

Physics 521, Quantum I

Lecture 4: Mathematical Foundations: Operator Algebra

These are important algebraic manipulations of linear operators that will be important in our study of quantum mechanics.

- Adjoint: By definition: $(\hat{A}|u\rangle)^+ = \langle u|\hat{A}^\dagger \Rightarrow (\hat{A}\hat{B})^+ = \hat{B}^\dagger\hat{A}^\dagger$

Proof: Let $|v\rangle = \hat{B}|u\rangle$, $|w\rangle = \hat{A}|v\rangle = \hat{A}\hat{B}|u\rangle$

$$\Rightarrow \langle w| = \langle w|^+ = \langle v|\hat{A}^\dagger = \langle u|\hat{B}^\dagger\hat{A}^\dagger = \langle u|(\hat{A}\hat{B})^+ \text{ q.e.d.}$$

- Commutator:

We can multiply operator through successive maps: $(\hat{A}\hat{B})|u\rangle = \hat{A}(\hat{B}|u\rangle)$

Operator multiplication satisfies associativity, i.e., $\hat{A}(\hat{B}\hat{C}) = (\hat{A}\hat{B})\hat{C}$

However, generally they do not satisfy commutativity

In general, $\hat{A}\hat{B} \neq \hat{B}\hat{A}$: operator order matters?

Define the "commutator" $[\hat{A}, \hat{B}] = \hat{A}\hat{B} - \hat{B}\hat{A} \Rightarrow \hat{A}\hat{B} = \hat{B}\hat{A} + [\hat{A}, \hat{B}]$

Properties of the commutator

- Antisymmetric: $[\hat{A}, \hat{B}] = -[\hat{B}, \hat{A}]$

- Linear: $[c_1\hat{A} + c_2\hat{B}, \hat{C}] = c_1[\hat{A}, \hat{C}] + c_2[\hat{B}, \hat{C}]$

- Product rule: $[\hat{A}, \hat{B}\hat{C}] = [\hat{A}, \hat{B}]\hat{C} + \hat{B}[\hat{A}, \hat{C}]$

- Conjugation: $[\hat{A}, \hat{B}]^+ = -[\hat{A}^\dagger, \hat{B}^\dagger] \Rightarrow$ if \hat{A} and \hat{B} are Hermitian
 $[\hat{A}, \hat{B}]$ is anti-Hermitian

- Jacobi identity: $[\hat{A}, [\hat{B}, \hat{C}]] + [\hat{C}, [\hat{A}, \hat{B}]] + [\hat{B}, [\hat{C}, \hat{A}]] = 0$

Note: The anticommutator is defined $\{\hat{A}, \hat{B}\} = \hat{A}\hat{B} + \hat{B}\hat{A}$

$$\Rightarrow \hat{A}\hat{B} = -\hat{B}\hat{A} + \{\hat{A}, \hat{B}\}$$

The anticommutator is important in the theory of fermions as we will see in 522.

Example: Spin- $\frac{1}{2}$: 2D Hilbert Space, basis: $\{|+\rangle = \text{spin-up along } z$
 $\quad\quad\quad |-\rangle = \text{spin-down along } z\}$

Pauli operators: $\hat{\sigma}_x = |+\rangle\langle -| + |-\rangle\langle +|$, $\hat{\sigma}_y = -i|+\rangle\langle -| + i|-\rangle\langle +|$
 $\hat{\sigma}_z = |+\rangle\langle +| - |-\rangle\langle -|$

Representation in $\{| \pm \rangle\}$ basis

$$\hat{\sigma}_x = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}, \quad \hat{\sigma}_y = \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}, \quad \hat{\sigma}_z = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$$

$$[\hat{\sigma}_i, \hat{\sigma}_j] = 2i\epsilon_{ijk}\hat{\sigma}_k \text{ (using Einstein summation)} \quad \text{e.g. } [\hat{\sigma}_x, \hat{\sigma}_y] = 2i\hat{\sigma}_z$$

$$\text{Check } \hat{\sigma}_x \hat{\sigma}_y = (|+\rangle\langle -| + |-\rangle\langle +|)(-i|+\rangle\langle -| + i|-\rangle\langle +|) = i(|+\rangle\langle +| - |-\rangle\langle -|)$$

