PHOT 301: Quantum Photonics

LECTURE 05

Michaël Barbier, Summer (2024-2025)

OVERVIEW

week	Topic	Reading
Week 1	Introduction & Required Mathematical Methods. Waves and Schrödinger's equation, Probability, Uncertainty and Time evolution. Infinite square well.	
Week 2	The harmonic oscillator, Creation and annihilation operators. Free particle, 1D Bound states & Scattering/Transmission, Finite well	
Week 3	Quantum mechanics formalism: Functions and operators, uncertainty. Approximation methods.	Ch. 3
Week 4	Angular momentum and the Hydrogen atom, Spin Magnetic fields, The Pauli equation, Minimal Coupling, Aharonov Bohm Perturbation: Fine Structure of Hydrogen, The Zeeman Effect	
Week 5	Identical particles, Periodic table, Molecular bonds, Periodic structures, Band structure, Bloch functions Time-dependent perturbation: Absorption, spontaneous emission, and stimulated emission	
Week 6	Final exam	

FOR NEXT WEEK

- Textbook Chapter 2: 2.31, 2.34, 2.41, 2.53
- Textbook Chapter 3: 2.31, 2.34, 2.41, 2.53
- Homework documents:
  - phot301_homework_braket.pdf
- Reading (by Thursday 7 August 2025): Chapter 4 of Griffiths

SUMMARY OF WHAT WE KNOW

- Time-independent Schrodinger equation
- Find eigenstates and eigenenergies:
  - **complete basis**: Solution is superposition of eigenstates
  - **orthonormal**: Solution is superposition of eigenstates
- Special case(?) of free particles:
  - Propagating waves $\Psi(x,t) \propto e^{i(kx-\omega t)}$
  - **All energies** can be reached
  - Real solutions are given by **wave packets**
  - **Uncertainty** between position and momentum

SUMMARY OF WHAT WE KNOW

- Evolution in time
  - Phase factor depending on energy: $e^{iE_n t/\hbar}$
  - Higher energies change faster
  - Superposition of bound states deform
  - Free particles: **wave packets** have faster and slower components (dispersion)

MATHEMATICS OF WAVE FUNCTIONS & OBSERVABLES?

Wave functions

- **Complete basis** of **orthonormal** eigenstates
- Superposition is solution of **linear** Schrodinger equation

Observables

- Observables are **linear operators**
- Applying an **operator** to a wave function gives another wave function

–> Quantum mechanics can be described with linear algebra

LINEAR ALGEBRA

FIELD OF COMPLEX NUMBERS

- The sets of rational ($\mathbb{Q}$), real ($\mathbb{R}$), and complex numbers ($\mathbb{C}$) are **fields**:
  - 2 operations: addition and multiplication
  - identity elements: addition (0), multiplication (1)
  - Inverse elements: addition (-x), multiplication (x^{-1})
  - Commutativity, associativity, distributivity

Complex numbers $z \in \mathbb{C}$:

- Imaginary identity $\quad i = \sqrt{-1}, \qquad i^2 = -1$
- Complex conjugate z^*: $\quad z = x + i\,y \longrightarrow z^* = x - i\,y$

FIELD OF COMPLEX NUMBERS: PROPERTIES

Assume $z = x + iy \in \mathbb{C}$:

$$\begin{aligned}
\text{Representation} \quad & z = x + i\,y = re^{i\theta} = r\,(\cos\theta + i\ \sin\theta) \\
\text{Complex conjugate} \quad & z^* = x - i\,y = re^{-i\theta} = r\,(\cos\theta - i\ \sin\theta) \\
\text{Magnitude} \quad & |z|^2 = z^*\,z = x^2 + y^2 = \Re\{z\}^2 + \Im\{z\}^2 \\
\text{Phase} \quad & \theta = -i\ln(z/|z|) = \arctan(y/x) \\
\text{Trigoniometry} \quad & \cos\theta = \frac{e^{i\theta} + e^{-i\theta}}{2}, \qquad \sin\theta = \frac{e^{i\theta} - e^{-i\theta}}{2i}
\end{aligned}$$

Operations:

$$\begin{aligned}
\text{Addition} \quad & z_1 + z_2 = (x_1 + x_2) + i\,(y_1 + y_2) \\
\text{Multiplication} \quad & z_1\,z_2 = r_1 r_2 e^{i(\theta_1 + \theta_2)}
\end{aligned}$$

VECTOR SPACES

A vector space $\mathcal{V} = \{|\alpha\rangle, |\beta\rangle, |\gamma\rangle, ...\}$ over field $F = \mathbb{C}$:

- Addition of vectors $|\alpha\rangle + |\beta\rangle \in \mathcal{V}$
- Scalar multiplication $c|\alpha\rangle \in \mathcal{V}$

Property name	rule
(Addition) Commutative	$|\alpha\rangle + |\beta\rangle = |\beta\rangle + |\alpha\rangle$
(Addition) Associative	$|\alpha\rangle + (|\beta\rangle + |\gamma\rangle) = (|\alpha\rangle + |\beta\rangle) + |\gamma\rangle$
(Addition) Identity	$\mathbf{0} + |\beta\rangle = |\beta\rangle$ for all $|\beta\rangle$
(Addition) Inverse element	for all $|\beta\rangle$, exists $-|\beta\rangle$: $-|\beta\rangle + |\beta\rangle = \mathbf{0}$
(Scalar) Compatible product	$c\,(d\,|\alpha\rangle) = (c\,d)\,|\alpha\rangle$
(Scalar) Identity	$1\,|\alpha\rangle = |\alpha\rangle$
(Scalar) Distributivity	$c(|\alpha\rangle + |\beta\rangle) = c\,|\beta\rangle + c\,|\alpha\rangle$
(Scalar) Distributivity	$(c + d)|\alpha\rangle = c\,|\alpha\rangle + d\,|\alpha\rangle$

BASIS VECTORS

Linear independence

A vector $|\xi\rangle$ is linearly independent of $\{|\alpha\rangle, |\beta\rangle, |\gamma\rangle, \ldots\}$

$\Leftrightarrow$ no linear combination: $|\xi\rangle = a|\alpha\rangle + b|\beta\rangle + c|\gamma\rangle + \ldots$

Example: in 3D vector space:

- Vector $(x, y, z) = (0, 1, 1)$ is linearly independent from $\{(1, 1, 0),\ (1, 0, 0)\}$
- BUT .. $(0, 1, 1)$ is dependent to $\{(-1, 1, 0),\ (1, 0, 1)\}$

Basis vectors:

- A vector set is linear independent if each of them is independent from the others.
- The span of a vector set is the subset of vectors formed by linear combinations
- A linear independent vector set is a basis if it spans the whole space

BASIS VECTORS

Suppose a finite set of n basis vectors:

$$\{|e_1\rangle,\ |e_2\rangle, \dots,\ |e_n\rangle\ \}$$

Each vector $|\alpha\rangle$ can be written as superposition:

$$|\alpha\rangle = a_1|e_1\rangle + a_2|e_2\rangle + \cdots + a_n|e_n\rangle$$

In component notation for **specific basis**:

$$|\alpha\rangle = (a_1, a_2, \dots, a_n)$$

$\longrightarrow$ Simplifies understanding the properties:

$$\begin{aligned}
|0\rangle + |\alpha\rangle = |\alpha\rangle \quad &\Longrightarrow |0\rangle = (0, 0, \dots, 0) \\
|\alpha\rangle + |-\alpha\rangle = |0\rangle \quad &\Longrightarrow |-\alpha\rangle = (-a_1, -a_2, \dots, -a_n) \\
|\alpha\rangle + c|\beta\rangle \quad &\Longrightarrow |\alpha\rangle + c|\beta\rangle = (a_1 + c\, b_1, a_2 + c\, b_2, \dots, a_n + c\, b_n)
\end{aligned}$$

NORMED VECTOR SPACE

- There exists a norm or length of a vector $|\beta\rangle$ given by $\|\beta\| \equiv \|\,|\beta\rangle\,\|$

Property name	**rule**
Non-negative	$\|\beta\| \geq 0$
Positive definite	$\|\beta\| = 0 \Leftrightarrow |\beta\rangle = |0\rangle$
Absolute homogeneity	$\|c\,\beta\| = |c|\,\|\beta\|$
Triangle inequality	$\|\,|\alpha\rangle + |\beta\rangle\,\| \leq \|\alpha\| + \|\beta\|$

- Distance corresponding to norm:

$$d(|\beta\rangle, |\alpha\rangle) = \|\,|\alpha\rangle - |\beta\rangle\,\|$$

- Example distance: $d\left((x_1, y_1),\, (x_2, y_2)\right) = \sqrt{(x_2 - x_1)^2 + (y_2 - y_1)^2}$
- Example norm: $\|(3,4)\| = \sqrt{3^2 + 4^2} = \sqrt{25} = 5$

INNER PRODUCT VECTOR SPACE

- An inner product of a vector space:

$$\langle\, \langle\alpha| \,,\, |\beta\rangle \,\rangle = \langle\alpha|\beta\rangle \longrightarrow c \in \mathbb{C}$$

Property name	**rule**
conjugate symmetry	$\langle\beta|\alpha\rangle^* = \langle\alpha|\beta\rangle$
linearity 2nd argument	$\langle\alpha\,|\,(\,c\,|\beta\rangle \,+\, d\,|\gamma\rangle)\rangle \;=\; c\,\langle\alpha|\beta\rangle \,+\, d\,\langle\alpha|\gamma\rangle$
$\Rightarrow$ conjugate linear 1st	$\langle\,(c\,|\alpha\rangle \,+\, d\,|\beta\rangle\,)\,|\,\gamma\rangle \;=\; c^*\,\langle\alpha|\gamma\rangle \,+\, d^*\,\langle\beta|\gamma\rangle$
positive definite	$\langle\beta|\beta\rangle > 0$

- The norm is defined by

$$||\beta|| = \sqrt{\langle\beta|\beta\rangle}$$

ORTHONORMAL BASIS VECTORS

- A vector $|\beta\rangle$ is normalized $\quad \Leftrightarrow \quad \|\beta\| = 1$
- A vector $|\beta\rangle \perp |\alpha\rangle \quad \Leftrightarrow \quad \langle\alpha|\beta\rangle = 0$
- Orthonormal set of vectors: $\langle\alpha_i|\alpha_j\rangle = \delta_{ij}$
- Always possible to find an orthonormal basis!

