

# Mathematical Structure of Quantum mechanics (C-T II)

Stationary states are assumed to form a complete, orthonormal set

$$\int dx \varphi_n^*(x) \varphi_m(x) = \delta_{nm}$$

(Orthonormality)

$$\sum_n \varphi_n^*(x) \varphi_m(x') = \delta(x-x')$$

(Completeness/  
Closure relation)

The Dirac delta  $\delta(x-x')$  is not a function, also known as a distribution, and only has meaning inside an integral

$$\int dx f(x) \delta(x-x') = f(x')$$

(Lebesgue integral of an ordinary function over a set of measure zero is zero, so removing a point cannot change the value of an integral. But clearly removing  $x'$  makes the integral above zero, so  $\delta(x-x')$  cannot be an ordinary function.)

## Some Dirac delta identities

$$① f(x) \delta(x-x') = f(x') \delta(x-x')$$

$$\Rightarrow = \int dy f(y) \delta(y) \quad \square$$

$$② \delta(ax) = \frac{1}{|a|} \delta(x)$$

$$③ y=ax \Rightarrow \int dx f(x) \delta(ax) = \int dy \frac{f(y/a)}{|a|} \delta(y) = \frac{f(0)}{|a|}$$

$$④ \delta(g(x)) = \sum_{\substack{x_j, \\ g(x_j)=0}} \frac{1}{|g'(x_j)|} \delta(x-x_j)$$

Since  $\delta(g(x))$  is nonzero only at zeroes of  $g$ , we split the integral into several integrals around those zeroes:

$$\int dx f(x) \delta(g(x)) = \sum_j \int_{x_j-\epsilon}^{x_j+\epsilon} dx f(x) \delta(g(x))$$

Taylor expand  $g$  around  $x_j$  and keeps only the first nonzero term.

$$\delta(g(x)) = \delta\left[g(x_j) + (x - x_j) g'(x_j) + \mathcal{O}(x^2)\right]$$

Then by identity ②,

$$\begin{aligned} \int_{x_j-\epsilon}^{x_j+\epsilon} dx f(x) \delta(g(x)) &= \int_{x_j-\epsilon}^{x_j+\epsilon} dx f(x) \delta\left[g'(x_j)(x - x_j)\right] \\ &= \int_{x_j-\epsilon}^{x_j+\epsilon} dx f(x) \frac{\delta(x - x_j)}{|g'(x_j)|} \end{aligned}$$

□

$$\delta^2 \text{ is nonsensical } \int dx \delta^2(x) = \delta(0) = \infty$$

$\delta(x)$  can be built as the "limit" of a sequence of functions

$$① \quad \delta(x) = \lim_{\epsilon \rightarrow 0} \frac{1}{\epsilon} \Theta\left(\frac{\epsilon}{2} - |x|\right)$$

Heaviside step function  $\Theta(x) = \begin{cases} 1, & x \geq 0 \\ 0, & \text{otherwise} \end{cases}$

$$\Theta\left(\frac{\epsilon}{2} - |x|\right) = \begin{cases} 1, & |x| \leq \epsilon/2 \\ 0, & \text{otherwise} \end{cases}$$

Squishing the top hat function, keeping the area under the graph constant.

$$\int_{-\epsilon/2}^{\epsilon/2} dx \Theta\left(\frac{\epsilon}{2} - |x|\right) f(x) = \frac{1}{\epsilon} \int_{-\epsilon/2}^{\epsilon/2} dx f(x)$$

↓ Antiderivative of  $f$

$$= \frac{F(a/2) - F(-a/2)}{2} = \frac{1}{2} \left[ \frac{F(0+a/2) - F(0)}{a/2} + \frac{F(0-a/2) - F(0)}{-a/2} \right]$$

$$\lim_{\epsilon \rightarrow 0} \frac{F'(0) + F'(0)}{2} = F'(0) = f(0)$$

□

## Other representations

$$\textcircled{2} \quad \delta(x) = \lim_{\epsilon \rightarrow 0} \frac{1}{\pi \epsilon} e^{-x^2/\epsilon}$$

$$\textcircled{3} \quad \delta(x) = \lim_{\epsilon \rightarrow 0} \frac{1}{\pi} \frac{\epsilon}{x^2 + \epsilon^2}$$

$$\textcircled{4} \quad \delta(x) = \lim_{n \rightarrow \infty} \frac{\sin(nx)}{\pi x}$$

