Mathematical Structure of Quantum mechanics (C-T II)

Stationary states are assumed to form a complete, orthonormal set

$$\boxed{\begin{aligned} \int dx\, \varphi_n^*(x)\varphi_m(x) &= \delta_{nm} \\ \sum_n \varphi_n^*(x)\varphi_m(x') &= \delta(x-x') \end{aligned}}$$

(Orthonormality)

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

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

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

$$= \int \frac{dy}{|a|} f(y)\delta(y) \quad \square$$

③ $$\delta(g(x)) = \sum_{\substack{x_j,\\ g(x_j)=0}} \frac{1}{|g'(x_j)|}\delta(x-x_j)$$

- 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.

$$\delta(g(x)) = \delta\left[\overset{0}{g(x_j)} + (x-x_j)\,g'(x_j) + \mathcal{O}(x^2)\right]$$

Then by identity ②,

$$\int_{x_j-\epsilon}^{x_j+\epsilon} dx\, f(x)\,\delta(g(x)) = \int_{x_j-\epsilon}^{x_j+\epsilon} dx\, f(x)\,\delta\left[g'(x_j)(x-x')\right]$$

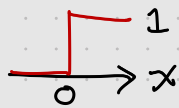
$$= \int_{x_j-\epsilon}^{x_j+\epsilon} dx\, f(x)\,\frac{\delta(x-x')}{|g'(x_j)|} \qquad \square$$

δ^2 is nonsensical $\int dx\, \delta^2(x) = \delta(0) = \infty$

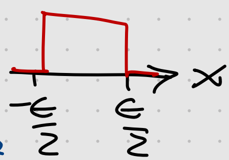
$\delta(x)$ can be built as the "limit" of a sequence of functions

① $\delta(x) = \lim\limits_{\epsilon \to 0} \frac{1}{\epsilon}\, \Theta\left(\frac{\epsilon}{2} - |x|\right)$

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.

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

↓ Antiderivative of f

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

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

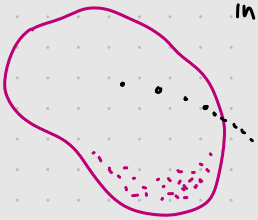
Other representations

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

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

④ $\delta(x) = \lim_{n \to \infty} \frac{\sin(nx)}{\pi x}$ ← (Does not actually converge to $\delta(x)$. Only converge in the sense of distributions)

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



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

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

Suppose that $\boxed{\psi(x) = \sum_n c_n \varphi_n(x)}$ $*$, 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 $\{\varphi_n(x)\}_n$

$$* = \int dx'\, \psi(x') \underbrace{\sum_n \varphi_n^*(x')\varphi_n(x)}_{\text{Must be } \delta(x-x') \text{ to return } \psi(x)}$$

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

$\psi(x) \in L^2$
Square-integrable func.

$$|c_n|^2 = \begin{pmatrix}\text{Probability that the} \\ \text{energy is } E_n\end{pmatrix} < \infty$$

$\{c_n\}_n \in \ell^2$
Square-summable sequence

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

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

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 space, just different "bases"!

$$= \sum_n d_n^* c_n = [d_1^* d_2^* \cdots] \begin{bmatrix} c_1 \\ c_2 \\ \vdots \end{bmatrix}$$

$\psi(x)$ 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 $\|\cdot\|: V \to \mathbb{R}^+$

① Positive definiteness $\|\psi\| = 0$ iff $\psi = 0$ (zero vector)

② Triangle inequality $\|\psi + \phi\| \leq \|\psi\| + \|\phi\|$

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

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 $\|\psi\|_\infty = \max_j |c_j|$

Instance of the family of 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.

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

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

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

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

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

Ex Dirac delta $\int dx \underbrace{\delta(x-x')}_{\text{Linear functional}} \underbrace{f(x)}_{\text{Vector}} = \underbrace{f(x')}_{\text{Value in } \mathbb{C}}$

Not a vector but a perfectly valid linear functional $\underbrace{\langle x|}_{\text{Bra}} : V \to \mathbb{C}$

Scalar $\underbrace{\langle\phi|\psi\rangle}_{\text{Bra-ket}}$

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

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

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

$$\begin{pmatrix}\text{Linear}\\ \text{functional}\end{pmatrix} \overset{\text{Finite}}{\underset{\text{dim}}{\Longleftrightarrow}} \begin{pmatrix}\text{1-by-}n\\ \text{matrix}\end{pmatrix} \qquad [x \; x \; \cdots \; x]\begin{bmatrix} c_1 \\ c_2 \\ \vdots \\ c_d \end{bmatrix}$$

