagger \hat{U} = \hat{\mathbb{1}}}$

Similarly, $\boxed{\hat{U} \hat{U}^\dagger = \hat{\mathbb{1}}}$

$\hat{U}^{-1} = \hat{U}^\dagger$ – Unitary operator

$$\det(\underline{U}\,\underline{U}^\dagger) = (\det U)(\det U^\dagger) = \det(\mathbb{1}) = 1.$$

Matrix representing $\hat{U}$

$$= (\det U)(\det (U^T)^*)$$

$$= (\det U)(\det U)^*$$

$$= |\det U|^2 \qquad = 1$$

$$\rightarrow \boxed{|\det U| = 1}$$

☆ Scalar product is invariant under change of basis.

(c.f. $\vec{a}\cdot\vec{b}$ invariant under rotations)

Do this — $|v'\rangle = \hat{U}|v\rangle, \quad |w'\rangle = \hat{U}|w\rangle$

$$\langle w'|v'\rangle = \langle \hat{U}w|\hat{U}v\rangle$$

$$= \langle w|\underbrace{\hat{U}^\dagger\hat{U}}_{\mathbb{1}}|v\rangle$$

OR

$$\boxed{\langle w'|v'\rangle = \langle w|v\rangle}$$

Instead of acting on vectors (active) can act on operators (passive) – c.f. rotating vectors vs. rotating coordinates.

Do this — $\langle i'|\hat{A}|j'\rangle = \langle i|\hat{U}^\dagger\hat{A}\hat{U}|j\rangle \rightarrow \boxed{\hat{A}' = \hat{U}^\dagger\hat{A}\hat{U}}$

Not both!

Hermitian Operators

Hermitian = self-adjoint

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

$\hat{A}^\dagger = -\hat{A}$ anti-Hermitian

Every operator can be written as a sum of a Hermitian and anti-Hermitian operator.

$$\hat{A} = \underbrace{\frac{\hat{A}+\hat{A}^\dagger}{2}}_{\text{Hermitian}} + \underbrace{\frac{\hat{A}-\hat{A}^\dagger}{2}}_{\text{anti-Hermitian}}$$

★ For a Hermitian operator (not a general operator):

$$A_{ij} = \langle i|\hat{A}|j\rangle = \left(\langle j|\hat{A}^\dagger|i\rangle\right)^*$$

$$= \left(\langle j|\hat{A}|i\rangle\right)^* \quad \text{— because } \hat{A}^\dagger = \hat{A}$$

$$= A_{ji}^*$$

Suppose we want an <u>eigenvector</u> of the operator $\hat{A}$, i.e. a solution to

$$\hat{A}|v\rangle = \underset{\substack{\uparrow \\ \text{eigenvalue}}}{\lambda}|v\rangle = \lambda\hat{\mathbb{1}}|v\rangle.$$

eigenvalue — $\lambda \in \mathbb{C}$ complex #.

$$(\hat{A} - \lambda\hat{\mathbb{1}})|v\rangle = 0$$

$$\langle u|(\hat{A} - \lambda\hat{\mathbb{1}})|v\rangle = 0$$

$$\rightarrow \underline{A} - \lambda\mathbb{1} = 0 \quad \text{Matrix eq.}$$

$$\boxed{\det(\underline{A} - \lambda\mathbb{1}) = 0}$$

— Eigenvalue condition

- determines eigenvalues λ.

<u>Theorem</u>: All eigenvalues of a Hermitian op. are real.

<u>Proof</u>: Suppose $|v\rangle$ is an eigenvector of $\hat{A} = \hat{A}^\dagger$ with eigenvalue λ:

$$\hat{A}|v\rangle = \lambda|v\rangle \rightarrow \langle v|\hat{A}|v\rangle = \lambda\,\|v\|^2$$

Also, $(\hat{A}|v\rangle)^\dagger = \lambda^*\langle v|$

$$= \langle v|\hat{A}^\dagger = \langle v|\hat{A} \Rightarrow \langle v|\hat{A}|v\rangle = \lambda^*\langle v|v\rangle$$

↑ Hermitian

$$= \lambda^*\,\|v\|^2$$

$$\Rightarrow \boxed{\lambda = \lambda^*} \quad \text{real}$$

<u>Theorem</u>: For a Hermitian operator, $\exists$ orthonormal basis of eigenvectors for V.

In that basis: $\underline{A} = \begin{pmatrix} \lambda_1 & & & 0 \\ & \lambda_2 & & \\ & & \ddots & \\ 0 & & & \lambda_n \end{pmatrix}$ diagonal

$\Rightarrow$ We can always diagonalize a Hermitian operator by a unitary transformation s.t.

$$\boxed{(\hat{U}^\dagger \hat{A} \hat{U})_{ij} = \lambda_i \delta_{ij}}$$

Hilbert Spaces — vector space with a scalar product

and corresponding norm s.t. all vectors can be normalized to $\|v\|=1$ (proper vectors), with continuity & completeness with respect to the inner product.

- If $\|v\|^2 = \langle v|v\rangle = 1$, then

with $|v\rangle = \sum_i v_i |i\rangle$,

basis vector.

$$1 = \langle v|v\rangle = \sum_{i,j} \langle j| v_j^* v_i |i\rangle$$

$$= \sum_{i,j} v_j^* v_i \langle j|i\rangle$$

$$= \sum_{i,j} v_j^* v_i \delta_{ij}$$

$$= \sum_i v_i^* v_i = \sum_i |v_i|$$

$$= \sum_i |\underbrace{\langle i|v\rangle}_{v_i}|^2$$

☆ The state space for quantum mechanics is a Hilbert space.