

Phys 521

Lectures 7-11

Mathematical structure of quantum mechanics

Example: Particle in 1-dim. box:

$$V(x) = \begin{cases} 0, & 0 < x < a \\ \infty, & \text{otherwise} \end{cases}$$

$$0 < x < a: -\frac{\hbar^2}{2m} \frac{d^2 \psi}{dx^2} = E \psi \iff \frac{d^2 \psi}{dx^2} + k^2 \psi = 0$$

$$k^2 = \frac{2mE}{\hbar^2}$$

$$\text{B.C.: } \psi(x=0) = 0 = \psi(x=a)$$

$$\text{Solution: } \psi_n(x) = \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi x}{a}\right)$$

Normalized Fourier
functions on the
interval $0 < x < a$.

↑
Orthonormal and complete

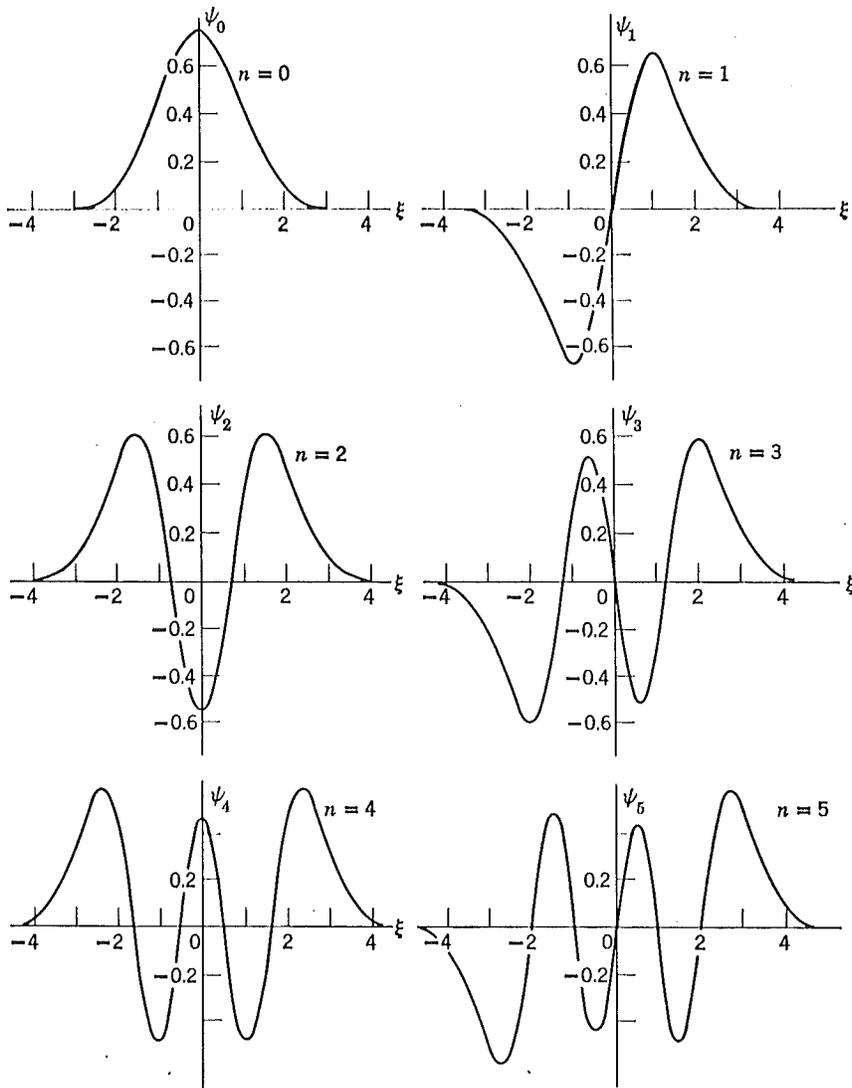
$$V(x) = \frac{1}{2} kx^2 = \frac{1}{2} m\omega^2 x^2 \quad (1b)$$

Energy eigenfunctions for SHO:

$$\psi_n(x) = \frac{1}{\sqrt{2^n n!}} \left(\frac{m\omega}{\pi\hbar} \right)^{1/4} \exp\left(-\frac{m\omega}{2\hbar} x^2\right) H_n\left(\sqrt{\frac{m\omega}{\hbar}} x\right)$$

↑
nth Hermite polynomial

§3 Study of the Eigenfunctions



From
Quantum Mechanics,
by E. Merzbacher

Figure 5.1. The eigenfunctions of the linear harmonic oscillator for the quantum numbers $n = 0$ to 5. ψ_n is plotted versus $\xi = \sqrt{m\omega/\hbar} x$, and all eigenfunctions are normalized as $\int_{-\infty}^{+\infty} |\psi_n(\xi)|^2 d\xi = 1$.