Convergence  
in the sense of  
distributions  
outside the space  
of square-integrable functions

(Does not actually converge to  
 $\delta(x)$ . Only converge in the sense  
of distributions)

Walter Appel, Mathematics for  
Physicists & Physicists, p. 233

$$\textcircled{5} \quad \delta(x - x') = \int_{-\infty}^{\infty} \frac{dk}{2\pi} e^{ik(x-x')} \quad \leftarrow \text{Inverting the Fourier transform}$$

Suppose that  $\psi(x) = \sum_n c_n \varphi_n(x)$ , \* orthonormality implies that

$$\int dx \varphi_n^*(x) \psi(x) = \sum_m c_m \underbrace{\int dx \varphi_n^*(x) \varphi_m(x)}_{\delta_{nm}} = c_n$$

Completeness says that an arbitrary wave function  $\psi(x)$  is amenable to the expansion \* in terms of the set  $\{\varphi_n(x)\}_n$

$$* = \int dx' \psi(x') \sum_n \varphi_n^*(x') \varphi_n(x)$$

$\underbrace{\qquad\qquad\qquad}_{\text{Must be } \delta(x-x')}$   
to return  $\psi(x)$

$$|\psi(x)|^2 dx = \left( \text{Probability to find the particle within } dx \right) < \infty$$

Square-integrable func.

$$|c_n|^2 = \left( \text{Probability that the energy is } E_n \right) < \infty$$

$\{c_n\}_n \in l^2$   
Square-summable sequences

$$\psi(x) = \sum_n c_n \varphi_n(x),$$

$$\phi(x) = \sum_n d_n \varphi_n(x)$$

Inner product  $\int dx \phi^*(x) \psi(x) = \sum_{nm} d_m^* c_n \int dx \varphi_m^*(x) \varphi_n(x)$

"Same" inner product  $\int dx \phi^*(x) \psi(x) = \sum_n d_n^* c_n = [d_1^* d_2^* \dots] \begin{bmatrix} c_1 \\ c_2 \\ \vdots \end{bmatrix}$   
space, just different "bases"!

$\psi(x)$  and  $\{c_n\}_n$  are different representations of the same abstract vector, denoted as a ket  $|\psi\rangle$ .

# of L.I. vectors 

Finite dimensional  
Infinite dimensional

## Normed and inner product spaces

Norm  $\|\cdot\| : V \rightarrow \mathbb{R}^+$

- ① Positive definiteness  $\|\psi\| = 0$  iff  $\psi = 0$  (zero vector)
- ② Triangle inequality  $\|\psi + \phi\| \leq \|\psi\| + \|\phi\|$

Inner product  $(\cdot, \cdot) : V \times V \rightarrow \mathbb{C}$

- ① Linearity in the 2nd argument

$$(\phi, a\psi_1 + b\psi_2) = a(\phi, \psi_1) + b(\phi, \psi_2)$$

- ② Conjugate symmetry  $(\psi, \phi) = (\phi, \psi)^*$

- ③ Positive definiteness  $(\psi, \psi) \geq 0$  with equality iff  $\psi = 0$

① + ②  $\Rightarrow$  Conjugate linearity in the 1st argument

Ex Inner product on  $\mathbb{R}^2$ :  $(\vec{x}, \vec{y}) = 5x_1y_1 + x_1y_2 + x_2y_1 + 3x_2y_2$

$$(\vec{x}, \vec{x}) = 5x_1^2 + 2x_1x_2 + 3x_2^2 = (x_1 + x_2)^2 + 4x_1^2 + 2x_2^2 \geq 0$$

with equality iff  $x_1 = x_2 = 0$

Inner product  $\Rightarrow$  Norm. But not necessarily true that Norm  $\Rightarrow$  inner product. CEx Max norm  $\|\psi\|_\infty = \max_j |c_j|$

$$\text{p-norm } \|\psi\|_p = \sqrt[p]{\sum_j |c_j|^p}$$

But when an inner product can be recovered from a norm, it is through a so-called polarization identity.