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

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

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

Antilinear map $\qquad \langle \psi | \xleftrightarrow{\dagger} |\psi\rangle$

in an ONB

$$c_1^* \langle e_1| + \cdots + c_d^* \langle e_d| \longleftrightarrow c_1 |e_1\rangle + \cdots + c_d |e_n\rangle$$

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

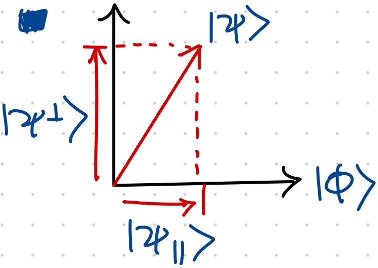
ONB $\qquad \langle \phi | \psi \rangle = \sum_{jk} d_j^* c_k \overbrace{\langle e_j | e_k \rangle}^{\delta_{jk}} = \sum_j d_j^* c_j$

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

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. $\langle x |$

Cauchy-Schwarz inequality $(\text{C-T } A_{\text{II}})$

$$\boxed{|\langle\phi|\psi\rangle|^2 \leq \langle\phi|\phi\rangle\langle\psi|\psi\rangle}$$



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

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

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

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

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

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

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

$$\boxed{\begin{aligned} \langle e_j|e_k\rangle &= \delta_{jk} \\ \sum_j |e_j\rangle\langle e_j| &= \hat{\mathbb{1}} \end{aligned}}$$

(Orthonormality)

(Completeness/ Closure relation)

Linear map

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

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

$$\boxed{\varphi_j = \sum_k T_{jk}\psi_k,} \qquad \boxed{\hat{T}|e_j\rangle = \sum_k T_{kj}|e_k\rangle}$$

(Definition of matrix elements)

$$\hat{T} = \hat{\mathbb{1}}\hat{T}\hat{\mathbb{1}} = \sum_{jk} |e_j\rangle\underbrace{\langle e_j|\hat{T}|e_k\rangle}\langle e_k| = \sum_{jk} T_{jk}|e_j\rangle\langle e_k|$$

Matrix element T_{jk}

Row

Column

(Derive transformation rules from the previous page)

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

Ex Pauli matrices

$$\hat{\sigma}_1 = \hat{\sigma}_x \equiv \hat{X} = |0\rangle\langle 1| + |1\rangle\langle 0| \longleftrightarrow \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

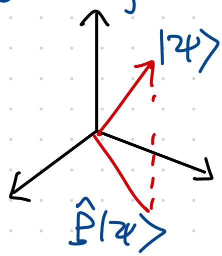
$$\hat{\sigma}_2 \equiv \hat{\sigma}_y \equiv \hat{Y} = -i|0\rangle\langle 1| + i|1\rangle\langle 0| \longleftrightarrow \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$$

$$\hat{\sigma}_3 \equiv \hat{\sigma}_z \equiv \hat{Z} = |0\rangle\langle 0| - |1\rangle\langle 1| \longleftrightarrow \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

Projection operator (1st pass)

Outer products $|\psi\rangle\langle\phi|$ are linear operators e.g. $\hat{\mathbb{1}} = \sum_j |e_j\rangle\langle e_j|$

ONB for a subspace



Index set for the subspace

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

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

Suppose $|\psi\rangle = \sum_k \psi_k |e_k\rangle$, then $\hat{P}|\psi\rangle = \sum_j \psi_j |e_j\rangle$, $j \in S$

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

HW C-T H_{II} Problem 5.

The trace Two equivalent definitions

① $\mathrm{Tr}\,\hat{T} = \sum_j T_{jj}$ (Obviously linear)

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

Let us prove the equivalence only in an ONB (Not ONB ⇒ Need dual basis)

① ⇒ ② $\mathrm{Tr}(|\psi\rangle\langle\phi|) = \sum_j \langle e_j|\psi\rangle\langle\phi|e_j\rangle = \langle\phi|\psi\rangle$

↑ Only in ONB

② ⇒ ① $\mathrm{Tr}\,\hat{T} = \mathrm{Tr}\left[\sum_{jk} T_{jk}|e_j\rangle\langle e_k|\right] = \sum_{jk} T_{jk}\,\mathrm{Tr}(|e_j\rangle\langle e_k|) = \sum_j T_{jj}$

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

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

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

Ex $\mathrm{Tr}[\hat{\sigma}_j,\hat{\sigma}_k] = i\epsilon_{jkl}\,\mathrm{Tr}\,\hat{\sigma}_l = 0$