$\longrightarrow$ In component notation: $\langle\alpha|\beta\rangle = a_1^* b_1 + \cdots + a_n^* b_n \qquad \textbf{with} \quad a_i = \langle e_i|\alpha\rangle$

The norm is given by:

$$\|\alpha\|^2 = \langle\alpha|\alpha\rangle = a_1^* b_1 + \cdots + a_n^* b_n \qquad \textbf{with} \quad a_i = |a_1|^2 + \cdots + |a_n|^2$$

In $\mathbb{R}^n$ the angle between two vectors is $\mathbf{a} \cdot \mathbf{b} = \|\mathbf{a}\|\,\|\mathbf{b}\| \cos(\theta)$:

$$\cos\theta = \frac{\sqrt{\langle\alpha|\beta\rangle\,\langle\beta|\alpha\rangle}}{\|\alpha\|\|\beta\|}$$

IMPORTANT THEOREMS

- The dimension n (= number of basis vectors) is constant for a vector space.
- Gram-Schmidt procedure: **any** basis $\longrightarrow$ **orthonormal** basis.
- Schwartz inequality:

$$|\langle\alpha|\beta\rangle|^2 \leq \langle\alpha|\alpha\rangle\,\langle\beta|\beta\rangle$$

- Triangle inequality:

$$\|\,|\alpha\rangle + |\beta\rangle\,\| \leq \|\alpha\|^2 + \|\beta\|^2$$

OPERATORS: LINEAR TRANSFORMATIONS

- linear transformations $\hat{T}$:

$$|\alpha'\rangle = \hat{T}\,|\alpha\rangle \qquad \text{linearity:} \quad \hat{T}(c|\alpha\rangle + d|\beta\rangle) = a\,\hat{T}|\alpha\rangle + b\,\hat{T}|\beta\rangle$$

- If we know the basis vectors $|e_1\rangle, \ldots, |e_n\rangle$:

$$\begin{aligned}
|\alpha'\rangle &= \hat{T}\,|\alpha\rangle \\
&= \hat{T}\;(a_1|e_1\rangle + \cdots + a_n|e_n\rangle) \\
&= \hat{T}\,a_1|e_1\rangle + \cdots + \hat{T}\,a_n|e_n\rangle \\
&= a_1\,\hat{T}\,|e_1\rangle + \cdots + a_n\,\hat{T}\,|e_n\rangle \\
&= \sum_{i=1}^{n} a_i\,\hat{T}\,|e_i\rangle
\end{aligned}$$

OPERATORS: MATRIX NOTATION

- If we know the basis vectors $|e_1\rangle, \dots, |e_n\rangle$:

$$\hat{T}\,|\alpha\rangle = \sum_{j=1}^{n} a_j\,\hat{T}\,|e_j\rangle$$

The $\hat{T}\,|e_i\rangle$ can be written as superposition:

$$\begin{aligned}
\hat{T}\,|e_1\rangle &= T_{11}|e_1\rangle + T_{21}|e_2\rangle + \cdots + T_{n1}|e_n\rangle \\
\hat{T}\,|e_2\rangle &= T_{12}|e_1\rangle + T_{22}|e_2\rangle + \cdots + T_{n2}|e_n\rangle \\
&\dots \\
\hat{T}\,|e_n\rangle &= T_{1n}|e_1\rangle + T_{2n}|e_2\rangle + \cdots + T_{nn}|e_n\rangle
\end{aligned}$$

$$\Rightarrow \hat{T}\,|\alpha\rangle = \sum_{j=1}^{n} a_j\,\hat{T}\,|e_j\rangle = \sum_{j=1}^{n}\sum_{i=1}^{n} a_j T_{ij}|e_i\rangle = \sum_{i=1}^{n}\left(\sum_{j=1}^{n} T_{ij}a_j\right)|e_i\rangle$$

OPERATORS: MATRIX NOTATION

$$\Rightarrow \hat{T}\,|\alpha\rangle = \sum_{j=1}^{n} a_j\,\hat{T}\,|e_j\rangle = \sum_{j=1}^{n}\sum_{i=1}^{n} a_j T_{ij}|e_i\rangle = \sum_{i=1}^{n}\left(\sum_{j=1}^{n} T_{ij}a_j\right)|e_i\rangle$$

Operator $\hat{T}$ as a matrix T_{ij} for basis $\{|e_1\rangle\,,\,\ldots\,,\,|e_n\rangle\}$

$$a_i' = \sum_{j=1}^{n} T_{ij}a_j$$

And the matrix:

$$T_{ij} = \begin{pmatrix} T_{11} & T_{12} & \cdots & T_{1n} \\ T_{21} & T_{22} & \cdots & T_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ T_{n1} & T_{n2} & \cdots & T_{nn} \end{pmatrix} \qquad \text{with} \qquad T_{ij} = \langle e_i|\hat{T}|e_j\rangle$$

MATRICES AND VECTORS

If we have a basis basis $\{|e_1\rangle, \ldots, |e_n\rangle\}$

$$|\alpha\rangle = \begin{pmatrix} a_1 \\ a_2 \\ \vdots \\ a_n \end{pmatrix}$$

An operator acting on a vector $|\alpha\rangle$:

$$\hat{T}|\alpha\rangle \longrightarrow \sum_{j=1}^{n} T_{ij} a_j = \begin{pmatrix} T_{11} & T_{12} & \cdots & T_{1n} \\ T_{21} & T_{22} & \cdots & T_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ T_{n1} & T_{n2} & \cdots & T_{nn} \end{pmatrix} \begin{pmatrix} a_1 \\ a_2 \\ \vdots \\ a_n \end{pmatrix}$$

OPERATORS AND MATRIX PROPERTIES

- Adding two operators:

$$\hat{U} = \hat{S} + \hat{T} \longrightarrow U_{ij} = S_{ij} + T_{ij}$$

- Performing multiple operators $\hat{U} = \hat{S}\hat{T}$:

$$\hat{U}|\alpha\rangle = \hat{S}\hat{T}|\alpha\rangle \longrightarrow U_{ij} = \sum_k S_{ik}T_{kj}$$

INTERMEZZO: MATRIX PRODUCTS

The matrix product between matrices A and B is defined as

$$A \cdot B = \begin{pmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \end{pmatrix} \begin{pmatrix} b_{11} & b_{12} & b_{13} \\ b_{21} & b_{22} & b_{23} \\ b_{31} & b_{32} & b_{33} \end{pmatrix}$$

$$= \sum_j a_{ij} b_{jk}$$

- Rows of A are multiplied by columns of B.
- $A_{MN} \cdot B_{NK} \leftarrow$ No. columns of A must equal No. rows of B

OPERATORS AND MATRIX PROPERTIES

- Transpose of a matrix $\tilde{T} = T_{ji}$
  - **symmetric:** $\tilde{T} = T$
  - **antisymmetric:** $\tilde{T} = -T$
- Complex conjugate of a matrix $T^* = T_{ij}^*$
  - **real:** $T^* = T$
  - **imaginary:** $T^* = -T$
- Hermitian conjugate of a square matrix $T^\dagger = \tilde{T}^* = T_{ji}^*$
  - **Hermitian:** $T^\dagger = T$
  - **skew hermitian:** $T^\dagger = -T$

BRA-KET NOTATION AND INNER PRODUCTS

- The inner product for orthonormal basis $\{|e_1\rangle, \dots, |e_n\rangle\}$

$$\langle\alpha|\beta\rangle = a_1^* b_1 + a_2^* b_2 + \cdots + a_n^* b_n = \mathbf{a}^\dagger \mathbf{b}$$

- ket $|\beta\rangle$ is a column vector
- bra $\langle\alpha|$ is a complex conjugate row vector

In vector notation:

$$\langle\alpha| \longrightarrow \vec{a} = \begin{pmatrix} a_1^* & a_2^* & \dots & a_N^* \end{pmatrix} \qquad |\beta\rangle \longrightarrow \vec{b} = \begin{pmatrix} b_1 \\ b_2 \\ \vdots \\ b_N \end{pmatrix}$$

OPERATORS AND MATRIX PROPERTIES

- Transpose of a matrix product $\widetilde{ST} = \tilde{T}\tilde{S}$
- Hermitian of a matrix product $(ST)^\dagger = T^\dagger S^\dagger$
- **Inverse matrix** $T^{-1}T = TT^{-1} = 1 = \delta_{ij}$
- Inverse of a matrix product $(ST)^{-1} = T^{-1}S^{-1}$
- **Unitary matrix** $U^\dagger = U^{-1}$
- Unitary operators preserve inner product:

$$\langle\alpha'|\beta'\rangle = \mathbf{a}'^\dagger\mathbf{b}' = (U\mathbf{a})^\dagger(U\mathbf{b}) = \mathbf{a}^\dagger U^\dagger U\mathbf{b} = \mathbf{a}^\dagger\mathbf{b} = \langle\alpha|\beta\rangle$$

CHANGE OF BASIS

- Unitary matrices $U(\longleftarrow U^\dagger = U^{-1})$ preserve inner product
  - Norm doesn't change
  - Angles between vectors don't change

$\longrightarrow$ Apply unitary transformation to orthonormal basis is again orthonormal basis

$$\{|e_1\rangle, |e_2\rangle, \ldots, |e_n\rangle\} \qquad |e_i'\rangle = U|e_i\rangle \quad \text{is orthonormal}$$

If T transforms a basis: $a_i\rangle = T|e_i\rangle$ to another orthonormal one: $\langle a_j|a_i\rangle = \delta_{ij} \Longrightarrow T$ is unitary:

$$\begin{aligned} \delta_{ij} &= \langle a_j|a_i\rangle \\ &= \langle a_j|T|e_i\rangle \qquad \Rightarrow \quad T^\dagger T = 1 \quad \Rightarrow \quad T^\dagger = T^{-1} \\ &= \langle e_j|T^\dagger T|e_i\rangle \end{aligned}$$

COMMUTATORS

- Matrix-multiplication not commutative $\longleftrightarrow$ Order of operators!
- Commutator of two operators/matrices

$$[\hat{S}, \hat{T}] = \hat{S}\hat{T} - \hat{T}\hat{S} \longleftrightarrow [S, T] = S\,T - T\,S$$

- Anti-commutator of two operators/matrices

$$\{\hat{S}, \hat{T}\} = \hat{S}\hat{T} + \hat{T}\hat{S} \longleftrightarrow \{S, T\} = S\,T + T\,S$$