$$(\phi, \psi) = \operatorname{Re}(\phi, \psi) + i \operatorname{Re}(i\phi, \psi)$$

$$\operatorname{Re}(\phi, \psi) = \frac{1}{2} (\|\psi\|^2 + \|\phi - \psi\|^2 - \|\phi + \psi\|^2)$$

Orthonormal basis  
(ONB)  $(e_j, e_k) = \delta_{jk}$

### Linear functional and the bra $\langle \psi |$

An inner product with a fixed vector  $\phi$  can always be thought of as a linear map  $(\phi, \cdot) : V \rightarrow \mathbb{C}$

$$\psi \mapsto (\phi, \psi)$$

Ex Dirac delta  $\int dx \delta(x-x') f(x) = f(x')$

Linear functional Vector Value in  $\mathbb{C}$

Bra

Not a vector but a perfectly valid linear functional  $\langle \phi | : V \rightarrow \mathbb{C}$

Scalar  $\langle \phi | \psi \rangle$   
Bra-ket

$\langle \phi |$  Many names: linear functional, dual vector, 1-form

The dual space  $V^*$  is the vector space of linear functionals with addition defined as  $\langle (\phi_1 + \phi_2) | \psi \rangle = \langle \phi_1 | \psi \rangle + \langle \phi_2 | \psi \rangle, \psi \in V$

( $V^*$  can be defined without prior notion of an inner product)

$\begin{pmatrix} \text{Linear} \\ \text{Functional} \end{pmatrix} \xleftrightarrow[\text{dim}]{} \begin{pmatrix} \text{Finite} \\ \text{matrix} \end{pmatrix}$

$$\begin{bmatrix} x & x & \dots & x \end{bmatrix} \begin{bmatrix} c_1 \\ c_2 \\ \vdots \\ c_d \end{bmatrix}$$

Dual basis  $\langle f_j | e_k \rangle = \delta_{jk} \Rightarrow \dim V^* = \dim V$

An inner product gives a correspondence between dual vector in  $V^*$  and vectors in  $V$

$$\langle \phi | \psi \rangle = (|\phi\rangle, |\psi\rangle)$$

Antilinear map

$$\langle \psi | \xleftarrow{+} |\psi\rangle$$

in an ONB

$$c_1^* \langle e_1 | + \cdots + c_d^* \langle e_d | \xleftarrow{+} c_1 |e_1\rangle + \cdots + c_d |e_n\rangle$$

The conjugate is there to make sure that  $\|\psi\| = \sqrt{\langle \psi | \psi \rangle}$  is a norm (real and positive).

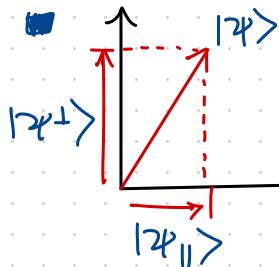
ONB  $\langle \phi | \psi \rangle = \sum_{jk} d_j^* c_k \underbrace{\langle e_j | e_k \rangle}_{\delta_{jk}} = \sum_j d_j^* c_j$

$$\langle \psi | \psi \rangle = \sum_j |c_j|^2$$

Reminder (Ballentine):  $\langle \phi | \psi \rangle$  is often thought of as a shorthand for an inner product, but this interpretation is not valid when there is no corresponding  $|\phi\rangle$  for the bra  $\langle \phi |$  e.g.  $\langle \times |$

## Cauchy-Schwarz inequality (C-T A<sub>II</sub>)

$$|\langle \psi | \phi \rangle|^2 \leq \langle \phi | \phi \rangle \langle \psi | \psi \rangle$$



Many approaches to proving the ineq. This one uses the Pythagorean thm.

$$|\psi\rangle = |\psi_{\perp}\rangle + |\psi_{\parallel}\rangle = \frac{\langle \phi | \psi \rangle}{\langle \phi | \phi \rangle} |\phi\rangle, \quad |\psi_{\perp}\rangle = |\psi\rangle - \frac{\langle \phi | \psi \rangle}{\langle \phi | \phi \rangle} |\phi\rangle$$

$$\langle \psi | \psi \rangle = \langle \psi_{\perp} | \psi_{\perp} \rangle + \langle \psi_{\parallel} | \psi_{\parallel} \rangle$$

$$\langle \psi | \psi \rangle - \frac{|\langle \phi | \psi \rangle|^2}{\langle \phi | \phi \rangle} = \langle \psi_{\perp} | \psi_{\perp} \rangle \geq 0$$

$$\langle \phi | \phi \rangle \langle \psi | \psi \rangle \geq |\langle \phi | \psi \rangle|^2$$