Dirac δ -function: $\delta(x)$

Not really a function. To do things right requires the theory of generalized functions. For us, however, we shall think of $\delta(x)$ as a "function" ^(∞) sharply peaked at $x=0$ that it has a unit integral. We do not make mistakes as long as we always (in the end) put the δ -function under an integral.

$$f(x) = \int_{-\infty}^{\infty} dx' \delta(x-x') f(x') \quad \text{for any function } f(x')$$

$$\Rightarrow \int_{x_1}^{x_2} \delta(x) dx = \begin{cases} 1, & \text{if } x_1 < 0 < x_2 \\ 0, & \text{otherwise} \end{cases}$$

Representations:

$$\textcircled{1} \delta(x-x') = \int_{-\infty}^{\infty} \frac{dk}{2\pi} e^{ik(x-x')} \quad \leftarrow \text{inverting a Fourier transform}$$

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

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

$$\textcircled{4} \delta(x) = \lim_{N \rightarrow \infty} \frac{\sin Nx}{\pi x}$$

$$\textcircled{5} \delta(x) = \frac{1}{2} \frac{d^2}{dx^2} |x|$$

$\delta^2(x)$ is nonsense.

Properties:

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

② $f(x') \delta(x-x') = f(x) \delta(x-x')$

③ $\delta(g(x)) = \sum_i \frac{1}{|g'(x_i)|} \delta(x-x_i), \quad g(x_i) = 0$

Expand $g(x)$ about its zeroes.

Arbitrary wave function: $\Psi(x) = \sum_n c_n \varphi_n(x)$

Orthonormality $\Rightarrow c_n = \int dx \varphi_n^*(x) \Psi(x)$ Derive
└ probability amplitude

Where does completeness come in? Ability to expand any function.

$$\textcircled{1} \Psi(x) = \sum_n c_n \varphi_n(x) = \int dx' \underbrace{\left(\sum_n \varphi_n^*(x') \varphi_n(x) \right)}_{\delta(x-x')} \Psi(x')$$

Use this backwards to derive the expansion

$$\textcircled{2} \delta(x-x') = \sum_n c_n \varphi_n(x) \quad , \quad c_n = \int dx \varphi_n^*(x) \delta(x-x') = \varphi_n^*(x')$$
$$= \sum_n \varphi_n^*(x') \varphi_n(x)$$

$|\Psi(x)|^2 dx =$ (probability that particle lies between x and $x+dx$)

$\Psi(x)$ is a probability amplitude

Normalization: $1 = \int dx |\Psi(x)|^2$

$|c_n|^2 =$ (probability that energy is E_n)

↕ show in both directions

c_n is a probability amplitude

Normalization: $1 = \sum_n |c_n|^2$

Inner (scalar) product of two wave functions:

$$\psi(x) = \sum_n c_n \varphi_n(x), \quad \phi(x) = \sum_n d_n \varphi_n(x)$$

$$\text{(inner product)} = \int dx \phi^*(x) \psi(x) = \sum_n d_n^* c_n = (d_1^* \ d_2^* \ \dots) \begin{pmatrix} c_1 \\ c_2 \\ \vdots \\ c_n \end{pmatrix}$$

Abstract to a complex vector space

- Why? Notational ease
- Calculational convenience
- Better understanding

Dirac bra-ket formulation:

Complex vector space

Vector (ket) $|\psi\rangle$

Vector space rules

Examples:

- ① $\psi(x), -\infty < x < \infty$ (SHO)
 - $|\psi\rangle \leftrightarrow \psi(x) \quad L^2$
 - no x -dependence rules
 - $|\varphi_n\rangle$ are basis vectors

- ② Particle in a box
 - $|\psi\rangle \leftrightarrow \psi(x) \quad L^2$ on $[0, a]$
 - rules
 - $|\varphi_n\rangle$ are a basis

- ③ Spin- $\frac{1}{2}$
 - $|\uparrow\rangle, |\downarrow\rangle, |\psi\rangle = \alpha|\uparrow\rangle + \beta|\downarrow\rangle$

Inner product: $(|\phi\rangle, |\psi\rangle) = \text{(complex number)}$

① Complex bilinear

② Complex symmetric: $(|\phi\rangle, |\psi\rangle) = (|\psi\rangle, |\phi\rangle)^*$

③ $(|\psi\rangle, |\psi\rangle) \geq 0$, $(|\psi\rangle, |\psi\rangle) = 0 \Rightarrow |\psi\rangle = 0$.