EIGENVALUE PROBLEMS

Eigenvector $\mathbf{x} \neq \mathbf{0}$ and eigenvalues λ of matrix A:

$$A\mathbf{x} = \lambda\mathbf{x} \Leftrightarrow (\lambda 1 - A)\mathbf{x} = \mathbf{0}$$

Because $\mathbf{x} \neq \mathbf{0}$ the inverse of $\lambda 1 - A$ cannot exist, because if it would:

$$\begin{aligned}
(\lambda 1 - A)\mathbf{x} &= \mathbf{0} \\
\implies (\lambda 1 - A)^{-1}(\lambda 1 - A)\mathbf{x} &= (\lambda 1 - A)^{-1}\mathbf{0} \\
\implies (\lambda 1 - A)^{-1}(\lambda 1 - A)\mathbf{x} &= \mathbf{0} \\
\implies \mathbf{x} &= \mathbf{0}
\end{aligned}$$

EIGENVALUE PROBLEMS

- Matrix $(\lambda 1 - A)$ not invertible $\longrightarrow$ the determinant has to be zero
- Solve characteristic equation:

$$\det(\lambda 1 - A) = 0$$

- Determinant is a “characteristic” polynomial in λ
- Highest order of λ is the dimension N of the $N \times N$ matrix
- Solving it means finding λ values

EXAMPLE EIGENVALUE PROBLEM

$$A = \begin{pmatrix} -5 & 2 \\ -7 & 4 \end{pmatrix}$$

This gives for the characteristic equation: $\det(\lambda 1 - A) = 0$:

$$\det\left[\lambda\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} - \begin{pmatrix} -5 & 2 \\ -7 & 4 \end{pmatrix}\right] = 0$$

$$\Longrightarrow \det\left[\begin{pmatrix} \lambda + 5 & -2 \\ 7 & \lambda - 4 \end{pmatrix}\right] = 0$$

The determinant is:

$$\lambda^2 + \lambda - 6 = 0 \longrightarrow (\lambda - 2)(\lambda + 3) = 0$$

EXAMPLE EIGENVALUE PROBLEM CTU'D

- Find eigenvalues λ_i
- Eigenvectors by filling in a specific eigenvalue λ_i

$$A\mathbf{x} = \begin{pmatrix} -5 & 2 \\ -7 & 4 \end{pmatrix} \qquad \lambda_1 = 2, \quad \lambda_2 = -3$$

Eigenvector $\mathbf{x}_1 = (x, y)$ for $\lambda_1 = 2$

$$A = \begin{pmatrix} \lambda_1 + 5 & -2 \\ 7 & \lambda_1 - 4 \end{pmatrix} \begin{pmatrix} x \\ y \end{pmatrix} = \begin{pmatrix} 7 & -2 \\ 7 & -2 \end{pmatrix} \begin{pmatrix} x \\ y \end{pmatrix} = 0$$

$$\implies \mathbf{x} = c \begin{pmatrix} 2 \\ 7 \end{pmatrix}$$

EIGENVALUE PROBLEMS: LARGE MATRICES

- Inverse exists $\Leftrightarrow$ determinant is nonzero
- Determinants of 3×3 or higher order matrices A:

$$\det(A) = \det \begin{pmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{pmatrix}$$

$$= \begin{vmatrix} a_{22} & a_{23} \\ a_{32} & a_{33} \end{vmatrix} a_{11} - \begin{vmatrix} a_{21} & a_{23} \\ a_{31} & a_{33} \end{vmatrix} a_{12} + \begin{vmatrix} a_{21} & a_{22} \\ a_{31} & a_{32} \end{vmatrix} a_{13}$$

$$= (a_{22}a_{33} - a_{23}a_{32})a_{11} - \ldots$$

Characteristic polynomial in λ of order N for $N \times N$ matrix

EIGENVALUE PROBLEMS: SIMPLIFY

- Reduce matrix A to simpler matrix B
- Transform matrix A by invertible matrix T:

$$B = T^{-1}AT \qquad \Longrightarrow \qquad \{\lambda_i\} \quad \text{the same}$$

- Characteristic equation of upper (or lower) triangle matrices B:

$$(\lambda - b_{11})(\lambda - b_{22}) \ldots (\lambda - b_{nn}) = 0$$

- Derive eigenvalues and eigenvectors for B:

$$\Longrightarrow \quad \begin{cases} \text{Eigenvalues} & \lambda_i = b_{ii} \\ \text{Eigenvectors} & \mathbf{x}'_i \text{ of } B = T\mathbf{x}_i \end{cases}$$

QUANTUM MECHANICS & HILBERT SPACE

MATRIX-FORMALISM OF QUANTUM MECHANICS

- Works if only a **finite** sum of basis functions is used
- Approximations possible ?

! General case is PROBLEMATIC !

- Often: infinite number of basis functions
- Inner products might not be finite $\longrightarrow$ not normalizable
- Operators can have infinite expectation values ? Undefined ?

GENERAL QUANTUM MECHANICAL FORMALISM

Mathematical correspondence:

- States: vectors in **Hilbert** space: L^2 square integrable functions
- Observables: **Hermitian** operators: $T^\dagger = T$
- Measurements: Orthogonal **projections**
- Symmetries of the system: **unitary operators**: $U^\dagger = U^{-1}$

Dirac "bra-ket" notation: $\langle \mathrm{bra}|, \quad |\mathrm{ket}\rangle$

- A convenient way of writing
- Implicitly expresses the mathematical properties.

PRE-HILBERT SPACES OR BANACH SPACES

A **Cauchy series**:

- an (infinite) sequence of vectors $v_n \in \mathcal{V} : v_1, v_2, v_3, \ldots$
- has property: for every small value ϵ we can find a finite N:

$$\forall\ m,\ n > N : \quad \|v_n - v_m\| < \varepsilon \quad \text{with } v_n, v_m \in \mathcal{V}$$

- A Cauchy series converges to a certain “vector” v that can be outside $\mathcal{V}$.

A **Banach space**:

- Is a *normed vector space*
- *Every Cauchy series converges* to an element v of the vector space: $v \in \mathcal{V}$.
    - Example: any Cauchy series of real numbers $x_n \in \mathbb{R}$ converges in $\mathbb{R}$
    - Example: Cauchy series of rational numbers $x_n = \frac{1}{2^n} \in \mathbb{Q}$ doesn’t converge in $\mathbb{Q}$

HILBERT SPACES

A **Hilbert space**

- Has an *inner product*
- Has its norm derived from the inner product: $\|\alpha\| = \sqrt{\langle\alpha|\alpha\rangle}$
- Is a Banach space

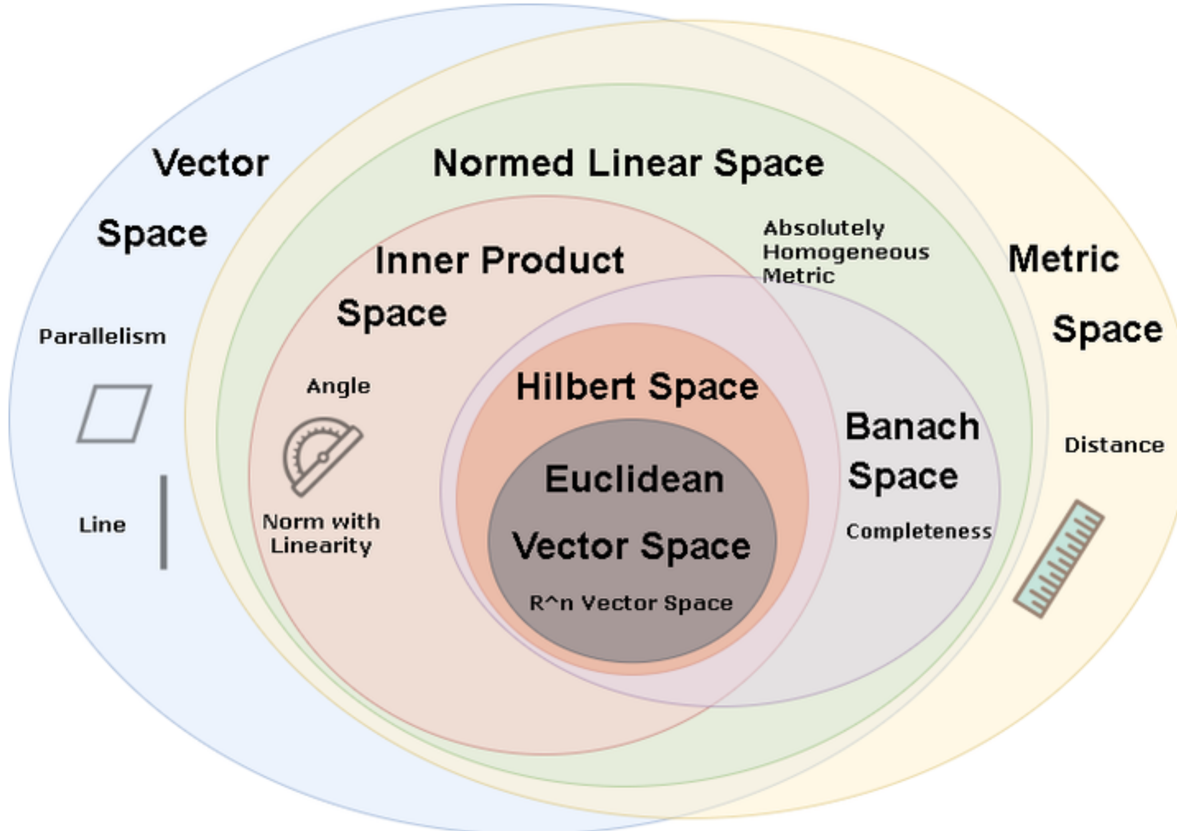
Vectors in Hilbert space are **well-behaved**

- Similar to vectors in $\mathbb{R}^N$
- Existance of complete orthonormal basis
- Applying **most** linear operators gives again a vector in the same space
- Definition Hermitian conjugate of an operator:

$$\langle\hat{T}^\dagger\alpha|\beta\rangle = \langle\alpha|\hat{T}\beta\rangle$$

SUMMARY OF VECTOR SPACES/PROPERTIES

- Vector space:
  - Addition: $|\alpha\rangle + |\beta\rangle$
  - Scalar multiplication: c |
- Inner product: $\langle\alpha|\beta\rangle$
- Norm: $\|\alpha\| = \langle\alpha|\alpha\rangle$
- Banach space: Cauchy complete
- Hilbert space:
  - Cauchy complete
  - Inner product with norm