$$\hat{\sigma}_y \hat{\sigma}_x = (-i|+\rangle\langle -| + i|-\rangle\langle +|)(|+\rangle\langle -| + |-\rangle\langle +|) = -i(|+\rangle\langle +| - |-\rangle\langle -|)$$

$$\Rightarrow [\hat{\sigma}_x, \hat{\sigma}_y] = 2i(|+\rangle\langle +| - |-\rangle\langle -|) = 2i\hat{\sigma}_z \quad \checkmark$$

$$\text{Using matrices: } \hat{\sigma}_x \hat{\sigma}_y = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix} = \begin{bmatrix} i & 0 \\ 0 & -i \end{bmatrix} = i\hat{\sigma}_z$$

$$\hat{\sigma}_y \hat{\sigma}_x = \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix} \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} = \begin{bmatrix} -i & 0 \\ 0 & i \end{bmatrix} = -i\hat{\sigma}_z$$

$$\text{Anticommutator: } \{\hat{\sigma}_i, \hat{\sigma}_j\} = \delta_{ij}, \quad \hat{\sigma}_x \hat{\sigma}_y + \hat{\sigma}_y \hat{\sigma}_x = 0 \quad \checkmark$$

Eigenvalues and Eigenvectors

Generally $M|u\rangle = |v\rangle$ (map)

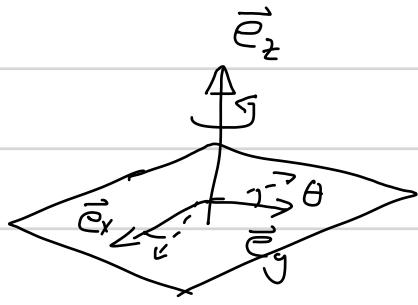
There can exist a set of characteristic (eigen) vectors: $\{|u_\lambda\rangle\}$
such that

$$\boxed{\hat{M}|u_\lambda\rangle = \lambda|u_\lambda\rangle}$$

\hat{M} acts like multiplication
by $\lambda = \text{eigenvalue}$

Note: If $|u_\lambda\rangle$ is an eigenvector of $|u_\lambda'\rangle$ with same eigenvalue..
 $|u_\lambda'\rangle = |\emptyset\rangle$ (null vector of all zeroes) trivial

Example from 3D space \mathbb{R}^3 : Rotation about the z -axis



$$\hat{R}_z(\theta) |e_x\rangle = \cos \theta |e_x\rangle + \sin \theta |e_y\rangle$$

$$\hat{R}_z(\theta) |e_y\rangle = -\sin \theta |e_x\rangle + \cos \theta |e_y\rangle$$

$$\hat{R}_z(\theta) |e_z\rangle = |e_z\rangle$$

$$\Rightarrow \hat{R}_z(\theta) = \begin{bmatrix} \cos \theta & -\sin \theta & 0 \\ \sin \theta & \cos \theta & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

$$\begin{array}{c} \hat{R}_z |e_x\rangle \\ \hat{R}_z |e_y\rangle \\ \hat{R}_z |e_z\rangle \end{array}$$

We immediately see $|e_z\rangle$ is an eigenvector of $\hat{R}_z(\theta)$

$\hat{R}_z(\theta) |e_z\rangle = +|e_z\rangle$, eigenvalue +1 (trivial operation \rightarrow identity)

Can we find other eigenvectors?

Theorem: An operator \hat{M} on a finite d -dimensional Hilbert space has d orthonormal eigenvectors iff $[\hat{M}, \hat{M}^\dagger] = 0$ (\hat{M} is called "normal")

Examples of normal operators:

- Hermitian operators $\hat{M} = \hat{M}^\dagger \Rightarrow [\hat{M}, \hat{M}^\dagger] = 0$

- Unitary operators $\hat{U}^\dagger \hat{U} = \hat{U} \hat{U}^\dagger = \hat{\mathbb{1}} \Rightarrow [\hat{U}, \hat{U}^\dagger] = 0$

$\hat{R}_z(\theta)$ is a unitary operator, $\hat{R}_z^{-1}(\theta) = \hat{R}_z(-\theta) = \hat{R}_z^T(\theta) = \hat{R}_z^+(\theta)$
(since real)

(Typically, we would call $\hat{R}_z(\theta)$ an "orthogonal matrix"

defined by $\hat{O}^{-1} = \hat{O}^T$, but orthogonal matrices are unitary when everything is real)

$\Rightarrow \hat{R}_z(\theta)$ has 3 eigenvectors that can form an orthonormal basis.