State vectors (quantum states): are normalized vectors:

$(|\psi\rangle, |\psi\rangle) = 1$.

Dual vectors (bras): $\langle\psi|$

Linear functions on vectors: $\langle\psi|\phi\rangle = \begin{matrix} \text{complex} \\ \text{number} \end{matrix}$

Make up a vector space

The inner product induces a map from kets to bras:

$|\psi\rangle \longleftrightarrow \langle\psi| : \langle\psi|\phi\rangle \equiv (|\psi\rangle, |\phi\rangle)$

①, ②, + ③
above

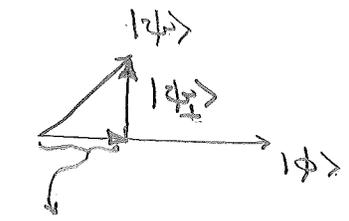
This map is antilinear

$|\psi\rangle = c_1|\psi_1\rangle + c_2|\psi_2\rangle \longleftrightarrow \langle\psi| = c_1^*\langle\psi_1| + c_2^*\langle\psi_2|$

Generally drop (,) notation for inner product, but caution!

This map is 1-1 for finite-dimensional vector spaces.

Schwarz inequality: $|\langle\phi|\psi\rangle|^2 \leq \langle\phi|\phi\rangle\langle\psi|\psi\rangle$



$\frac{|\phi\rangle\langle\phi|\psi\rangle}{\langle\phi|\phi\rangle}$

$|\psi_{\perp}\rangle = |\psi\rangle - \frac{|\phi\rangle\langle\phi|\psi\rangle}{\langle\phi|\phi\rangle}$

$\langle\psi_{\perp}|\psi_{\perp}\rangle = \langle\psi|\psi\rangle - \frac{\langle\psi|\phi\rangle\langle\phi|\psi\rangle}{\langle\phi|\phi\rangle}$

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

Representation of a vector:

Complete, orthonormal basis $|\varphi_n\rangle$

Examples:
energy eigenstates

Orthonormality: $\langle\varphi_m|\varphi_n\rangle = \delta_{nm}$

Completeness: $\mathbb{1} = \sum_n |\varphi_n\rangle\langle\varphi_n| = \hat{\mathbb{1}}$

Expansion of arbitrary vector:

$|\psi\rangle = \sum_n c_n |\varphi_n\rangle = \sum_n |\varphi_n\rangle\langle\varphi_n|\psi\rangle$

Meaning of
Completeness

$\downarrow = \langle\varphi_n|\psi\rangle = \left(\begin{matrix} \text{components in} \\ |\varphi_n\rangle\text{-representation} \end{matrix} \right)$

$\langle\psi| = \sum_n \langle\varphi_n| c_n^* = \sum_n \langle\psi|\varphi_n\rangle\langle\varphi_n|$

Inner product \rightarrow normalization

Linear operators:

\hat{O}

hat distinguishes
operators

C-T uses caps for operators

$\hat{O}|\psi\rangle$ is a ket

$\hat{O}(c_1|\psi_1\rangle + c_2|\psi_2\rangle) = c_1(\hat{O}|\psi_1\rangle) + c_2(\hat{O}|\psi_2\rangle)$

Unit operator: $\hat{\mathbb{1}}|\psi\rangle = |\psi\rangle$ for all $|\psi\rangle$

Outer product: $|\phi\rangle\langle\psi|$ is an operator

Projection operator:

1-d: $\hat{P}_{|\psi\rangle} = |\psi\rangle\langle\psi|$

Subspace S , spanned by $|\varphi_n\rangle$: $\hat{P}_S = \sum_n |\varphi_n\rangle\langle\varphi_n|$

$\hat{P}_S^2 = \hat{P}_S$

Unit operator $\hat{\mathbb{1}} = \sum_n |\varphi_n\rangle\langle\varphi_n|$

Matrix representation

$$\hat{O}|\psi\rangle = \sum_n |\varphi_n\rangle \underbrace{\langle \varphi_n | \hat{O} | \psi \rangle}_{d_n} = \sum_{nm} |\varphi_n\rangle \underbrace{\langle \varphi_n | \hat{O} | \varphi_m \rangle}_{O_{nm}} \underbrace{\langle \varphi_m | \psi \rangle}_{c_m}$$

$$\begin{pmatrix} d_1 \\ d_2 \\ \vdots \end{pmatrix} = O \begin{pmatrix} c_1 \\ c_2 \\ \vdots \end{pmatrix}$$

$$\hat{O} = \hat{1} \hat{O} \hat{1} = \sum_{nm} |\varphi_n\rangle \langle \varphi_n | \hat{O} | \varphi_m \rangle \langle \varphi_m |$$

matrix elements of \hat{O} in $|\varphi_n\rangle$ -rep

Operator products: $(\hat{N}\hat{O})|\psi\rangle = \hat{N}(\hat{O}|\psi\rangle)$ matrix rep?