WAVE FUNCTIONS IN HILBERT SPACE

Quantum mechanics $\longrightarrow$ specific Hilbert space: $L^2(a, b)$

- functions $f(x)$ square integrable over interval $[a, b]$

$$\|f\|^2 = \int_a^b |f(x)|^2 dx < \infty$$
$$\Longrightarrow f(x) \quad \text{normalizable}$$

- Inner product $\langle f|g\rangle$ given by:

$$\langle f|g\rangle = \int_a^b f(x)^* g(x) dx \leq 1 \qquad \text{norm: } \|f\| = \sqrt{\langle f|f\rangle}$$

The last inequality requires normalized $f(x)$ and $g(x)$

WAVE FUNCTIONS IN HILBERT SPACE

- Schwartz inequality $\Longrightarrow$ inner product is finite

$$|\langle f|g\rangle| \leq \sqrt{\langle f|f\rangle\langle g|g\rangle}$$

- Orthonormal complete set of basis vectors $\{|f_n\rangle\}$

$$\langle f_m|f_n\rangle = \int_a^b f_m(x)^* f_n(x)dx = \delta_{mn}$$

$$|f\rangle = \sum_n c_n\,|f_n\rangle, \qquad c_n = \langle f_n|f\rangle = \int_a^b f_n(x)^* f(x)dx$$

$\longrightarrow$ We will use sometimes f, g instead of $|\psi\rangle$, $|\psi_n\rangle$, etc. for (wave) functions

OBSERVABLES

- Observables are represented by measurement operators

$$\langle Q \rangle = \int \Psi^* \hat{Q} \Psi \, dx = \langle \Psi | \hat{Q} \Psi \rangle$$

Since measurements need to be real: $\langle Q \rangle = \langle Q \rangle^*$

$$\langle \Psi | \hat{Q} \Psi \rangle = \langle \hat{Q} \Psi | \Psi \rangle$$

$\implies$ The operator $\hat{Q} = \hat{Q}^\dagger$ is Hermitian

- In a finite basis: Hermitian operators $\iff$ Hermitian matrices

WHICH OPERATORS ARE HERMITIAN?

- Check this for $\hat{p} = -i\hbar \frac{d}{dx}$:

$$\begin{aligned}
\langle f|\hat{p}g\rangle &= \langle f| -i\hbar \frac{d}{dx} g\rangle \\
&= -i\hbar \int f(x)^* \frac{dg(x)}{dx} dx \\
&= -f(x)^* g(x)\Big|_{-\infty}^{+\infty} + i\hbar \int \frac{df(x)^*}{dx} g(x) dx \\
&= i\hbar \int \frac{df(x)^*}{dx} g(x) dx \\
&= \langle -i\hbar \frac{d}{dx} f|g\rangle \\
&= \langle \hat{p} f|g\rangle
\end{aligned}$$

$\longrightarrow$ Important that f and g become zero at $x = \pm\infty$

DETERMINATE STATES OF OBSERVABLES

- Perform independent measurements $\longrightarrow$ different outcomes (probabilistic)
- A determinate state $\longrightarrow$ every time the same outcome
- For a determinate state $|\Psi\rangle$ for Q: $\quad Q \longrightarrow \langle Q \rangle = q$ is a constant

$$\Longrightarrow \sigma^2 = \langle (Q - \langle Q \rangle)^2 \rangle = \langle \Psi | (Q - q)^2 \Psi \rangle = \langle (Q - q)\Psi | (Q - q)\Psi \rangle = 0$$

$$\Longrightarrow (Q - q)|\Psi\rangle = |0\rangle \quad \Longrightarrow \quad Q|\Psi\rangle = q|\Psi\rangle$$

- Hermitian operator $\hat{Q}$ has eigenvalue q
- The determinate state is an eigenstate of $\hat{Q}$

SPECTRUM: EIGENVALUES OF AN OPERATOR

- Spectrum of an operator: all eigenvalues
- Multiplicity or degeneracy: same eigenvalue for 2 or more eigenstates
- Hamiltonian operator is the standard example

$$\hat{H}|\psi\rangle = E|\psi\rangle$$

- Two types of spectra:
  - **Discrete spectrum**: spaced eigenvalues, normalizable eigenstates (e.g. infinite well)
  - **Continuous spectrum**: Continuous range of eigenvalues, **non-normalizable eigenstates** (e.g. free particle)
  - Possible mixture of both (e.g. finite well)

SPECTRUM: EIGENVALUES OF AN OPERATOR

Eigenvalues spectrum

↙ ↓ ↘

Discrete spectrum
Eigenfunctions: normalizable
(q_n, Ψ_n)

Continuous spectrum
Eigenfunctions: NOT normalizable
(q_n, f_n)

Mixture of discrete & continuous spectrum

DISCRETE SPECTRUM

1. Eigenvalues of operator $\hat{Q}$ are real:

$$\text{Assume eigenvalue } q \quad \hat{Q}f = qf$$

$$\Longrightarrow q\langle f|f\rangle = \langle f|\hat{Q}f\rangle = \langle \hat{Q}f|f\rangle = q^*\langle f|f\rangle$$

2. Eigenfunction of different eigenvalues are orthogonal

$$\text{Assume:} \quad \hat{Q}f = qf \qquad \hat{Q}g = q'g$$

$$\Longrightarrow q'\langle f|g\rangle = \langle f|\hat{Q}g\rangle = \langle \hat{Q}f|g\rangle = q^*\langle f|g\rangle$$
$$\Longrightarrow q' = q^* = q$$

DISCRETE SPECTRUM

Properties

1. Real eigenvalues
2. Eigenfunction of different eigenvalues are orthogonal: $\langle f_m | f_n \rangle = \delta_{mn}$
3. Degenerate eigenvalues can exist, but we can choose orthonormal basis of those eigenfunctions
4. Finite dimensional spaces are complete

Axiom: Any **observable operator** in Hilbert space has a complete basis of eigenfunctions

$$f(x) = \sum_n c_n f_n(x), \qquad \text{with} \quad c_n = \langle f_n | f \rangle = \int f_n(x)^* f(x) dx$$

$\Longrightarrow$ Observable operators are **Hermitian** and have a **complete basis of eigenfunctions**

DISCRETE SPECTRUM: STATISTICAL INTERPRETATION

- wave function $\Psi(x,t)$ and eigenfunctions f_n : $\hat{Q} f_n = q_n f_n$
- Wave function can be expanded in f_n:

$$\Psi(x,t) = \sum_n c_n(t) f_n(x), \qquad \text{with} \quad c_n(t) = \langle f_n | \Psi \rangle = \int f_n(x)^* \Psi(x,t) dx$$

- Measure expectation with **observable** operator $\hat{Q}$: $\langle \Psi | \hat{Q}\, \Psi \rangle$

$$\begin{aligned} \langle \hat{Q} \rangle = \langle \Psi | \hat{Q}\, \Psi \rangle &= \left\langle \sum_m c_m(t) f_m(x) \middle| \hat{Q} \sum_n c_n(t) f_n(x) \right\rangle \\ &= \sum_m \sum_n c_m(t)^* c_n(t) q_n \langle f_m(x) | f_n(x) \rangle \\ &= \sum_m \sum_n c_m(t)^* c_n(t) q_n \delta_{mn} = \sum_n |c_n(t)|^2 q_n \end{aligned}$$

SPECTRUM: EIGENVALUES OF AN OPERATOR

Eigenvalues spectrum

Discrete spectrum
Eigenfunctions: normalizable
(q_n, Ψ_n)

Continuous spectrum
Eigenfunctions: NOT normalizable
(q_n, f_n)

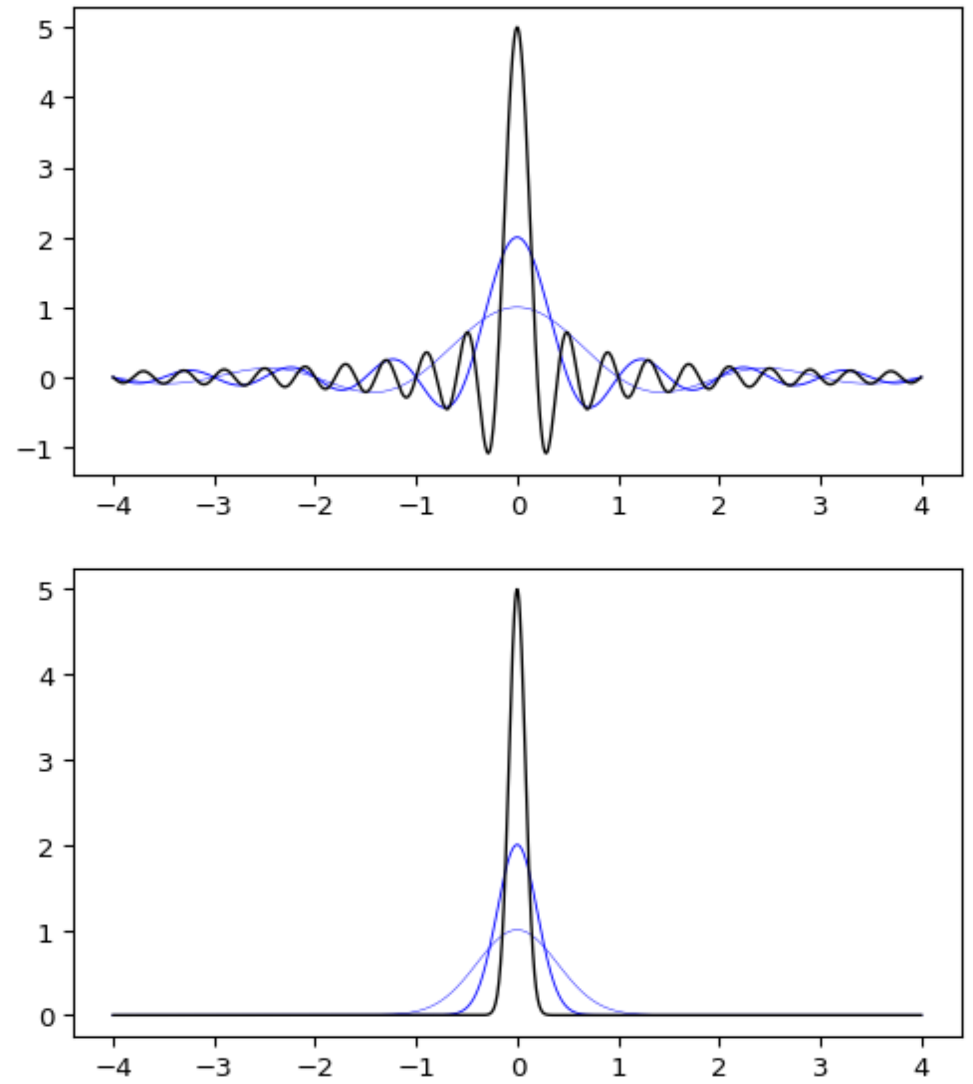
Mixture of discrete & continuous spectrum

