

Lecture 4: Foundations Continued

Eigenvalues and diagonal representations

Given an operator \hat{A} , its "characteristic" equation

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

\uparrow eigenvector \uparrow eigenvalue

Here I am using a short hand of labeling the eigenvectors by their eigenvalues.

A Hermitian operator is self-adjoint $\hat{A} = \hat{A}^\dagger$
The operators have real eigenvalues

Proof: $\langle a|\hat{A}|a\rangle = a \langle a|a\rangle$
 $\Rightarrow \langle a|\hat{A}|a\rangle^* = \langle a|\hat{A}^\dagger|a\rangle = a^* \langle a|a\rangle^*$

But $\hat{A} = \hat{A}^\dagger$ and $\langle a|a\rangle^* = \langle a|a\rangle$

$\Rightarrow a = a^*$ a is real

Theorem: The eigenvectors associated with non-degenerate eigenvalues of a Hermitian operator are orthogonal

Proof: Consider $\langle a'| \hat{A} |a\rangle$ where $\hat{A}|a\rangle = a|a\rangle$
 $\hat{A}|a'\rangle = a'|a'\rangle$

$$\begin{aligned} \langle a'| \hat{A} |a\rangle &= \langle a'| (\hat{A} |a\rangle) = a \langle a'|a\rangle \\ &= (\langle a'| \hat{A}) |a\rangle = a' \langle a'|a\rangle \end{aligned}$$

If $a \neq a'$ $\Rightarrow \langle a'|a\rangle = 0$

The set of eigenvectors form a resolution of the identity (we will prove this)

$$\hat{1} = \sum_a |a\rangle\langle a|$$

• $\{|a\rangle\}$ = orthonormal basis

$$\hat{A} = \hat{1} \hat{A} \hat{1} = \sum_{a,a'} |a\rangle\langle a| \hat{A} |a'\rangle\langle a'| = \sum_a a |a\rangle\langle a|$$

Action of \hat{A} = Project onto eigenvector $|a\rangle$ and multiply by eigenvalue a

Matrix representation of \hat{A} in basis of eigenvectors

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

$$\hat{A} \equiv \begin{bmatrix} a_1 & & & 0 \\ & a_2 & & \\ & & a_3 & \\ 0 & & & \dots \end{bmatrix} \quad \begin{array}{l} \text{Diagonal} \\ \text{Matrix} \end{array}$$

Finding eigenvalues of $\hat{A} \equiv$ "diagonalizing the matrix"

Diagonalizing a matrix

Not every matrix has a complete set of eigenvectors and eigenvalues. Thus that are called "normal operators" which satisfy

$$[\hat{A}, \hat{A}^\dagger] = 0$$

Examples of normal operators: Hermitian $\hat{A} = \hat{A}^\dagger$
Unitary $\hat{U}^\dagger \hat{U} = \hat{U} \hat{U}^\dagger = \hat{1}$

Given a normal operator in finite dimension D we can find all of the eigenvalues and eigenvectors through the process of diagonalization.

Consider a normal operator \hat{O} where

$$\hat{O}|\lambda\rangle = \lambda|\lambda\rangle \quad \text{where } |\lambda\rangle \neq \text{zero vector}$$

$$\Rightarrow (\hat{O} - \lambda \hat{1})|\lambda\rangle = 0$$

Since $|\lambda\rangle \neq 0$ vector $\hat{O} - \lambda \hat{1}$ is not invertible

$$\det[\hat{O} - \lambda \hat{1}] = 0 \quad (\text{from linear algebra})$$

Characteristic polynomial D roots \Rightarrow eigenvalues

Example: 2D Rotation matrix in real space is a normal matrix

$$\hat{R}^\dagger = \hat{R}^T \quad \hat{R}^T \hat{R} = \hat{1} \quad \Rightarrow [\hat{R}, \hat{R}^\dagger] = 0 \quad \checkmark$$

The matrix representation w.r.t. $\{|e_x\rangle, |e_y\rangle\}$ basis

$$\hat{R} = \begin{bmatrix} \cos\theta & -\sin\theta \\ \sin\theta & \cos\theta \end{bmatrix}$$