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

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

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

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

Adjoint Suppose $\hat{T}: V \to W$, $|\psi\rangle \in V$, $|\varphi\rangle = \hat{T}|\psi\rangle \in W$

$\langle\phi| \in W^*$

$$\begin{tikzcd} V \arrow[r, "\hat{T}"] \arrow[dr] & W \arrow[d, "\langle\phi|"] \\ & \mathbb{C} \end{tikzcd}$$

$$\langle\phi|\underbrace{\left(\hat{T}|\psi\rangle\right)}_{W} = \underbrace{\left(\langle\phi|\hat{T}\right)}_{V^*}|\psi\rangle$$

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

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

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

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

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

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

Normal operators: $[\hat{T}, \hat{T}^\dagger] = 0 \iff \hat{T}\hat{T}^\dagger = \hat{T}^\dagger\hat{T}$

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

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

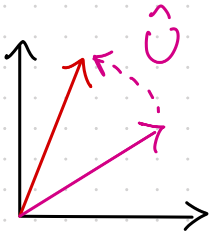
$\hat{T}^{-1}$ = left inverse and right inverse. One implies the other in finite dim but not necessary in ∞ dim.

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

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

$\hat{L} = \hat{R}^\dagger$, $\hat{L}\hat{R} = \mathbb{1}$ but $\hat{R}\hat{L} \neq \mathbb{1}$

Change of basis (Sakurai ed. 3, 1.5.1)



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

Active transformation

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

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

$$\langle e_j|\hat{U}|e_k\rangle = \langle e_j|e'_k\rangle \quad \therefore U \xleftrightarrow{\text{old}} \begin{bmatrix} \langle e_1|e'_1\rangle & \langle e_1|e'_2\rangle & \cdots \\ \langle e_2|e'_1\rangle & \langle e_2|e'_2\rangle & \\ \vdots & & \ddots \end{bmatrix}$$

$|\psi\rangle = \sum_j \psi_j |e_j\rangle$, $\psi_j = \langle e_j|\psi\rangle$ old expansion coefficient

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

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

In particular, to preserve the orthonormality,

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

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

Diagonalization (Spectral theorem)

Motivation: operator functions (C-T B_{II})

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

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

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

Eigenvalue

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

Eigenvector

How to determine the eigenvalues

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

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

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 $|\psi\rangle$ in a set of A-eigenvectors: $|\psi\rangle = \psi_1|a_1\rangle + \psi_2|a_2\rangle + \dots$

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

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

Special case $\hat{A}^\dagger = \hat{A}$; Hermitian $\hat{A}$ is 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

$$\langle a_j|\hat{A}|a_k\rangle \overset{\text{Hermiticity}}{=} \langle a_j|\hat{A}^\dagger|a_k\rangle = \langle a_k|\hat{A}|a_j\rangle^*$$

$$\langle a_j|\hat{A}|a_k\rangle = a_k\langle a_j|a_k\rangle, \qquad \langle a_k|\hat{A}|a_j\rangle^* = a_j^*\langle a_k|a_j\rangle^* = a_j^*\langle a_j|a_k\rangle$$

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

□

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

$\hat{A}|a_j\rangle = a|a_j\rangle$ Eigenvalue equation

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

$\sum_j |a_j\rangle\langle a_j| = \hat{\mathbb{1}}$ Completeness

A-representation

Spectral decomposition

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

P_j Projection onto the degenerate subspace

Degeneracy label

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 $\hat{B}\underbrace{|a\rangle}_{\text{A-eigenvector}}$.

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

→ Diagonalize $\hat{B}$ in this subspace ⇒ Simultaneous eigenvector. □

Properties of continuous "bases" $|x\rangle$ and $|p\rangle$

[They don't lie in the physical Hilbert space]

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

$$\langle x|x'\rangle = \delta(x-x')$$ Delta orthogonality

$$\int dx\, |x\rangle\langle x| = \hat{\mathbb{1}}$$ Completeness

x-representation:

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

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

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

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

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

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

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

$$\int dp\, |p\rangle\langle p| = \int dx \int dx'\, |x\rangle\langle x'| \underbrace{\int \frac{dp}{2\pi\hbar} e^{ip(x-x')/\hbar}}_{\delta(x-x')}$$

$$= \int dx\, |x\rangle\langle x| = \hat{\mathbb{1}}$$

p-representation:

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

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

q-representation of $\hat{A}$, $\hat{A}_{|q\rangle}$, is defined to be

$$\hat{A}_{|q\rangle}\langle q|\psi\rangle \equiv \langle q|\hat{A}|\psi\rangle$$

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

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

$\hat{x}$ in p-representation

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