INTERMEZZO: THE DIRAC DELTA FUNCTION

Dirac delta distribution:

$$\begin{cases} \delta(x \neq 0) = 0 \\ \delta(x = 0) = +\infty \end{cases}$$

$$\int_{-\infty}^{+\infty} \delta(x) = 1$$



Limit of series of functions:

- peaked such as sinc(x) or Gaussian
- limit to infinitely *thin* and *high*
- Area kept normalized

Filters out single point:

$f(a) = \int_{-\infty}^{+\infty} f(x)\,\delta(x-a)\,dx$

CONTINUOUS SPECTRA

- Eigenfunctions/values continuous variable $z \longrightarrow f_z$
- Eigenfunctions are **NOT** normalizable
- Solution: **Assume real eigenvalues**
- New definitions:

$$\text{Orthonormality} \qquad \langle f_{z'} | f_z \rangle = \delta(z' - z)$$

$$\text{Completeness} \qquad f(x) = \int c(z) f_z dz \qquad \text{with} \quad c(z) = \langle f_z | f \rangle$$

$$\langle f_{z'} | f \rangle = \int c(z) \langle f_{z'} | f_z \rangle dz = \int c(z) \delta(z' - z) dz = c(z')$$

CONTINUOUS SPECTRA: EXAMPLE

Momentum operator for a free particle

Momentum eigenvalue equation:

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

- Filling in momentum operator $\hat{p} = -i\hbar\frac{d}{dx}$:

$$\frac{d\psi_p(x)}{dx} = \frac{ip}{\hbar}\psi_p(x)$$

This differential equation has solution:

$$\psi_p(x) = Ae^{ipx/\hbar} = \frac{1}{\sqrt{2\pi}}e^{ipx/\hbar}$$

CONTINUOUS SPECTRA: EXAMPLE

Momentum operator for a free particle

Eigenvalues and eigenfunctions:

$$-i\hbar\frac{d}{dx}f_p(x) = pf_p(x) \quad \text{with} \qquad f_p(x) = Ae^{ipx/\hbar}$$

If eigenvalues $p \in \mathbb{R}$ then $\{f_p\}$ is orthogonal:

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

Completeness follows from Fourier analysis:

$$f(x) = \int c(p)f_p(x)dp = \frac{1}{\sqrt{2\pi\hbar}}\int c(p)e^{ipx/\hbar}dp$$

CONTINUOUS SPECTRA: EXAMPLE

Momentum operator for a free particle

Completeness follows from Fourier analysis:

$$f(x) = \int c(p) f_p(x) dp = \frac{1}{\sqrt{2\pi\hbar}} \int c(p) e^{ipx/\hbar} dp$$

The coefficients $c(p)$ are as expected:

$$\langle f_{p'} | f_p \rangle = \int c(p) f^*_{p'} \, f_p \, dp = \int c(p) \delta(p - p') dp = c(p')$$

- Eigenfunctions f_p NOT normalizable $\longrightarrow$ don't exist
- BUT: Dirac orthonormal ($\langle f_{p'} | f_p \rangle = \delta(p - p')$) + complete

$\longrightarrow$ Create normalized wave function from superposition

QUANTUM STATES

WAVE FUNCTION VERSUS STATE

State of a system at t represented by vector in Hilbert space: $|S(t)\rangle$

- Represented by the wave function $\Psi(x,t) = \langle x|S(t)\rangle$
- Represented by the wave function in momentum space $\Phi(p,t) = \langle p|S(t)\rangle$
- Represented in the basis of stationary eigenstates $c_n(t) = \langle n|S(t)\rangle$

We can write the state in any basis:

$$|S(t)\rangle \quad \longrightarrow \quad \int \Psi(x,t)\delta(x-x')\,dx'$$
$$= \int \Phi(p,t)\frac{1}{\sqrt{2\pi\hbar}}e^{ipx/\hbar}\,dp'$$
$$= \sum_{n=1}^{+\infty} c_n(t)e^{-iE_nt/\hbar}\psi_n(x)$$

EIGENSTATES AS BASIS IN HILBERT SPACE

- The wave function of a quantum state $|\Psi(t)\rangle$

$$\Psi(x,t) = \langle x|\Psi(t)\rangle, \qquad \hat{x}|x\rangle = x_0|x\rangle$$

$\longrightarrow \quad x_0$ are eigenvalues of position operator $\hat{x}$

$$\langle x_0|\Psi(t)\rangle = \int_{-\infty}^{\infty} \delta(x - x0)\psi(x)dx = \psi(x_0)$$

MOMENTUM EIGENVECTORS?

Momentum eigenvalue equation:

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

- Filling in momentum operator $\hat{p} = -i\hbar\frac{d}{dx}$:

$$\frac{d\psi_p(x)}{dx} = \frac{ip}{\hbar}\psi_p(x)$$

This differential equation has solution:

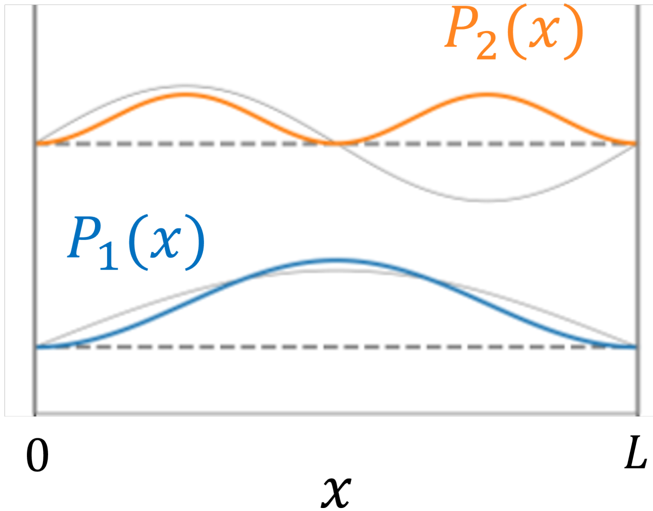
$$\psi_p(x) = Ae^{ipx/\hbar} = \frac{1}{\sqrt{2\pi}}e^{ipx/\hbar}$$

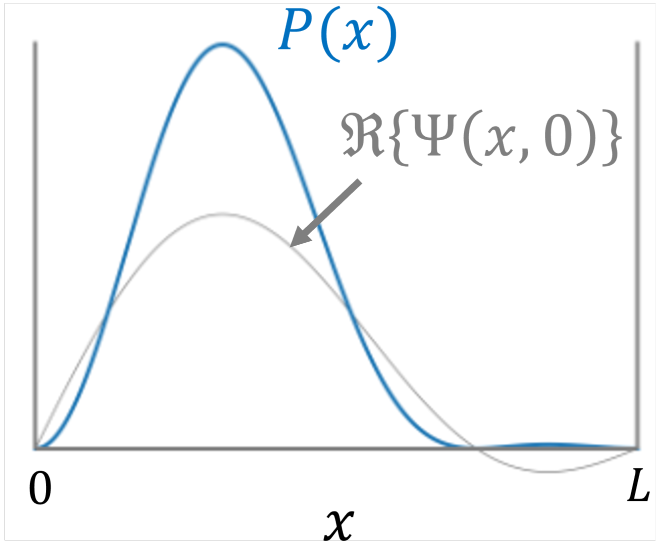
OPERATORS, MEASUREMENTS, AND COLLAPSE

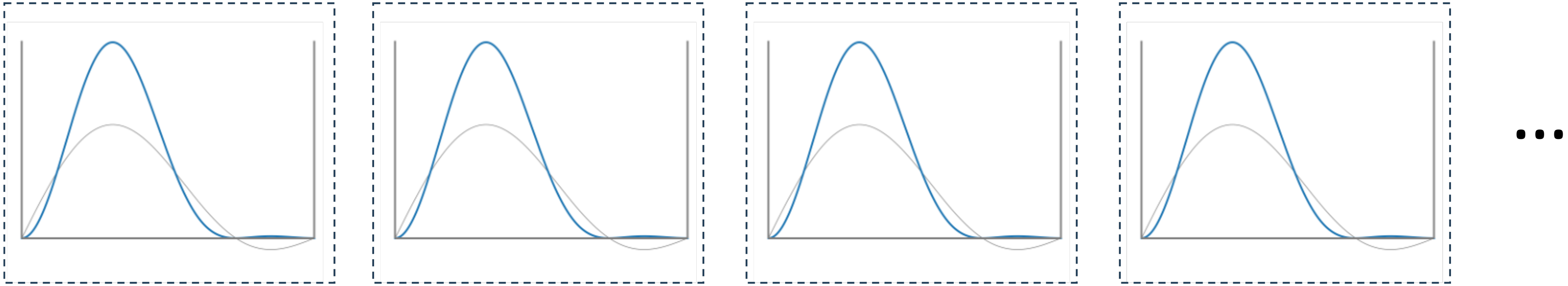
OBSERVABLES, OPERATORS AND COLLAPSE

- We can measure observables:
  - position and momentum of a particle,
  - energy of a particle in a potential,
  - excitation-level of an electron in an atom
  - spin of an electron
  - …
- Before measurement
  - superposition of eigenstates
  - Probability to find a particle in x: $|\Psi(x,t)|^2$
  - $\Psi(x,t) = \sum c_n(t)\psi_n(x) \longrightarrow P(n) = |c_n(t)|^2$
- Measurement: system collapses to single eigenstate