Characteristic equation

$$\det(\hat{R} - \lambda \hat{I}) = \det \begin{bmatrix} \cos\theta - \lambda & -\sin\theta \\ \sin\theta & \cos\theta - \lambda \end{bmatrix} = (\cos\theta - \lambda)^2 + \sin^2\theta$$

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

\Rightarrow Rotation operator has complex eigenvalues

\Rightarrow Must think now in a complex vector space

\Rightarrow There are no real vectors that are eigenvectors of \hat{R} unless $\theta = m\pi$ (makes sense geometrically)

Define eigenvectors of \hat{R} . $\hat{R}|\pm\rangle = e^{\mp i\theta}|\pm\rangle$

(sign choice will become clear below).

To find these eigenvectors, we expand them in the $|e_x\rangle, |e_y\rangle$ basis

$$|\pm\rangle \doteq \begin{bmatrix} \alpha_{\pm} \\ \beta_{\pm} \end{bmatrix}$$

$$\hat{R}|\pm\rangle = \begin{bmatrix} \cos\theta & -\sin\theta \\ \sin\theta & \cos\theta \end{bmatrix} \begin{bmatrix} \alpha_{\pm} \\ \beta_{\pm} \end{bmatrix} = e^{\mp i\theta} \begin{bmatrix} \alpha_{\pm} \\ \beta_{\pm} \end{bmatrix}$$

$$\Rightarrow \begin{cases} \cos\theta \alpha_{\pm} - \sin\theta \beta_{\pm} = e^{\mp i\theta} \alpha_{\pm} = \cos\theta \alpha_{\pm} \mp i \sin\theta \alpha_{\pm} \\ \sin\theta \alpha_{\pm} + \cos\theta \beta_{\pm} = e^{\mp i\theta} \beta_{\pm} = \cos\theta \beta_{\pm} \mp i \sin\theta \beta_{\pm} \end{cases}$$

Both of these equations lead to the same thing (as they must).

$$\Rightarrow \frac{\beta_{\pm}}{\alpha_{\pm}} = \pm i$$

Because $|\lambda\rangle$ and $C|\lambda\rangle$ are both eigenvectors with same eigenvalue, we fix $|C|$ by normalization. The phase is arbitrary and of no physical importance in quantum mechanics

Thus let $\alpha_{\pm} = 1 \Rightarrow \beta_{\pm} = \pm i$

$$|\pm\rangle \doteq \begin{bmatrix} 1 \\ \pm i \end{bmatrix} \xrightarrow{\text{normalize}} |\pm\rangle = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ \pm i \end{bmatrix}$$

$$\Rightarrow |\pm\rangle = \frac{|e_x\rangle \pm i|e_y\rangle}{\sqrt{2}} \quad \left(\text{Normalized eigenvectors of the rotation operator in 2D} \right)$$

We recognize this from optics as circular polarization!

The combination $x \pm iy$ is very important in the theory of rotations of functions around the z -axis. Stay tuned.

Change of basis

Given a matrix representation in one basis, we can transform this matrix to a different basis using a "similarity transformation"

We can use Dirac notation to make our lives easier.

Let $\{|\alpha\rangle\}$ be one orthonormal basis

$\{|\alpha'\rangle\}$ be another orthonormal basis

$A_{\alpha'\alpha} = \langle \alpha' | \hat{A} | \alpha \rangle$ are the matrix elements in basis - 1

$A_{i'i} = \langle i' | \hat{A} | i \rangle$ are the matrix elements in basis - 2

Use the completeness relation to transform between basis

$$A_{\alpha'\alpha} = \langle \alpha' | \hat{1} \hat{A} \hat{1} | \alpha \rangle = \sum_{i,i'} \langle \alpha' | i' \rangle \underbrace{\langle i' | \hat{A} | i \rangle}_{A_{i'i}} \langle i | \alpha \rangle$$