Equality iff  $|\psi\rangle$  is a scalar multiple of  $|\phi\rangle$ . □

⚠ From this point onward, we assume an ONB  $\{|\psi_j\rangle\}_j$  ⚡

$$\langle \psi_j | \psi_k \rangle = \delta_{jk}$$

$$\sum_j |\psi_j\rangle \langle \psi_j| = \hat{\mathbb{I}}$$

(Orthonormality)

(Completeness/  
Closure relation)

Linear map

$$\hat{T}(|\psi\rangle + |\varphi\rangle) = a \hat{T}|\psi\rangle + b \hat{T}|\varphi\rangle$$

$$\psi_j = \langle \psi_j | \psi \rangle, \varphi_j = \langle \psi_j | \varphi \rangle, \hat{T}|\psi\rangle = |\psi\rangle$$

$$\psi_j = \sum_k T_{jk} \psi_k,$$

$$\hat{T}|\psi_j\rangle = \sum_k T_{kj} |\psi_k\rangle$$

Definition of  
matrix elements

$$\hat{T} = \hat{\mathbb{I}} \hat{T} \hat{\mathbb{I}} = \sum_{jk} |\psi_j\rangle \underbrace{\langle \psi_j |}_{\text{Matrix element}} \hat{T} |\psi_k\rangle \langle \psi_k| = \sum_{jk} T_{jk} |\psi_j\rangle \langle \psi_k|$$

Matrix  
element  
Row  $\uparrow$   
 $T_{jk}$   $\uparrow$   
Column

Derive transformation rules from  
the previous page

$$\hat{T} \hat{S} = \sum_{jkl} T_{jl} S_{lk} |\psi_j\rangle \langle \psi_l|$$

Ex Pauli matrices

$$\hat{\sigma}_x = \hat{\sigma}_x \equiv \hat{X} = |0\rangle \langle 1| + |1\rangle \langle 0| \leftrightarrow \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

$$\hat{\sigma}_y = \hat{\sigma}_y \equiv \hat{Y} = -i |0\rangle \langle 1| + i |1\rangle \langle 0| \leftrightarrow \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$$

$$\hat{\sigma}_z = \hat{\sigma}_z \equiv \hat{Z} = |0\rangle \langle 0| - |1\rangle \langle 1| \leftrightarrow \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

## Projection operator (1st pass)

Outer products  $|v\rangle\langle v|$  are linear operators e.g.  $\hat{I} = \sum_j |e_j\rangle\langle e_j|$

ONB for a subspace

$$\{ |e_j\rangle \mid j \in S \} \subset \{ |e_k\rangle \mid k=1, 2, \dots, \dim V \}$$

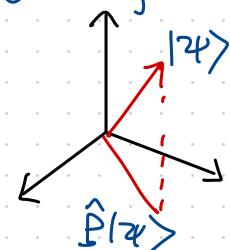
Index set for the subspace

$$\hat{P} = \sum_j |f_j\rangle\langle f_j|$$

$$\text{Suppose } |v\rangle = \sum_k c_k |e_k\rangle, \text{ then } \hat{P}|v\rangle = \sum_j c_j |e_j\rangle, j \in S$$

Projectors for the union or the intersection of two subspaces?  $\Rightarrow$

HW C-T H<sub>II</sub> Problem 5.



## The trace Two equivalent definitions

$$\textcircled{1} \quad \text{Tr } \hat{T} = \sum_j T_{jj} \quad (\text{Obviously linear})$$

$$\textcircled{2} \quad \text{Tr}(|\psi\rangle\langle\phi|) = |\phi\rangle\langle\psi| \quad (\text{Obviously basis-independent})$$