Acting to left: $\langle \phi | \hat{O} | \psi \rangle = \langle \phi | (\hat{O} | \psi \rangle) = \langle \phi | \hat{O} | \psi \rangle$

Adjoint operator (Hermitian conjugate):

$$\hat{O}|\psi\rangle = |\psi'\rangle \iff \langle \psi' | = \langle \psi | \hat{O}^\dagger$$

$$\langle \phi | \hat{O} | \psi \rangle = \langle \phi | \psi' \rangle = \langle \psi' | \phi \rangle^* = \langle \psi | \hat{O}^\dagger | \phi \rangle^*$$

$$= \langle \psi | \hat{O}^\dagger | \phi \rangle^* \iff \langle \phi | \hat{O} | \psi \rangle$$

No way to write this in Dirac notation except as $\langle \phi | \hat{O} | \psi \rangle$

The map \hat{O}^\dagger is antilinear

$$(\alpha \hat{O} + \beta \hat{N})|\psi\rangle \iff \langle \psi | (\alpha \hat{O} + \beta \hat{N})^\dagger$$

$$\alpha \langle \hat{O} | \psi \rangle + \beta \langle \hat{N} | \psi \rangle \iff \alpha^* \langle \psi | \hat{O}^\dagger + \beta^* \langle \psi | \hat{N}^\dagger = \langle \psi | (\alpha^* \hat{O}^\dagger + \beta^* \hat{N}^\dagger)$$

$$\implies (\alpha \hat{O} + \beta \hat{N})^\dagger = \alpha^* \hat{O}^\dagger + \beta^* \hat{N}^\dagger$$

How to determine the eigenvalues:

characteristic equation

$$(\hat{A} - \lambda_n \hat{1}) |\psi_n\rangle = 0 \Rightarrow \det(\hat{A} - \lambda_n \hat{1}) = 0$$

What does this mean?

Rep in a particular orthonormal basis.

Basis-dependence

D dimensions \rightarrow D roots, including multiple roots

Dealing with degeneracies

Eigenvectors of a Hermitian operator \hat{A} form a complete orthonormal basis, the A-representation.

A-representation: $\hat{A} |\psi_n\rangle = \lambda_n |\psi_n\rangle$

Orthonormality: $\langle \psi_n | \psi_m \rangle = \delta_{nm}$

Completeness: $\hat{1} = \sum_n |\psi_n\rangle \langle \psi_n|$

Spectral decomposition: $\hat{A} = \sum_n \lambda_n |\psi_n\rangle \langle \psi_n| = \sum_\lambda \lambda \hat{P}_\lambda$

Describe situation for non-Hermitian operators. For QM Hermitian is enough.

Unitary operators: Operators that preserve inner products

$$\langle \phi | \psi \rangle = \langle \phi | \hat{U}^\dagger \hat{U} | \psi \rangle \quad \text{for all } |\phi\rangle, |\psi\rangle$$

$$\Leftrightarrow \hat{U}^\dagger \hat{U} = \hat{1} = \hat{U} \hat{U}^\dagger$$

Eigenvalues of \hat{U} are phases

$$\hat{U} = e^{i\hat{A}} \quad \text{for some Hermitian } \hat{A}$$

Normal operators: diagonalized in a complete orthonormal basis $\Leftrightarrow [\hat{A}, \hat{A}^\dagger] = 0$

Polar decomposition

Change of representation:

$$\hat{I} = \sum_n |\varphi_n\rangle\langle\varphi_n| = \sum_m |\chi_m\rangle\langle\chi_m|$$

$$\text{Kets: } |\psi\rangle = \sum_n |\varphi_n\rangle\langle\varphi_n|\psi\rangle = \sum_m |\chi_m\rangle\langle\chi_m|\psi\rangle$$

$$\langle\chi_m|\psi\rangle = \sum_n \underbrace{\langle\chi_m|\varphi_n\rangle}_{u_{mn}} \langle\varphi_n|\psi\rangle$$

Matrix form

u unitary matrix

Bras:

Operators:

Commutators and simultaneous eigenstates:

$$\text{Commutator: } [\hat{A}, \hat{B}] = 0$$

Theorem: \hat{A} and \hat{B} normal. $[\hat{A}, \hat{B}] = 0 \Leftrightarrow \hat{A}$ and \hat{B} have a complete, orthonormal set of simultaneous eigenstates.