Let $U_{i\alpha} = \langle i | \alpha \rangle$. These numbers when put in a row-column array form the elements of unitary matrix

$$(U^\dagger)_{\alpha'i'} = U_{i\alpha'}^* = \langle i' | \alpha' \rangle^* = \langle \alpha' | i' \rangle$$

$$\text{Thus } A_{\alpha'\alpha} = \sum_{i,i'} U_{\alpha'i'}^\dagger A_{i'i} U_{\alpha i}$$

$$\begin{aligned} \text{The matrix is unitary } (U^\dagger U)_{\alpha'\alpha} &= \sum_i U_{\alpha'i}^\dagger U_{i\alpha} = \sum_i \langle \alpha' | i \rangle \langle i | \alpha \rangle \\ &= \langle \alpha' | \alpha \rangle = \delta_{\alpha'\alpha} \Rightarrow U^\dagger U = \mathbb{1} \end{aligned}$$

Since $U^\dagger = U^{-1}$, this is a similarity transformation

There is another way to look at this. Consider the active basis map

$$\text{e.g. } \hat{U} = |+\rangle\langle e_x| + |-\rangle\langle e_y| \quad \left(\begin{array}{l} \text{maps one basis} \\ \text{to another} \end{array} \right)$$

the representation in $\{|e_x\rangle, |e_y\rangle\}$ basis

$$U_{xx} = \langle e_x | \hat{U} | e_x \rangle = \langle e_x | + \rangle, \quad U_{xy} = \langle e_x | \hat{U} | e_y \rangle = \langle e_x | - \rangle$$

$$U_{yx} = \langle e_y | \hat{U} | e_x \rangle = \langle e_y | + \rangle, \quad U_{yy} = \langle e_y | \hat{U} | e_y \rangle = \langle e_y | - \rangle$$

$$\Rightarrow \hat{U} = \begin{bmatrix} \langle e_x | + \rangle & \langle e_x | - \rangle \\ \langle e_y | + \rangle & \langle e_y | - \rangle \end{bmatrix} : \text{Change of basis matrix} \\ x, y \Rightarrow +, -$$

Let us "diagonalize" $\tilde{R}^{(x,y)}$ by a similarity transformation

$$U = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 1 \\ i & -i \end{bmatrix} \Rightarrow \tilde{R}^{(+,-)} = U^\dagger \tilde{R}^{(x,y)} U$$

$$\begin{aligned} \Rightarrow \tilde{R}^{(+,-)} &= \frac{1}{2} \begin{bmatrix} 1 & -i \\ 1 & +i \end{bmatrix} \begin{bmatrix} \cos\theta & -\sin\theta \\ \sin\theta & \cos\theta \end{bmatrix} \begin{bmatrix} 1 & 1 \\ i & -i \end{bmatrix} = \frac{1}{2} \begin{bmatrix} 1 & -i \\ 1 & +i \end{bmatrix} \begin{bmatrix} e^{-i\theta} & e^{i\theta} \\ ie^{-i\theta} & -ie^{i\theta} \end{bmatrix} \\ &= \begin{bmatrix} e^{-i\theta} & 0 \\ 0 & e^{i\theta} \end{bmatrix} \quad \text{q.e.d.} \end{aligned}$$

Infinite dimensional Hilbert Space and Continuous Variables

In our discussion of matrix mechanics, we have focussed on finite dimensional Hilbert spaces. The Hilbert space we have encountered so far, $L_2(\mathbb{R})$, square normalizable complex functions on the real line, is an infinite dimensional Hilbert space. Such Hilbert spaces are much more complicated than the finite dimensional case, with many subtleties that we won't fully address here.

One particular difference is the existence of operators with a continuous spectrum

Consider the position and momentum operators \hat{x} and \hat{p} they have eigenvectors and eigenvalues: $\hat{x}|x\rangle = x|x\rangle$, $\hat{p}|p\rangle = p|p\rangle$. Here the eigenvalues are continuous variables $-\infty \leq x \leq \infty$, $-\infty \leq p \leq \infty$ on the real line. Thus the elements of these bases are not countable as the representations of vectors or operators in these bases are not matrices.

These are bases, nonetheless, in the sense that they span the space. The most important manifestation of this fact are the "completeness relations" which are now expressed as integrals rather than sums

$$\int_{-\infty}^{\infty} dx |x\rangle\langle x| = \hat{1}, \quad \int_{-\infty}^{\infty} dp |p\rangle\langle p| = \hat{1}$$

These bases are orthonormal in the Dirac delta sense $\langle x'|x\rangle = \delta(x-x')$, $\langle p'|p\rangle = \delta(p'-p)$.