Let us prove the equivalence only in an ONB (Not ONB  $\Rightarrow$  Need dual basis)

$$\textcircled{1} \Rightarrow \textcircled{2} \quad \text{Tr}(|\psi\rangle\langle\phi|) = \sum_j \underbrace{\langle e_j | \psi \rangle}_{\text{Only in ONB}} \langle \phi | e_j \rangle = \langle \phi | \psi \rangle \sum_j T_{jj}$$

$$\textcircled{2} \Rightarrow \textcircled{1} \quad \text{Tr } \hat{T} = \text{Tr} \left[ \sum_{j,k} T_{jk} |e_j\rangle\langle e_k| \right] = \sum_{j,k} T_{jk} \text{Tr}(|e_j\rangle\langle e_k|)$$

$$\text{Ex} \quad \text{Tr } \hat{\mathbb{1}}_{d \times d} = d, \quad \text{Tr } \hat{P}_S = \dim S, \quad \text{Tr } \hat{\sigma}_j = 0, \quad j=1,2,3$$

Cyclic property:  $\text{Tr}(\hat{A}\hat{B}) = \text{Tr}(\hat{B}\hat{A}) \Rightarrow \text{Tr}[\hat{A}, \hat{B}] = 0$

$$\text{Tr}(\hat{A}\hat{B}\hat{C}) \neq \text{Tr}(\hat{B}\hat{A}\hat{C})$$

$$\text{Ex} \quad \text{Tr}[\hat{\sigma}_j^2, \hat{\sigma}_k^2] = i \epsilon_{jkl} \text{Tr} \hat{\sigma}_l = 0$$

Paradox  $0 = \text{Tr}[\hat{x}, \hat{p}] = i\hbar \text{Tr} \hat{\mathbb{1}} = i \cdot \infty$  What's going on?

( $\hat{x}$  and  $\hat{p}$  are unbounded operator ( $\|\hat{x}\psi(x)\| = \|x\psi(x)\|$  is not bounded)).  $\Rightarrow$  Mathematicians work with the Weyl form of the canonical commutation relation

$$e^{ix\hat{x}} e^{ip\hat{p}} = e^{-i\eta\xi/\hbar} e^{i\xi\hat{p}} e^{ix\hat{x}}$$

whose eigenvalues are bounded within the unit circle  $|z| \leq 1$ .

Adjoint Suppose  $\hat{T}: V \rightarrow W$ ,  $|v\rangle \in V$ ,  $\langle \phi | = \hat{T}^* |v\rangle \in W^*$

$$\begin{array}{ccc} & \uparrow & \\ V & \xrightarrow{\hat{T}} & W \\ & \searrow & \downarrow \langle \phi | \\ & & \mathbb{C} \end{array}$$

$$\langle \phi | (\hat{T} | v \rangle) = (\langle \phi | \hat{T}) | v \rangle$$

Inner product  $\Rightarrow \exists$  a ket in  $V$  corresponding to the bra  $\langle \phi | \hat{T}$ . We write this ket as  $\hat{T}^+ | \phi \rangle$ .

Equivalently,  $(\hat{T}^+ | \phi, v \rangle) = (\phi | \hat{T} v \rangle)$  or  $\langle \phi | \hat{T}^+ | v \rangle = \langle v | \hat{T} | \phi \rangle^*$

Properties:  $(a\hat{T} + b\hat{S})^+ = a^* \hat{T}^+ + b^* \hat{S}^+$

$$(\hat{T} \hat{S})^+ = \hat{S}^+ \hat{T}^+$$

${}^+$  Antilinear

$$(\hat{T}^+)^+ = \hat{T}$$

In ONB,  $(\hat{T}^+)^{jk} = \langle e_j | \hat{T}^+ | e_k \rangle = \langle e_k | \hat{T} | e_j \rangle^* = \hat{T}_{kj}^*$  Conjugate transpose

Normal operators:  $[\hat{T}, \hat{T}^+] = 0 \Leftrightarrow \hat{T} \hat{T}^+ = \hat{T}^+ \hat{T}$

Hermitian  $\hat{T}^+ = \hat{T}$

Unitary  $\hat{T}^+ = \hat{T}^{-1}$

$\hat{T}^{-1}$  = left inverse and right inverse. One implies the other in finite dim but not necessary in  $\infty$  dim.