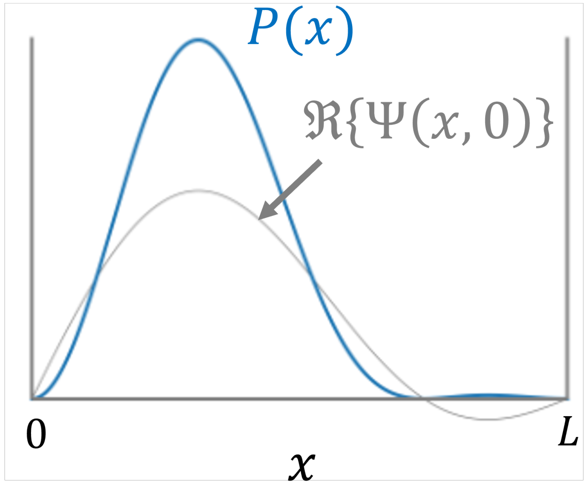
INFINITE WELL



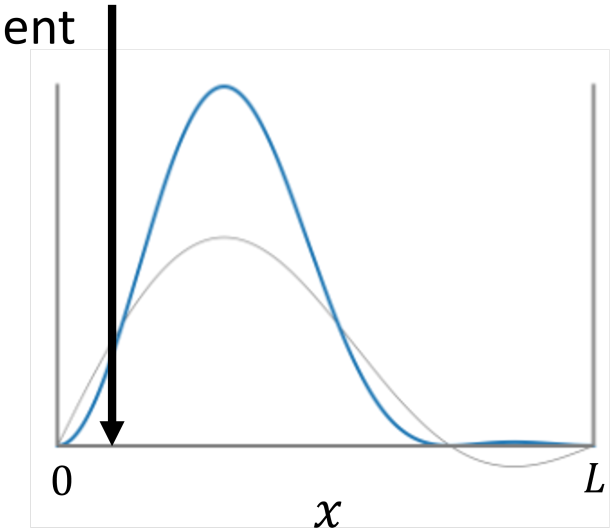




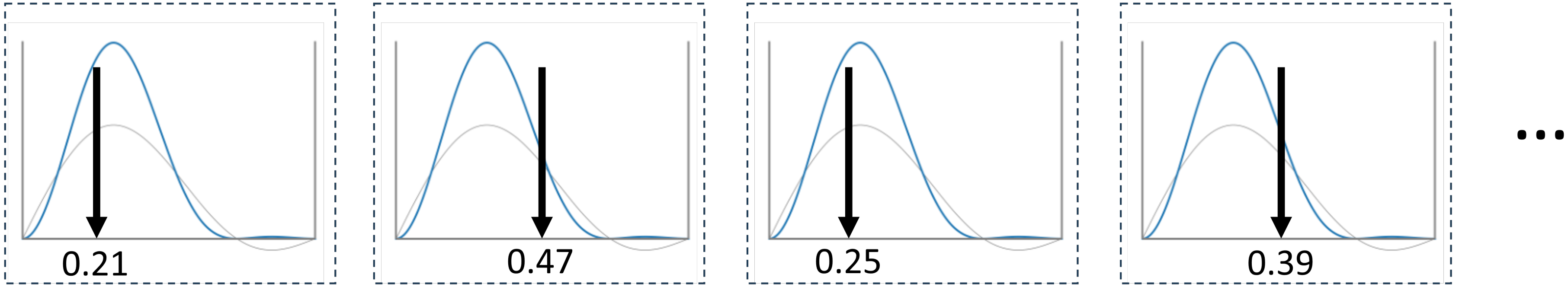
INFINITE WELL: OBSERVABLE POSITION



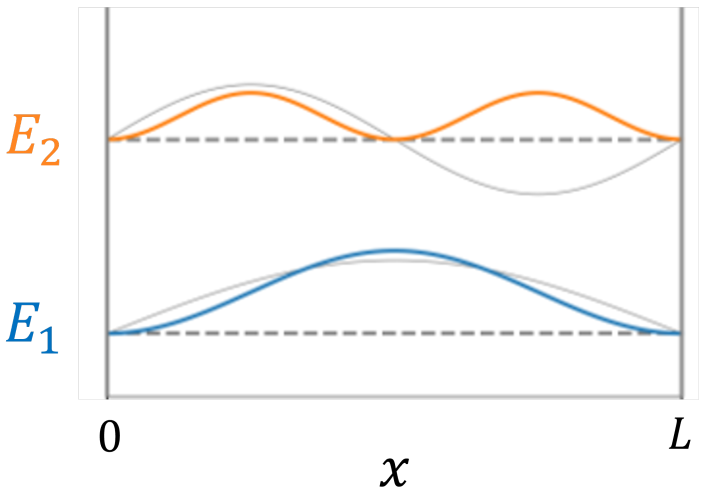
Position (x)
measurement



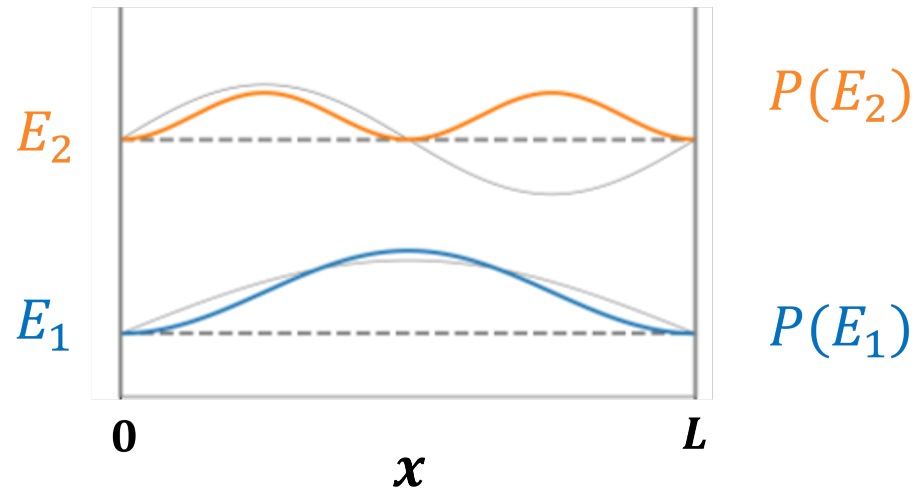
Every measurement probabilistic BUT average position $\langle x \rangle \propto \int_0^L P(x)\, x\, dx$