Note these continuous variable kets have units $|x\rangle = \frac{1}{\sqrt{\text{length}}}$, $|p\rangle = \frac{1}{\sqrt{\text{momentum}}}$

Using the completeness, we can decompose vectors and operators in these bases

$$|\psi\rangle = \hat{1}|\psi\rangle = \int_{-\infty}^{\infty} dx |x\rangle \underbrace{\langle x|\psi\rangle}_{\psi(x)} = \int_{-\infty}^{\infty} dx \psi(x) |x\rangle$$

Position-space wave function

$$|\psi\rangle = \hat{1}|\psi\rangle = \int_{-\infty}^{\infty} dp |p\rangle \underbrace{\langle p|\psi\rangle}_{\tilde{\psi}(p)} = \int_{-\infty}^{\infty} dp \tilde{\psi}(p) |p\rangle$$

Momentum-space wave function

The wave functions are functions of continuous variables, rather than entries in a column vector with a discrete index.

Change of basis: $|x\rangle \Leftrightarrow |p\rangle$

$$\psi(x) = \langle x|\psi\rangle = \langle x|\hat{1}|\psi\rangle = \int dp \langle x|p\rangle \underbrace{\langle p|\psi\rangle}_{\tilde{\psi}(p)}$$

The representation of one basis in another allows us to change basis. Here instead of matrices we have the function $\langle x|p\rangle = \psi_p(x) = \frac{1}{\sqrt{2\pi\hbar}} e^{ipx/\hbar}$. Plane wave = wave function of momentum eigenstate

$$\Rightarrow \psi(x) = \int \frac{dp}{\sqrt{2\pi\hbar}} e^{ipx/\hbar} \tilde{\psi}(p) \quad (\text{inverse Fourier transform}).$$

$$\text{Similarly, } \tilde{\psi}(p) = \langle p|\psi\rangle = \langle p|\hat{1}|\psi\rangle = \int dx \langle p|x\rangle \langle x|\psi\rangle = \int dx \frac{e^{-ipx/\hbar}}{\sqrt{2\pi\hbar}} \psi(x) \quad (\text{Fourier transform})$$

We can also see how inner products can be calculated using wave functions:

$$\begin{aligned} \langle \psi_1|\psi_2\rangle &= \int dx \langle \psi_1|x\rangle \langle x|\psi_2\rangle = \int dx \psi_1^*(x) \psi_2(x) \\ &= \int dp \langle \psi_1|p\rangle \langle p|\psi_2\rangle = \int dp \tilde{\psi}_1^*(p) \tilde{\psi}_2(p) \end{aligned}$$

$$\|\psi\|^2 = \langle \psi|\psi\rangle = \int dx \psi^*(x) \psi(x) = \int dx |\psi(x)|^2 = \int dp \tilde{\psi}^*(p) \tilde{\psi}(p) = \int dp |\tilde{\psi}(p)|^2 \quad (\text{Parseval's theorem}).$$

Operators The continuous variable analog of the matrix elements:

$$\text{In the basis of its eigenvectors: } \langle x'|\hat{x}|x\rangle = x \langle x'|x\rangle = x \delta(x-x')$$

$$\langle p'|\hat{p}|p\rangle = p \langle p'|p\rangle = p \delta(p-p')$$

$$\Rightarrow \hat{x} = \int dx x |x\rangle \langle x|, \quad \hat{p} = \int dp p |p\rangle \langle p| \quad (\text{like diagonal matrices})$$

Now consider position representation of the momentum operator

$$\begin{aligned} \langle x|\hat{p}|x'\rangle &= \int dp p \langle x|p\rangle \langle p|x'\rangle = \int dp p \frac{e^{-ip(x'-x)/\hbar}}{2\pi\hbar} = \left(\frac{1}{2\pi\hbar}\right) \left(\frac{-\hbar}{i} \frac{\partial}{\partial x'}\right) \int dp e^{\frac{-i}{\hbar} p(x'-x)} \\ &= \frac{1}{2\pi\hbar} \frac{-\hbar}{i} \frac{\partial}{\partial x'} \left[2\pi \delta\left(\frac{x-x'}{\hbar}\right) \right] = \boxed{\frac{-\hbar}{i} \frac{\partial}{\partial x'} \delta(x'-x)} \quad \text{Derivative of a delta function} \end{aligned}$$