CEx Right shift  $R: [c_1, c_2, \dots] \mapsto [0, c_1, c_2, \dots]$

Left shift  $L: [c_1, c_2, \dots] \mapsto [c_2, c_3, \dots]$

$$\hat{L} = \hat{R}^+, \quad \hat{L} \hat{R} = 1 \text{ but } \hat{R} \hat{L} \neq 1$$

## Change of basis (Sakurai ed. 3, 1.5.1)

ONBs  $\{|e_j\rangle\}$ ,  $\{|e'_j\rangle\}_j$

Active transformation

$$|e'_j\rangle = \hat{U}|e_j\rangle \Leftrightarrow \hat{U} = \sum_j |e'_j\rangle \langle e_j|$$

What are matrix elements of  $\hat{U}$  in the old (unprimed) basis?

$$\langle e_j | \hat{U} | e_k \rangle = \langle e_j | e'_k \rangle \quad \therefore U \xleftarrow{\text{old}} \begin{bmatrix} \langle e_1 | e_1 \rangle & \langle e_1 | e_2 \rangle & \dots \\ \langle e_2 | e_1 \rangle & \langle e_2 | e_2 \rangle & \dots \\ \vdots & \vdots & \ddots \end{bmatrix}$$

$$|\psi\rangle = \sum_j \psi_j |e_j\rangle, \quad \psi_j = \langle e_j | \psi \rangle \quad \text{old expansion coefficient}$$

$$\text{New coefficient } \langle e'_k | \psi \rangle = \sum_j \underbrace{\langle e'_k | e_j \rangle}_{(\hat{U}^\dagger)_{jk}} \psi_j$$

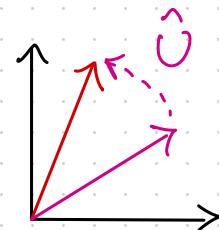
Transformation of matrix elements

$$\begin{aligned} \langle e'_j | \hat{T} | e'_k \rangle &= \langle e_j | \hat{U}^\dagger \hat{T} \hat{U} | e_k \rangle \\ &= \sum_{lm} \langle e_j | \hat{U}^\dagger | e_l \rangle \langle e_l | \hat{T} | e_m \rangle \langle e_m | \hat{U} | e_k \rangle \\ &= (\hat{U}^\dagger \hat{T} \hat{U})_{jk} \end{aligned}$$

In particular, to preserve the orthonormality,

$$\delta_{jk} = \langle e_j | e'_k \rangle = (\hat{U}^\dagger \hat{U})_{jk} \Leftrightarrow \hat{U}^\dagger \hat{U} = \hat{1} \quad (\hat{U} \text{ is unitary})$$

$$\therefore \text{Tr}(\hat{U}^\dagger \hat{T} \hat{U}) = \text{Tr}(\hat{U} \hat{U}^\dagger \hat{T}) = \text{Tr} \hat{T}$$



## Diagonalization (Spectral theorem)

Motivation: operator functions (C-T B<sub>II</sub>)

Defined by the power series of the function  $f(\hat{A}) = \sum_{n=0}^{\infty} f_n A^n$

e.g.  $e^{\hat{A}} = \sum_{n=0}^{\infty} \frac{\hat{A}^n}{n!} = \hat{1} + \hat{A} + \frac{\hat{A}^2}{2!} + \frac{\hat{A}^3}{3!} + \dots$

Can't take the function element-wise. CEx  $\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}^2 = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \neq \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$

If  $[\hat{A}, \hat{B}] \neq 0$ ,  $e^{\hat{A}+\hat{B}} \neq e^{\hat{A}} e^{\hat{B}}$   $\Rightarrow$  BCH formula (HW2 P5)

If  $|a\rangle$  is an eigenvector of  $\hat{A}$ ,

$$\hat{A}|a\rangle = a|a\rangle,$$

↓  
Eigenvalue  
↑  
Eigenvector

How to determine the eigenvalues

$$(\hat{A} - a_j \hat{1})|a_j\rangle = 0$$

$$\Rightarrow \det(\hat{A} - a_j \hat{1}) = 0$$

Not invertible

then  $f(\hat{A})|a\rangle = \sum_{n=0}^{\infty} f_n A^n |a\rangle = \sum_{n=0}^{\infty} f_n a^n |a\rangle = f(a)|a\rangle$ .

That is, one can take the function of the eigenvalue directly.

So  $A$ -action is simple if we can expand any  $|z\rangle$  in a set of  $A$ -eigenectors.  $|z\rangle = z_1|a_1\rangle + z_2|a_2\rangle + \dots$

When can one expect this to happen? When  $\hat{A}$  is a so-called "normal operator"

$$\hat{A} \text{ is normal if } [\hat{A}, \hat{A}^\dagger] = 0 \Leftrightarrow \hat{A}\hat{A}^\dagger = \hat{A}^\dagger\hat{A}$$

Special case Hermitian or unitary  $\hat{A}$  are normal.