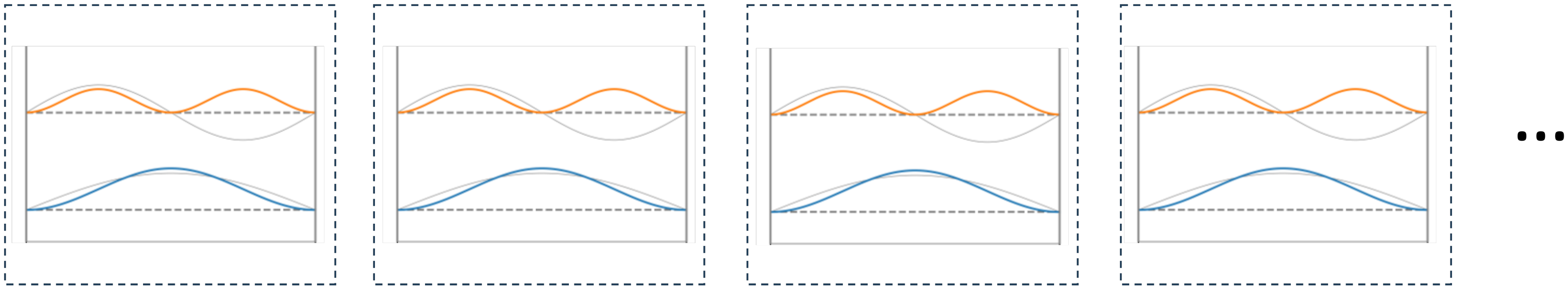


INFINITE WELL: ENERGIES



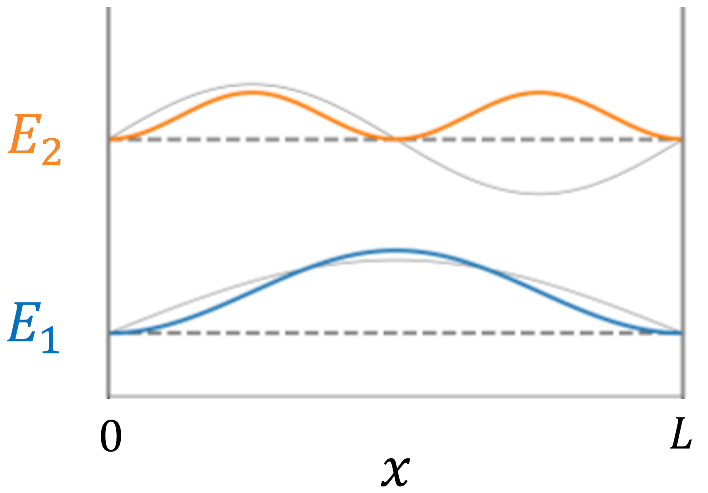
Energy (E_n) measurement

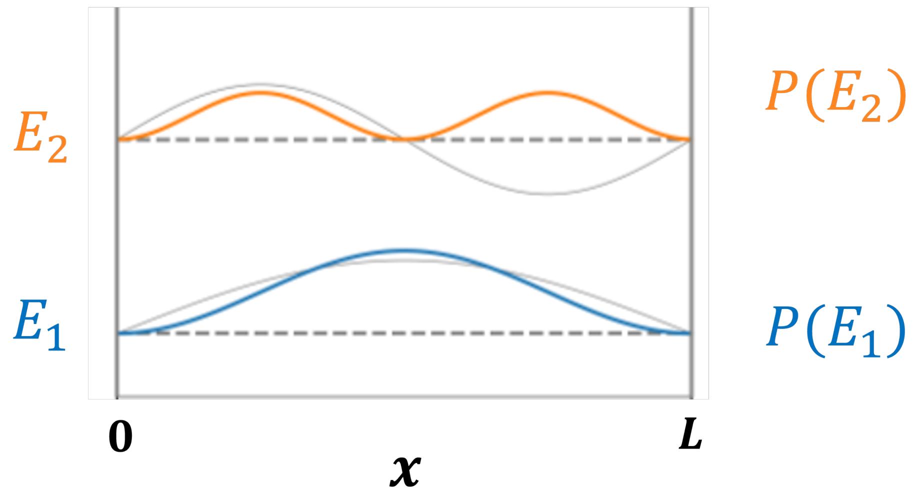




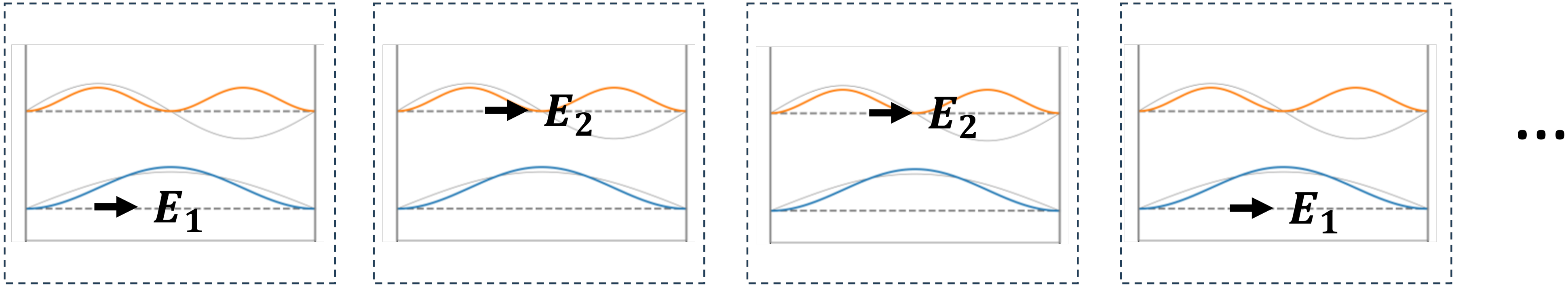
INFINITE WELL: OBSERVABLE ENERGY

Energy (E_n) measurement

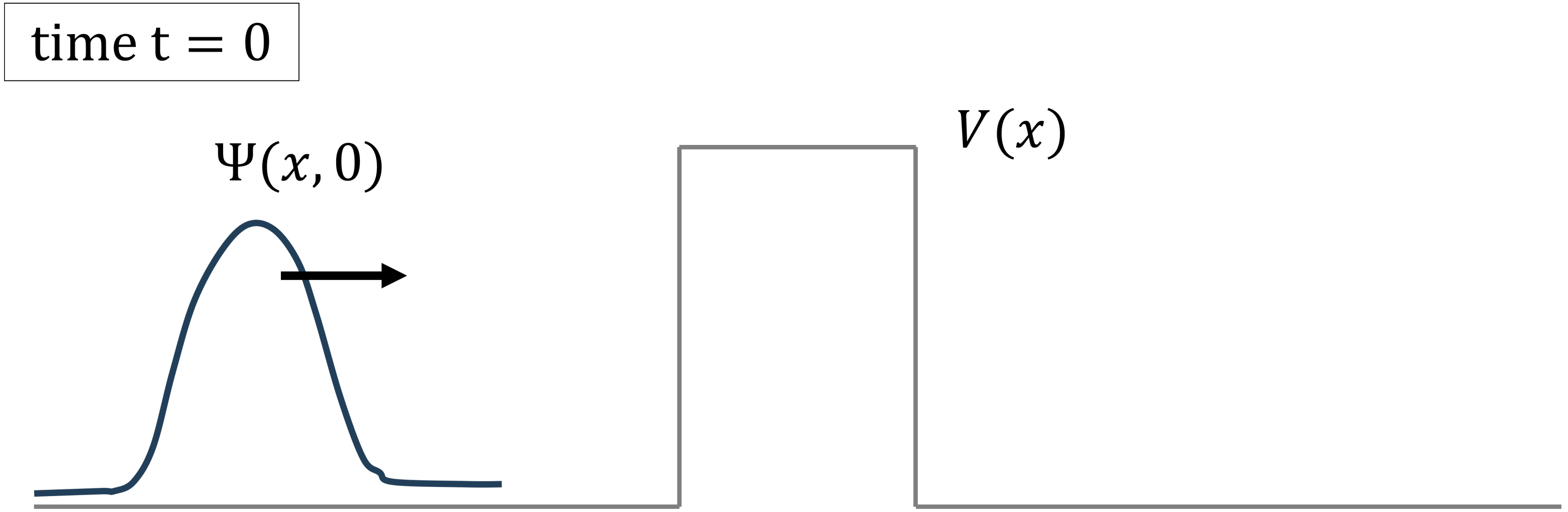


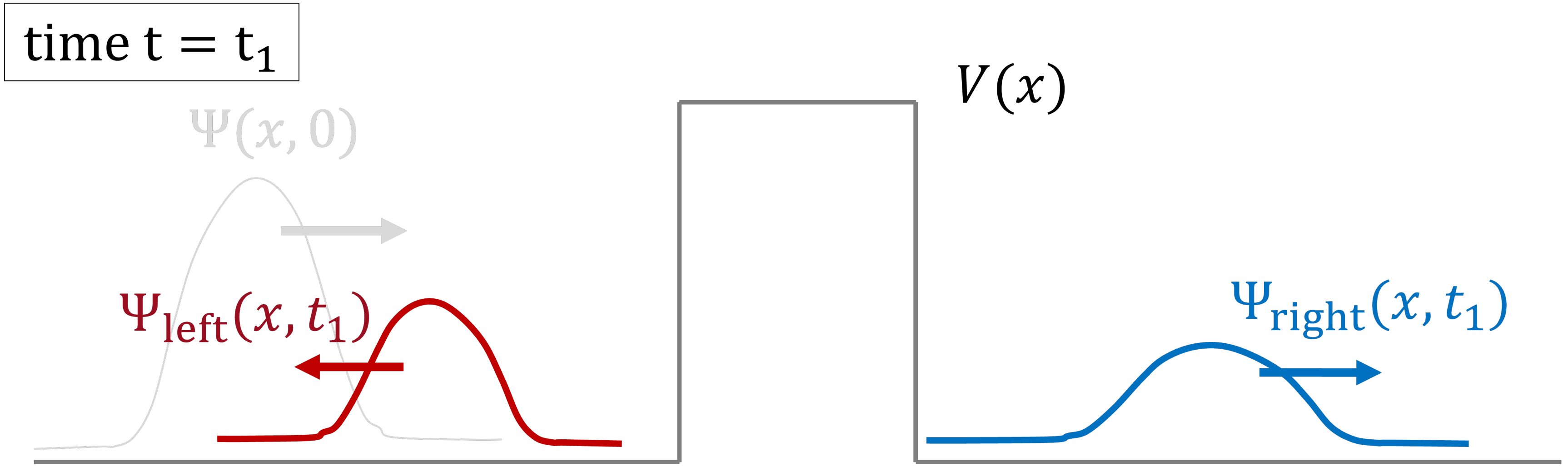


Every measurement probabilistic BUT average energy $\langle H \rangle \propto \sum_n P(E_n) E_n$

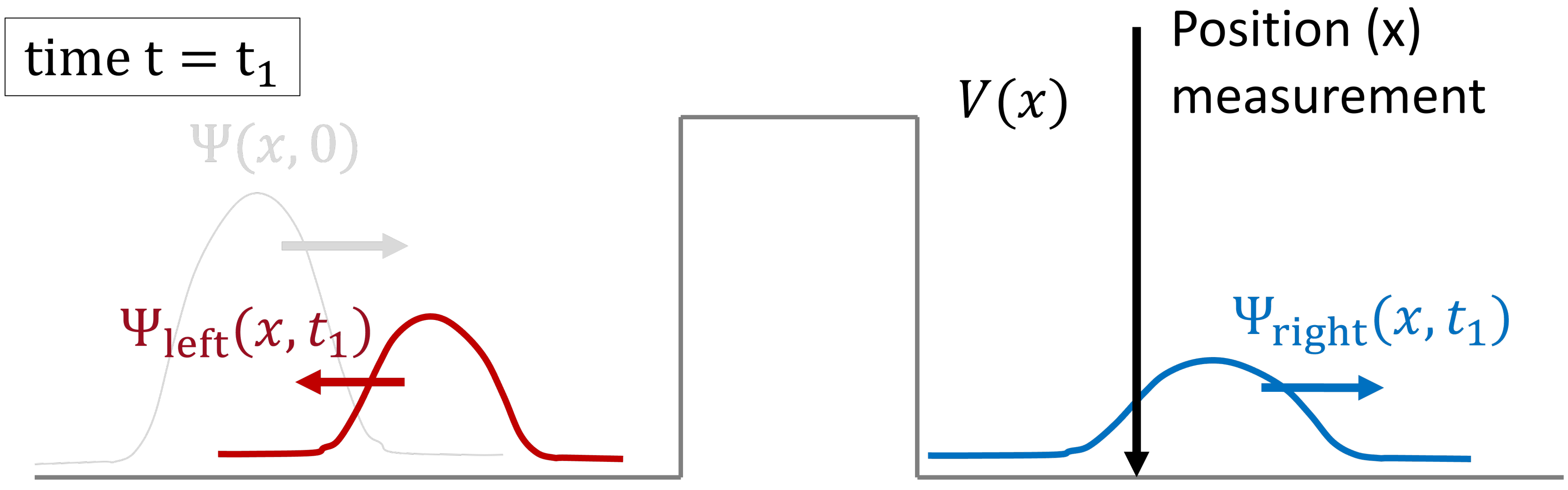


WAVEPACKET INCIDENT ON BARRIER

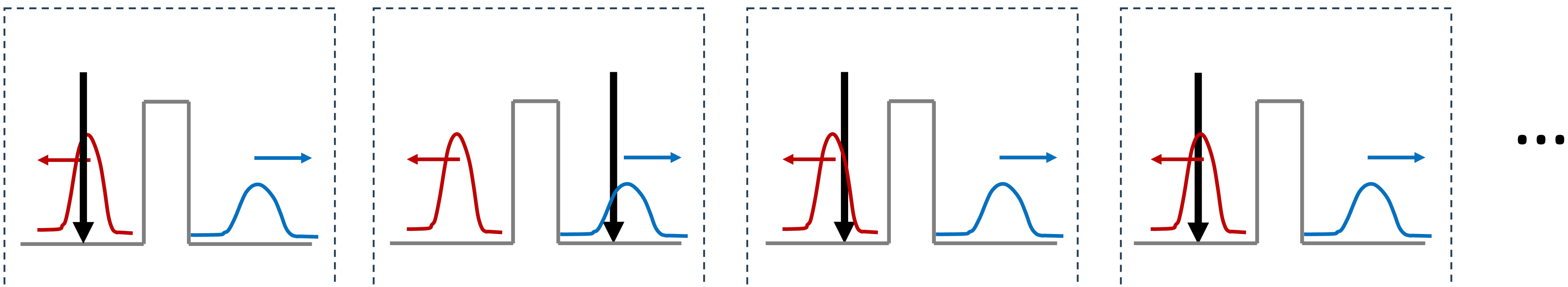




WAVEPACKET: OBSERVABLE POSITION



Every measurement probabilistic BUT average position $\langle x \rangle \propto \int_0^L P(x)\, x\, dx$



OBSERVABLES, OPERATORS AND COLLAPSE

- State of a quantum system: $|\Psi\rangle$
- Wave function represents state: $\langle x|\Psi(t)\rangle \longrightarrow \Psi(x,t)$
- Observable is something we can measure (a real number)
- Observable Q corresponds to an Hermitian operator $\hat{Q}$
- Measuring NOT same as applying operator $\hat{Q}|\Psi\rangle$

- Measurement operators DON'T always commute (**incompatible** observables)
- Incompatible observables $\longrightarrow$ **NO common basis** of eigenfunctions

UNCERTAINTY PRINCIPLE

- Heisenberg uncertainty principle

$$\sigma_x \sigma_p \geq \frac{\hbar}{2}$$

- Commutator is nonzero:

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

- Can’t measure position and momentum at the same time
- Measuring position *destroys* the momentum measurement

GENERALIZED UNCERTAINTY PRINCIPLE

- **General** uncertainty principle is related to the commutator

$$\boxed{\sigma_A^2 \sigma_B^2 \geq \left(\frac{1}{2i} \left\langle \left[\hat{A}, \hat{B} \right] \right\rangle \right)^2}$$

- Number between brackets is real but can be negative
- We need the square at the right-hand-side
- Commutating operators $\longrightarrow$ no restriction on σ_A, σ_B

How to proof this?