Like the delta-function itself, this is a tempered distribution, which only makes sense inside an integral. Thus, if $\psi(x) = \langle x|\psi\rangle$,

$$\langle x|\hat{p}|\psi\rangle = \int dx' \langle x|\hat{p}|x'\rangle \langle x'|\psi\rangle = \int dx' \frac{-\hbar}{i} \frac{\partial}{\partial x'} \delta(x'-x) \psi(x') \stackrel{\text{integration by parts}}{\downarrow} \int dx' \delta(x'-x) \frac{\hbar}{i} \frac{\partial \psi(x')}{\partial x'} = \frac{\hbar}{i} \frac{\partial \psi}{\partial x}$$

As expected

This is the formal way of showing $\hat{p} = \frac{\hbar}{i} \frac{\partial}{\partial x}$ as we did in 491
 Similarly we will find $\hat{x} = \frac{\hbar}{i} \frac{\partial}{\partial p}$ in momentum space. More formally

$$\langle p | \hat{x} | p' \rangle = \frac{\hbar}{i} \frac{\partial}{\partial p} \delta(p - p') \Rightarrow \langle p | \hat{x} | \psi \rangle = \frac{\hbar}{i} \frac{\partial}{\partial p} \tilde{\psi}(p)$$

Parity

In Quantum I we introduced the parity operator $\hat{\Pi}$ which reflects position and momenta. Classically $\Pi: x \rightarrow -x$, $\Pi: p \rightarrow -p$. Quantumly

$$\hat{\Pi} |x\rangle = |-x\rangle, \quad \hat{\Pi} |p\rangle = |-p\rangle$$

We can thus define $\hat{\Pi}$ in the position and momentum bases

$$\hat{\Pi} = \int dx | -x \rangle \langle x | = \int dp | -p \rangle \langle p |$$

Note $\hat{\Pi}^\dagger = \int dx |x\rangle \langle -x| = \hat{\Pi}$ (Hermitian), $\hat{\Pi}^2 = \hat{1}$.

$\Rightarrow \hat{\Pi}$ is Hermitian and Unitary. Its eigenvalues are ± 1 (even/odd parity)

$$\langle x | \hat{\Pi} = (\hat{\Pi}^\dagger |x\rangle)^\dagger = (\hat{\Pi} | -x \rangle)^\dagger = | -x \rangle = \langle -x |$$

Thus, if $\psi(x) = \langle x | \psi \rangle$, then $\langle x | \hat{\Pi} | \psi \rangle = \psi(-x)$

$$\left. \begin{aligned} \text{Note } \hat{\Pi}^\dagger \hat{x} \hat{\Pi} &= \int dx |x\rangle \langle -x| \hat{x} | -x \rangle \langle x| = - \int dx x |x\rangle \langle x| = -\hat{x} \\ \hat{\Pi}^\dagger \hat{p} \hat{\Pi} &= -\hat{p} \end{aligned} \right\} \text{Unitary transformation}$$

Hamiltonian: $\hat{H} = \frac{\hat{p}^2}{2m} + V(\hat{x}) \Rightarrow \hat{\Pi}^\dagger \hat{H} \hat{\Pi} = \frac{\hat{p}^2}{2m} + V(-\hat{x})$

Proof: For any unitary operator $\hat{U}^\dagger \hat{A} \hat{U} = (\hat{U}^\dagger \hat{A} \hat{U})^n$ since $\hat{U}^\dagger \hat{U} = \hat{1}$

By performing a power series $\hat{U}^\dagger f(\hat{A}) \hat{U} = f(\hat{U}^\dagger \hat{A} \hat{U})$

$$\Rightarrow \hat{\Pi}^\dagger \hat{p}^2 \hat{\Pi} = (-\hat{p})^2 = \hat{p}^2, \quad \hat{\Pi}^\dagger V(\hat{x}) \hat{\Pi} = V(-\hat{x})$$