Thm If  $\hat{A}^\dagger = \hat{A}$ , then eigenvalues of  $\hat{A}$  are real. Moreover, eigenvectors of  $\hat{A}$  that correspond to distinct eigenvalues are orthogonal

Hermiticity

$$\begin{aligned} \langle a_j | \hat{A} | a_k \rangle &= \langle a_j | \hat{A}^\dagger | a_k \rangle = \langle a_k | \hat{A} | a_j \rangle^* \\ &\quad \parallel \qquad \parallel \\ a_k \langle a_j | a_k \rangle & \qquad \qquad \qquad a_j^* \langle a_k | a_j \rangle^* \\ &\qquad \qquad \qquad \parallel \\ &\qquad \qquad \qquad a_j^* \langle a_j | a_k \rangle \end{aligned}$$

$$\Rightarrow (a_k - a_j^*) \langle a_j | a_k \rangle = 0 \Rightarrow \begin{cases} \text{Case I } j = k \Rightarrow a_j^* = a_j \\ \text{Case II } a_j \neq a_k \Rightarrow \langle a_j | a_k \rangle = 0 \end{cases}$$

### Spectral thm (special case)

For  $\hat{A}$  Hermitian, one can choose A-eigenvectors that form a complete, orthonormal set i.e. an ONB.

( $\hat{A}$  degenerate  $\Rightarrow$  Diagonalize  $\hat{A}$  in the degenerate subspace)

$$\hat{A}(a_j) = a_j a_j \quad \text{Eigenvalue equation}$$

$$\langle a_j | a_k \rangle = \delta_{jk} \quad \text{Orthonormality}$$

$$\sum_j \langle a_j | a_j \rangle = 1 \quad \text{Completeness}$$

Spectral decomposition

$$\hat{A} = \sum_j a_j |a_j\rangle \langle a_j| = \sum_j a_j \sum_\alpha |a_{j\alpha}\rangle \langle a_{j\alpha}|$$

Degeneracy label

$P_j$  Projection onto the degenerate subspace

Thm Suppose that Hermitian operators  $\hat{A}$  and  $\hat{B}$  commute. Then eigenvectors of  $\hat{A}$  can be chosen to be simultaneously eigenvectors of  $\hat{B}$ .

- Consider a vector  $\hat{B}|a\rangle$ .

$$\hat{A}\hat{B}|a\rangle = \hat{B}\hat{A}|a\rangle = a\hat{B}|a\rangle \Rightarrow \hat{B}|a\rangle \text{ is an } A\text{-eigenvector}$$

Case I Eigenvalue  $a$  is non-degenerate  $\Rightarrow \hat{B}|a\rangle \propto |a\rangle$

$|a\rangle$  is also a  $B$ -eigenvector

Case II  $\hat{B}$  transforms  $|a\rangle$  within the degenerate subspace

$\rightarrow$  Diagonalize  $\hat{B}$  in this subspace  $\Rightarrow$  Simultaneous eigenvector.  $\square$

Suppose  $\hat{A}$  Hermitian  $e^{i\hat{A}} = \sum_j e^{ia_j} |q_j\rangle \langle q_j|$

$$(e^{i\hat{A}})^+ = \sum_j \frac{1}{e^{ia_j}} |q_j\rangle \langle q_j| = (e^{i\hat{A}})^{-1} \Rightarrow e^{i\hat{A}}$$
 is unitary

and diagonalizable in an  $A$ -eigenbasis

Projection operator (2nd pass)

①  $\hat{P}^+ = \hat{P}$  CEX if this requirement is dropped  $\begin{pmatrix} 1 & 1 \\ 0 & 0 \end{pmatrix}$

②  $\hat{P}^2 = \hat{P} \Rightarrow$  Eigenvalues 0 or 1 ("Idempotent")

Positive operator  $\langle \psi | \hat{A} | \psi \rangle \geq 0 \forall \psi$

Ex  $\hat{T}^\dagger \hat{T}$  and  $\hat{T}^\dagger \hat{T}^\dagger$  are positive for any  $\hat{T} \Rightarrow$  SVD