Proof:

① Suppose \hat{A} and \hat{B} have simultaneous eigenstates $|\psi_n\rangle$. Then $\hat{A} = \sum_k A_k |\psi_k\rangle\langle\psi_k|$ and $\hat{B} = \sum_k B_k |\psi_k\rangle\langle\psi_k|$.

It is trivial to show that $[\hat{A}, \hat{B}] = 0$. (10)

Ⓔ Suppose $[\hat{A}, \hat{B}] = 0$. Let $|\psi_n\rangle$ be an eigenstate of \hat{A} with eigenvalue A_n , i.e., $\hat{A}|\psi_n\rangle = A_n|\psi_n\rangle$.

Consider the vector $\hat{B}|\psi_n\rangle$:

$$\hat{A}(\hat{B}|\psi_n\rangle) = \hat{B}(\hat{A}|\psi_n\rangle) = A_n(\hat{B}|\psi_n\rangle).$$

$\therefore \hat{B}|\psi_n\rangle$ is an eigenvector of \hat{A} with eigenvalue A_n . If A_n is nondegenerate, this implies that

$\hat{B}|\psi_n\rangle = B_n|\psi_n\rangle$. If A_n is degenerate, then it

implies that $\hat{B}|\psi_n\rangle$ lies in the subspace spanned by the degenerate eigenvectors. Diagonalizing \hat{B}

in all degenerate subspaces of \hat{A} yields

simultaneous eigenstates.

Continuous spectra: General - C-T
Example - position \hat{x} and momentum \hat{p}

Position eigenstates: $|x\rangle, -\infty < x < \infty$

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

x-representation for arbitrary ket $|\psi\rangle$: $|\psi\rangle = \int_{-\infty}^{\infty} dx |x\rangle \langle x|\psi\rangle$

$\psi(x) = \left(\begin{matrix} \text{wave} \\ \text{function} \end{matrix} \right) = \left(\begin{matrix} \text{amplitude to} \\ \text{be at } x \end{matrix} \right)$

If this is true, we must have

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

$$\Rightarrow \delta(x-x')$$

Orthonormality: $\langle x|x'\rangle = \delta(x-x')$ δ-for normalization

Completeness: $\int_{-\infty}^{\infty} dx |x\rangle \langle x| = \hat{1}$

Eigenstates $|x\rangle$ not normalizable $\Leftrightarrow \langle x|x'\rangle = \delta(x-x')$,
the wave function for position eigenstate $|x'\rangle$, is not square-integrable.

$|x\rangle$ not in Hilbert space

$\langle x|$ is in dual space

Position representation:

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

$$\langle\phi|\psi\rangle = \int_{-\infty}^{\infty} dx \langle\phi|x\rangle \langle x|\psi\rangle = \int_{-\infty}^{\infty} dx \phi^*(x) \psi(x)$$

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

Momentum representation: \hat{p} , $|p\rangle$, $\psi(p)$

Unitary transformation: $\langle x|p\rangle = \frac{1}{\sqrt{2\pi\hbar}} e^{\frac{i}{\hbar} px}$

$$|p\rangle = \int \frac{dx}{\sqrt{2\pi\hbar}} |x\rangle e^{\frac{i}{\hbar} px}$$

Changing this changes ... momentum integration measure

Orthogonality:

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

Completeness:

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

$$\hat{p}|p\rangle = p|p\rangle \leftarrow \text{defn of } \hat{p}$$

$$\langle x|\hat{p}|\psi\rangle = \int dp dx' \underbrace{\langle x|\hat{p}|p\rangle}_{p \langle x|p\rangle} \langle p|x'\rangle \langle x'|\psi\rangle$$

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

$$= \frac{\hbar}{i} \frac{d}{dx} \int dx' \langle x'|\psi\rangle \delta(x-x')$$

$$= \frac{\hbar}{i} \frac{d}{dx} \langle x|\psi\rangle$$

position representation of \hat{p}

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

momentum representation of \hat{x}

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

$$\langle x|\hat{p}\hat{x}|\psi\rangle = \frac{\hbar}{i} \frac{d}{dx} (x\psi(x)) = x \frac{\hbar}{i} \frac{d\psi}{dx} + \frac{\hbar}{i} \psi(x)$$

$$\Rightarrow [\hat{x}, \hat{p}] = i\hbar$$

Operator algebra