If the potential is reflection symmetric, $V(-\hat{x}) = V(\hat{x})$

$$\Rightarrow \hat{\Pi}^\dagger \hat{H} \hat{\Pi} = \hat{H} \text{ (parity invariant)} \Rightarrow \hat{H} \hat{\Pi} = \hat{\Pi} \hat{H}$$

$$\Rightarrow \boxed{[\hat{H}, \hat{\Pi}] = 0} \text{ if potential reflection symmetric}$$

⇒ For a reflection (parity) symmetric potential, there exist simultaneous eigenstates of \hat{H} and $\hat{\Pi}$: energy eigenstates are even or odd parity.

Countable bases in infinite dimensions

In an infinite dimensional Hilbert space, such as $L_2(\mathbb{R})$, we can always consider a basis with a countable number of elements. An example of such a basis are the eigenstates of the SHO (Fock states) $\{|n\rangle | n=0, 1, 2, \dots, \infty\}$ the complete relation is now $\sum_{n=0}^{\infty} |n\rangle\langle n| = \hat{1}$

All operators of the Hilbert space can be expanded in this basis. W.r.t. the operators are "infinite dimensional" matrices.

Examples: $\hat{\Pi}|n\rangle = (-1)^n |n\rangle$ (eigenstates of parity)

$$\Rightarrow \hat{\Pi} = \sum_{n=0}^{\infty} (-1)^n |n\rangle\langle n| = \begin{bmatrix} 1 & & & & \\ & -1 & & & \\ & & 1 & & \\ & & & -1 & \\ & & & & \ddots \end{bmatrix} \text{ diagonal matrix}$$

We can use the raising and lowering operators to find matrix representations of $\hat{x} = x_c \left(\frac{\hat{a} + \hat{a}^\dagger}{2}\right)$ and $\hat{p} = p_c \left(\frac{\hat{a} - \hat{a}^\dagger}{2i}\right)$

Characteristic units

$$\begin{pmatrix} x_c = \sqrt{\frac{\hbar}{2m\omega}} \\ p_c = \sqrt{2\hbar m\omega} \end{pmatrix}$$

$$\hat{a} = \sum_{n,n'} |n\rangle\langle n'| \hat{a} |n'\rangle\langle n| = \sum_{n=0}^{\infty} \sqrt{n} |n-1\rangle\langle n| = \begin{bmatrix} 0 & 1 & 0 & 0 & \dots \\ 0 & 0 & \sqrt{2} & 0 & \dots \\ 0 & 0 & 0 & \sqrt{3} & \dots \\ 0 & 0 & 0 & 0 & \dots \\ \vdots & \vdots & \vdots & \vdots & \ddots \end{bmatrix}$$

$$\hat{a}^\dagger = \sum_{n=0}^{\infty} \sqrt{n+1} |n+1\rangle\langle n| = \begin{bmatrix} 0 & 0 & 0 & \dots \\ 1 & 0 & 0 & \dots \\ 0 & \sqrt{2} & 0 & \dots \\ 0 & 0 & \sqrt{3} & \dots \\ \vdots & \vdots & \vdots & \ddots \end{bmatrix}$$

$$\Rightarrow \hat{x} = \sqrt{\frac{\hbar}{2m\omega}} \begin{bmatrix} 0 & 1 & 0 & 0 & \dots \\ 1 & 0 & \sqrt{2} & 0 & \dots \\ 0 & \sqrt{2} & 0 & \sqrt{3} & \dots \\ 0 & 0 & \sqrt{3} & 0 & \dots \\ \vdots & \vdots & \vdots & \vdots & \ddots \end{bmatrix}$$

$$\hat{p} = \sqrt{\frac{\hbar m\omega}{2}} \begin{bmatrix} 0 & -i & 0 & 0 & \dots \\ i & 0 & -i\sqrt{2} & 0 & \dots \\ 0 & i\sqrt{2} & 0 & -i\sqrt{3} & \dots \\ 0 & 0 & i\sqrt{3} & 0 & \dots \\ \vdots & \vdots & \vdots & \vdots & \ddots \end{bmatrix}$$