The general procedure for finding eigenvalues + eigenvectors is as follows.

Note: $\hat{M}|u_\lambda\rangle = \lambda|u_\lambda\rangle = \lambda\hat{1}|u_\lambda\rangle \Rightarrow (\hat{M} - \lambda\hat{1})|u_\lambda\rangle = |\phi\rangle$ (null vector)

Since $|u_\lambda\rangle \neq |\phi\rangle \Rightarrow (\hat{M} - \lambda\hat{1})$ is "singular" \Rightarrow it has no inverse

$\Rightarrow \det(\hat{M} - \lambda\hat{1}) = 0$ = Characteristic equation

- $\det(\hat{M} - \lambda\hat{1})$ is a d^{th} -order polynomial (characteristic polynomial).
- The d roots of the polynomial are the d eigenvalues.
 - If two eigenvalues are equal they are said to be **degenerate**.
 - If the characteristic polynomial is real and the eigenvalues are complex they come in conjugate pairs.

For the rotation operator, the characteristic equation is

$$\det \begin{bmatrix} \cos\theta - \lambda & -\sin\theta & 0 \\ \sin\theta & \cos\theta - \lambda & 0 \\ 0 & 0 & 1 - \lambda \end{bmatrix} = 0$$

$$\Rightarrow [(\cos\theta - \lambda)^2 + \sin^2\theta](1 - \lambda) = 0$$

Roots (eigenvalues): $1 - \lambda = 0 \Rightarrow \lambda = 1$

$$\lambda^2 - 2\cos\theta\lambda + 1 = 0 \Rightarrow \lambda_{\pm} = \cos\theta \pm \sqrt{\cos^2\theta - 1} = \cos\theta \pm i\sin\theta = e^{\pm i\theta}$$

Eigenvectors:

$$\lambda = 1: \quad |u_1\rangle = |e_z\rangle \quad (\text{by inspection})$$

$$\lambda_{\pm} = e^{\pm i\theta}$$

$$\begin{bmatrix} \cos\theta - e^{\pm i\theta} & -\sin\theta & 0 \\ \sin\theta & \cos\theta - e^{\mp i\theta} & 0 \\ 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} |u_x^{(\pm)}\rangle \\ |u_y^{(\pm)}\rangle \\ |u_z^{(\pm)}\rangle \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0 \end{bmatrix}$$

$$U_z^\pm = 0$$

$$\sin \theta \begin{bmatrix} -i & -1 \\ 1 & -i \end{bmatrix} \begin{bmatrix} U_x^{(\pm)} \\ U_y^{(\pm)} \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix}$$

$$\text{For } \theta \neq 0 \quad \mp i U_x^{(\pm)} - U_y^{(\pm)} = 0 \Rightarrow U_y^{(\pm)} = \mp i U_x^{(\pm)}$$

$$\Rightarrow |U^{(\pm)}\rangle = N_\pm \left(|e_x\rangle \mp i |e_y\rangle \right)$$

"Normalization constant"

$$\langle U^{(\pm)} | U^{(\pm)} \rangle = N_\pm^2 (\langle e_x | e_x \rangle + (-i)(+i) \langle e_y | e_y \rangle) = 2N_\pm^2$$

We "normalize" the eigenvector by setting $\langle U_\lambda | U_\lambda \rangle = 1$

$$\Rightarrow N_\pm = \frac{1}{\sqrt{2}}$$

\Rightarrow Eigenvalues and corresponding eigenvectors of a rotation about the z-axis by angle θ :

$$\{e^{-i\theta}, e^{i\theta}, 1\}; \left\{ \frac{|e_x\rangle + i|e_y\rangle}{\sqrt{2}}, \frac{|e_x\rangle - i|e_y\rangle}{\sqrt{2}}, |e_z\rangle \right\}$$