EXAMPLE UNCERTAINTY PRINCIPLE

- General uncertainty principle for position/momentum
- The commutator for $\hat{x}$ and $\hat{p}$:

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

Fill in in general uncertainty formula:

$$
\begin{aligned}
& \sigma_A^2 \sigma_B^2 \geq \left(\frac{1}{2i} \left\langle \left[\hat{A}, \hat{B} \right] \right\rangle \right)^2 \\
\Rightarrow \quad & \sigma_x^2 \sigma_p^2 \geq \left(\frac{1}{2i} \langle [\hat{x}, \hat{p}] \rangle \right)^2 = \left(\frac{1}{2i} \langle i\hbar \rangle \right)^2 = \frac{\hbar^2}{4} \\
\Rightarrow \quad & \sigma_x \sigma_p \geq \frac{\hbar}{2}
\end{aligned}
$$

$\longrightarrow$ Heisenberg uncertainty principle

COMMUTATORS AND UNCERTAINTY

$$\boxed{\sigma_A^2 \sigma_B^2 \geq \left(\frac{1}{2i} \left\langle \left[\hat{A}, \hat{B} \right] \right\rangle \right)^2}$$

- **Compatible observables**: Commutating observables $[\hat{A}, \hat{B}] = 0$
  - Measurements independent, order doesn't matter
  - No restriction on the common **uncertainty** of the measurement
  - A common basis of eigenstates can be found
- **Incompatible observables**: Non-commutating observables $[\hat{A}, \hat{B}] \neq 0$
  - **Order** of the measurement **matters** !
  - **Minimum uncertainty** on the measurements according to formula
  - **NO common basis** of eigenstates can be found

DIRAC NOTATION

BRACKETS: BRA'S AND KETS

- Inner product in matrix notation (separate "vectors")

$$\langle\alpha|\beta\rangle = \begin{pmatrix} a_1^* & a_2^* & \dots & a_n^* \end{pmatrix} \begin{pmatrix} b_1 \\ b_2 \\ \vdots \\ b_n \end{pmatrix} = a_1^* b_1 + a_2^* b_2 + \dots a_n^* b_n$$

- "bra" acts on the ket by row vector multiplication
- "bra" *vector* is separate from the "ket" vector: bra sits in a **dual vector space**
- Now with possible infinite basis:

$$\langle\alpha| = \sum_j a_j^* (\dots)_j \quad \longrightarrow \quad \langle\alpha| = \int \alpha^* (\dots) dx$$

BRACKETS: BRA'S AND KETS

- Kets are vectors in vector space
- Bra's are vectors in dual space
- In finite dimensions:
  - kets are column vectors
  - bra's are complex conjugate row vectors

$$\langle \text{bra}| = \langle \alpha| = \begin{pmatrix} a_1^* & a_2^* & \dots & a_n^* \end{pmatrix}$$

$$|\text{ket}\rangle = |\beta\rangle = \begin{pmatrix} b_1 \\ b_2 \\ \vdots \\ b_n \end{pmatrix}$$

DUAL SPACE AND HERMITIAN CONJUGATES

- Converting a $|\mathrm{ket}\rangle$ to a $\langle bra|$ and vice versa:

$$\langle\alpha| = |\alpha\rangle^\dagger$$

- An operator acting on a $\langle bra|$:

$$\langle\alpha|\hat{Q}^\dagger = \langle\hat{Q}\alpha| = \left(\hat{Q}|\alpha\rangle\right)^\dagger$$

$\longrightarrow$ operators can *act to the left* as this is allowed by associativity

- *Why is this?* See definition of Hermitian conjugate of operators:

$$\langle\hat{Q}^\dagger\alpha|\beta\rangle = \langle\alpha|\hat{Q}\beta\rangle$$

IN FINITE DIMENSIONS: MATRIX-FORMALISM

- Example in two dimensions, an operator acting on a $|\alpha\rangle = \begin{pmatrix} a_1 \\ a_2 \end{pmatrix}$:

$$\hat{Q}|\alpha\rangle = Q\mathbf{a} = \begin{pmatrix} Q_{11} & Q_{12} \\ Q_{21} & Q_{22} \end{pmatrix} \begin{pmatrix} a_1 \\ a_2 \end{pmatrix} = \begin{pmatrix} Q_{11}a_1 + Q_{12}a_2 \\ Q_{21}a_1 + Q_{22}a_2 \end{pmatrix}$$

The Hermitian conjugate gives

$$\langle\alpha|\hat{Q}^\dagger = \mathbf{a}^\dagger Q^\dagger = \begin{pmatrix} a_1^* & a_2^* \end{pmatrix} \begin{pmatrix} Q_{11}^* & Q_{21}^* \\ Q_{12}^* & Q_{22}^* \end{pmatrix} = \begin{pmatrix} Q_{11}^* a_1^* + Q_{12}^* a_2^* & Q_{21}^* a_1^* + Q_{22}^* a_2 \end{pmatrix}$$

For this example we indeed see that:

$$\langle\alpha|\hat{Q}^\dagger = \left(\hat{Q}|\alpha\rangle\right)^\dagger$$

THE PROJECTION OPERATOR

- The projection operator defined for a normalized $|\alpha\rangle$:

$$\hat{P}_\alpha = |\alpha\rangle\langle\alpha|$$

$\longrightarrow$ Projects any other vector $|\beta\rangle$ onto the direction of $|\alpha\rangle$:

$$\hat{P}_\alpha|\beta\rangle = (\langle\alpha|\beta\rangle)\,|\alpha\rangle$$

Example: projection in two dimensions

$$|\alpha\rangle = \frac{1}{\sqrt{5}}\begin{pmatrix} 1 \\ 2i \end{pmatrix}, \quad |\beta\rangle = \begin{pmatrix} 2 \\ 1 \end{pmatrix}$$

$$\hat{P}_\alpha|\beta\rangle = |\alpha\rangle\langle\alpha|\beta\rangle = \frac{1}{5}\begin{pmatrix} 1 \\ 2i \end{pmatrix}\begin{pmatrix} 1 & -2i \end{pmatrix}\begin{pmatrix} 2 \\ 1 \end{pmatrix} = \frac{2}{5}(1-i)\begin{pmatrix} 1 \\ 2i \end{pmatrix}$$

THE PROJECTION OPERATOR: EXAMPLE

Example: projection in two dimensions

$$|\alpha\rangle = \frac{1}{\sqrt{5}}\begin{pmatrix} 1 \\ 2i \end{pmatrix}, \quad |\beta\rangle = \begin{pmatrix} 2 \\ 1 \end{pmatrix}$$

$$\hat{P}_\alpha|\beta\rangle = |\alpha\rangle\langle\alpha|\beta\rangle = \frac{1}{5}\begin{pmatrix} 1 \\ 2i \end{pmatrix}\begin{pmatrix} 1 & -2i \end{pmatrix}\begin{pmatrix} 2 \\ 1 \end{pmatrix} = \frac{2}{5}(1-i)\begin{pmatrix} 1 \\ 2i \end{pmatrix}$$

The operator itself is an **outer product**:

$$\hat{P}_\alpha = |\alpha\rangle\langle\alpha| = \frac{1}{5}\begin{pmatrix} 1 \\ 2i \end{pmatrix}\begin{pmatrix} 1 & -2i \end{pmatrix} = \frac{1}{5}\begin{pmatrix} 1 & -2i \\ 2i & 4 \end{pmatrix}$$

Two-dimensional vector spaces are actually useful: Spin, the two-level atom approximation, etc.

IDENTITY OPERATORS

- If we have a complete basis $\{ |e_n\rangle \}$
- Projection operator:

$$\hat{P}_n = |e_n\rangle\langle e_n|$$

Then the identity operator can be written as:

$$\boxed{\sum_n \hat{P}_n = \sum_n |e_n\rangle\langle e_n| = \hat{1}}$$

Or for a continuous spectrum and eigenfunction basis:

$$\langle e_z|e'_z\rangle = \delta(z - z') \qquad \boxed{\int |e_z\rangle\langle e_z|\, dz = \hat{1}}$$

FUNCTIONS OF OPERATORS: POWER SERIES

- Sums and products of operators, **order is important**:

$$(\hat{Q} + c\hat{R})|\alpha\rangle = \hat{Q}|\alpha\rangle + c\hat{R}|\alpha\rangle \qquad \hat{Q}\hat{R}|\alpha\rangle = \hat{Q}\left(\hat{R}|\alpha\rangle\right)$$

- Functions of operators are represented by their **power series**
- Likewise with matrices (also operators in our case):

$$e^{\hat{Q}} = 1 + \hat{Q} + \frac{1}{2}\hat{Q}^2 + \frac{1}{3!}\hat{Q}^3 + \dots$$

$$\frac{1}{1-\hat{Q}} = 1 + \hat{Q} + \hat{Q}^2 + \hat{Q}^3 + \hat{Q}^4 + \dots$$

$$\ln(1+\hat{Q}) = \hat{Q} - \frac{1}{2}\hat{Q}^2 + \frac{1}{3}\hat{Q}^3 - \frac{1}{4}\hat{Q}^4 \dots$$