Properties of continuous "bases"  $|x\rangle$  and  $|p\rangle$  [They don't lie in the physical Hilbert space]

$$\hat{x}|x\rangle = x|x\rangle \quad \text{Eigenvalue equation}$$

$$\langle x|x'\rangle = \delta(x-x') \quad \text{Delta orthogonality}$$

$$\int dx |x\rangle \langle x| = \hat{1} \quad \text{Completeness}$$

$x$ -representation:

$$|\psi\rangle = \int dx \underbrace{\langle x|\psi\rangle}_{\psi(x)} |x\rangle$$

$\psi(x) = \begin{pmatrix} \text{Position-space} \\ \text{wave function} \end{pmatrix} = \begin{pmatrix} \text{Probability amplitude} \\ \text{to be at } x \end{pmatrix}$

$$\langle \phi|\psi\rangle = \int dx \langle \phi|x\rangle \langle x|\psi\rangle = \int dx \phi^*(x) \psi(x)$$

$$\hat{p}|p\rangle = p|p\rangle$$

$$\langle x|p\rangle = \frac{1}{\sqrt{2\pi\hbar}} e^{ipx/\hbar} \quad \begin{array}{l} \text{(Unitary change-of-basis)} \\ \text{from the } x\text{-rep} \end{array}$$

$\frac{1}{\sqrt{2\pi\hbar}}$  ← Conventional integration measure

$$\langle p|p'\rangle = \int dx \langle p|x\rangle \langle x|p'\rangle = \int_{2\pi\hbar} dx e^{i(p'-p)x/\hbar} = \delta(p-p')$$

$$\begin{aligned} \int dp |p\rangle \langle p| &= \int dx \int dx' |x\rangle \langle x'| \int \frac{dp}{2\pi\hbar} e^{ip(x-x')/\hbar} \\ &= \int dx |x\rangle \langle x| = \hat{1} \end{aligned}$$

$\delta(x-x')$

$p$ -representation:

$$|\varphi\rangle = \int dp \underbrace{\langle p|\varphi\rangle}_{\tilde{\varphi}(p)} |p\rangle$$

$$\tilde{\varphi}(p) = \begin{pmatrix} \text{Momentum-space} \\ \text{wave function} \end{pmatrix} = \begin{pmatrix} \text{Probability amplitude} \\ \text{to have momentum } p \end{pmatrix}$$

The representation of an operator  $\hat{A}$  in a continuous basis  $|q\rangle$ ,  $\hat{A}|q\rangle$  (its  $q$ -representation) is defined to be

$$\hat{A}|q\rangle \langle q|\psi\rangle = \langle q|\hat{A}|\psi\rangle$$

$\hat{p}$  in  $x$ -representation:

$$\begin{aligned}\langle x|\hat{p}|\psi\rangle &= \int dp \int dx' \langle x|\hat{p}|p\rangle \langle p|x'\rangle \langle x'|\psi\rangle \\ &= \int dx' \psi(x') \underbrace{\int dp}_{2\pi\hbar} p e^{\frac{i p(x-x')}{\hbar}} \underbrace{\delta(x-x')}_{\text{red}} \\ &= \int dx' \psi(x') \frac{\hbar}{i} \frac{d}{dx} \int \frac{dp}{2\pi\hbar} e^{\frac{i p(x-x')}{\hbar}} \\ &= \frac{\hbar}{i} \frac{d}{dx} \int dx' \psi(x') \delta(x-x') \\ &= \boxed{\frac{\hbar}{i} \frac{d}{dx} \psi(x)} \quad \leftarrow \hat{p}_{|x\rangle}\end{aligned}$$

$\hat{x}$  in  $p$ -representation

$$\langle p|\hat{x}|\psi\rangle = -\frac{\hbar}{i} \frac{d}{dp} \tilde{\psi}(p)$$

$(\hat{x}\hat{p})_{|x\rangle}$  and  $(\hat{p}\hat{x})_{|x\rangle}$ ?  $\Rightarrow$  HW C-T H<sub>II</sub> Problem 10.

$$\underbrace{(\hat{x}\hat{p} - \hat{p}\hat{x})_{|x\rangle}}_{(x\hat{p} - \hat{p}x)} \psi(x) = i\hbar \psi(x)$$