(Aside: we recognize the eigenvectors $\frac{|e_x\rangle \pm i|e_y\rangle}{\sqrt{2}}$ as circular polarization)

The eigenvectors of \hat{R}_z form an orthonormal basis as they must (since \hat{R}_z is unitary)

Diagonalization

The eigenvectors of a normal matrix \hat{M} form an orthonormal basis (a "complete set").

$$\Rightarrow \hat{1} = \sum_{\lambda}^{\text{def}} |U_\lambda\rangle \langle U_\lambda|$$

We can write a representation of \hat{M} in the basis of its eigenvectors

$$\hat{M} = \hat{1} \hat{M} \hat{1} = \sum_{\lambda} |U_\lambda\rangle \langle U_\lambda| \hat{M} |U_{\lambda'}\rangle \langle U_{\lambda'}| = \sum_{\lambda} \lambda \underbrace{|U_\lambda\rangle \langle U_\lambda|}_{\delta_{\lambda\lambda'} \text{ (orthonormal)}} \langle U_{\lambda'} |$$

$$\Rightarrow \boxed{\hat{M} = \sum_{\lambda} \lambda |U_\lambda\rangle \langle U_\lambda|} \quad \hat{M} \text{ is a diagonal matrix in the basis of its eigenvalues}$$

The process of finding the eigenvectors and eigenvalues is often known as "diagonalization." We thus can perform a unitary transformation (similarity transformation) from a normal matrix to a diagonal matrix.

Nature of the eigenvalues

- For a Unitary operator, $\hat{U}|u_\lambda\rangle = \lambda|u_\lambda\rangle$, $\langle u_\lambda|\hat{U}^\dagger = \lambda^* \langle u_\lambda|$
 $\Rightarrow \langle u_\lambda|\hat{U}^\dagger \hat{U}|u_\lambda\rangle = |\lambda|^2 \langle u_\lambda|u_\lambda\rangle = |\lambda|^2$ but $\hat{U}^\dagger \hat{U} = \hat{1} \Rightarrow \langle u_\lambda|\hat{U}^\dagger \hat{U}|u_\lambda\rangle = 1$
 \Rightarrow The eigenvalues of \hat{U} satisfy $|\lambda|=1 \Rightarrow$ eigenvalues are phases $e^{i\theta}$

- For a Hermitian operator $\hat{A} = \hat{A}^\dagger$, Let $\hat{A}|a\rangle = a|a\rangle$
normalized eigenvector labeled by eigenvalue

Consider $\langle a|\hat{A}|a\rangle = a$, $\langle a|\hat{A}|a\rangle^* = \langle a|\hat{A}^\dagger|a\rangle = a^* = \langle a|\hat{A}|a\rangle = a$

\Rightarrow The eigenvalues of a Hermitian matrix are real numbers

\Rightarrow Eigenvalue decomposition $\hat{A} = \sum_a a|a\rangle\langle a|$ (diagonal matrix with real eigenvalues).

The eigenvectors associated with different eigenvalues must be orthogonal

Proof: Consider $\hat{A}|a\rangle = a|a\rangle$ and $\hat{A}|a'\rangle = a'|a'\rangle$ with $a \neq a'$

$$\Rightarrow \langle a|\hat{A}|a\rangle = \langle a'|\hat{A}|a\rangle = a \langle a'|a\rangle = \langle a'|\hat{A}|a\rangle = a' \langle a'|a\rangle$$

(since $\langle a'|\hat{A} = (\hat{A}|a'\rangle)^+ = (a'|a'\rangle)^+ = \langle a'|a'$ (real a'))

$$\Rightarrow (a-a') \langle a'|a\rangle = 0, \text{ but since } a \neq a' \Rightarrow \langle a|a'\rangle = 0 \Rightarrow \text{orthogonal (q.e.d.)}$$

\Rightarrow If all of eigenvectors of a Hermitian operator are nondegenerate, they form an orthogonal basis, and can be normalized to an orthonormal basis.

The case of degeneracies

Suppose for a given eigenvalue λ of a normal operator \hat{M} , there are g_λ different eigenvectors (different means not parallel to one another) $\{|u_\lambda^{(i)}\rangle \mid i=1, 2, \dots, g_\lambda\}$

$$\Rightarrow \hat{M}|u_\lambda^{(i)}\rangle = \lambda|u_\lambda^{(i)}\rangle$$

Since $\{|u_\lambda^{(i)}\rangle\}$ are linearly independent, they span a subspace of \mathcal{H} of $\dim g_\lambda$.

\Rightarrow Any vector $|v_\lambda\rangle = \sum_{i=1}^{g_\lambda} \alpha_i |u_\lambda^{(i)}\rangle$ is also an eigenvector of \hat{M} with eigenvalue λ .

$\Rightarrow \{|u_\lambda^{(i)}\rangle\}$ spans an "eigensubspace" \mathcal{H}_λ .

\Rightarrow We can always find an orthonormal basis of eigenvectors, by choosing an orthonormal basis for the spaces \mathcal{H}_λ . Note, vectors in different subspaces, with different values of λ are orthogonal by the argument above (nondegenerate eigenvectors are orthogonal).

\Rightarrow There always exists an orthonormal basis of eigenvectors $\{|e_\lambda^{(i)}\rangle\}$

$$\langle e_\lambda^{(i)} | e_\lambda^{(j)} \rangle = \delta_{ij}, \quad \delta_{ii}$$

For a given λ $\{|e_\lambda^{(i)}\rangle \mid i=1, 2, \dots, g_\lambda\}$ spans a subspace \mathcal{H}_λ of dimension g_λ .

The different subspaces are orthogonal: $\mathcal{H}_\lambda \perp \mathcal{H}_{\lambda'}$ if $\lambda \neq \lambda'$

We can form a resolution of the identity:

$$\hat{1} = \sum_{\lambda} \sum_{i=1}^{g_\lambda} |e_\lambda^{(i)}\rangle \langle e_\lambda^{(i)}| = \sum_{\lambda} \hat{P}_\lambda$$

$\hat{P}_\lambda = \sum_{i=1}^{g_\lambda} |e_\lambda^{(i)}\rangle \langle e_\lambda^{(i)}|$ is a "projection operator" — it acts to "project" a vector onto the subspace \mathcal{H}_λ . $\hat{P}_\lambda |v\rangle = \sum_{i=1}^{g_\lambda} \langle e_\lambda^{(i)} | v \rangle |e_\lambda^{(i)}\rangle \in \mathcal{H}_\lambda$

The projection operators satisfies $\hat{P}_\lambda = \hat{P}_\lambda^+$ $\hat{P}_\lambda \hat{P}_{\lambda'} = \delta_{\lambda\lambda'} \quad (\text{orthogonal projection})$

The total Hilbert space is said to be the "direct sum" of all the orthogonal eigensubspaces:

$$\mathcal{H} = \bigoplus_{\lambda} \mathcal{H}_\lambda$$

"direct sum" = union

The matrix representation of \hat{M} in the basis of its eigenvalues has diagonal blocks

$$\hat{M} = \begin{bmatrix} \lambda_1 & & & & & \\ & \ddots & & & & \\ & & \lambda_2 & & & \\ & & & \ddots & & \\ & & & & \lambda_2 & \\ & & & & & \ddots \\ & & & & & & \lambda_3 \\ & & & & & & & \ddots \\ & & & & & & & & \lambda_3 \end{bmatrix} \quad \begin{array}{l} \leftarrow \text{eigenvalue } \lambda_1: \text{Nondegenerate} \\ \leftarrow \text{eigenvalue } \lambda_2: \text{triply degenerate} \\ \leftarrow \text{eigenvalue } \lambda_3: \text{doubly degenerate} \end{array}$$

zeros in all other elements

Commuting operators and eigenspaces

Consider two Hermitian operators that commute: $[\hat{A}, \hat{B}] = 0$

Suppose $|a\rangle$ is an eigenvector of \hat{A} , $\hat{A}|a\rangle = a|a\rangle \Rightarrow \hat{B}|a\rangle$ is an eigenvector of \hat{A} with the same eigenvalue: $\hat{A}(\hat{B}|a\rangle) = \hat{B}(\hat{A}|a\rangle) = a(\hat{B}|a\rangle)$ q.e.d.

If $|a\rangle$ is a nondegenerate eigenvector $\Rightarrow \hat{B}|a\rangle \propto |a\rangle \Rightarrow |a\rangle$ is also an eigenvector of \hat{B} , with a nondegenerate eigenvalue b . Thus we can write the vector $|a, b\rangle$ s.t. $\hat{A}|a, b\rangle = a|a, b\rangle$, $\hat{B}|a, b\rangle = b|a, b\rangle$

If $|a\rangle$ is degenerate, then we can say that $\hat{B}|a\rangle \in \mathcal{H}_a$, the eigensubspace spanned by the degenerate eigenvectors with eigenvalue a .

Note: If $|a\rangle$ and $|a'\rangle$ are nondegenerate $\Rightarrow \langle a'|\hat{B}|a\rangle = 0$

Thus, in the basis of eigenvectors of \hat{A} , $\{|a\rangle\}$, if $[\hat{A}, \hat{B}] = 0$, then the representation of \hat{B} will be "block diagonal"

$$\hat{B} = \begin{bmatrix} \hat{B}_1 & & & & & \\ & \ddots & & & & \\ & & \hat{B}_2 & & & \\ & & & \ddots & & \\ & & & & \hat{B}_3 & \\ & & & & & \ddots \end{bmatrix} \quad \begin{array}{l} \leftarrow \mathcal{H}_1 \\ \leftarrow \mathcal{H}_2 \\ \leftarrow \mathcal{H}_3 \end{array} = \hat{B}_1 \oplus \hat{B}_2 \oplus \hat{B}_3$$

The operators $\hat{B}_a = \hat{P}_a \hat{B} \hat{P}_a$ (\hat{B} projected in subspace \mathcal{H}_a) can each be diagonalized. Thus, with a subspace \mathcal{H}_a of degeneracy g_a , there are g_a eigenvectors of \hat{B} .

\Rightarrow If $[\hat{A}, \hat{B}] = 0$, there exist a set of common eigenvectors of \hat{A} and \hat{B} . We often say that \hat{A} and \hat{B} are mutually diagonalizable in the same basis.

Note: If $[\hat{A}, \hat{B}] \neq 0$, it doesn't mean that they can't share any eigenvectors. However they cannot share all eigenvectors. For if they did, they would be diagonal in the same basis, and thus they would commute.

Complete Set of Commuting Operators:

Now after we diagonalize \hat{B}_a , it might be the case that some of its eigenvectors are degenerate. In that case, the eigenvector is not uniquely specified by the two eigenvalues a and b . However, this means that there can be a third operator \hat{C} which mutually commutes with \hat{A} and \hat{B} : $[\hat{A}, \hat{B}] = [\hat{A}, \hat{C}] = [\hat{C}, \hat{B}] = 0$. In the subspaces $\hat{P}_{a,b}$, \hat{C} will be block diagonal. We can then diagonalize $\hat{C}_{a,b}$, and keep going until we have no more degeneracy.

\Rightarrow A complete set of mutually commuting operators $\{\hat{A}, \hat{B}, \hat{C}, \dots\}$ is the minimal set of normal operators that all commute with one another such that the common eigenvectors of all the operators are uniquely specified. I.e., there is only one vector $|a, b, c, \dots\rangle$ (up to multiplication by a scalar) such that

$$\hat{A}|a, b, c, \dots\rangle = a|a, b, c, \dots\rangle$$

$$\hat{B}|a, b, c, \dots\rangle = b|a, b, c, \dots\rangle$$

$$\hat{C}|a, b, c, \dots\rangle = c|a, b, c, \dots\rangle$$

The collection of eigenvalues $\{a, b, c, \dots\}$ specify the state.