Lecture 10: Coordinate and Momentum Representations

• We will start by considering the quantum description of the motion of a particle in one dimension.

• In classical mechanics, the state of the particle is given by its position and momentum coordinates, $x$ and $p$.

• In quantum mechanics, we will consider position and momentum as observables and therefore represent them by Hermitian operators, $X$ and $P$, respectively.

• Based on experimental evidence, we have deduced that:

$$[X,P] = i\hbar I$$
Incompatible Observables

- If two operators do not commute, then an eigenstate of one cannot be an eigenstate of the other.

Proof:

- Strategy: assume opposite and show contradiction
- Assume \( |a,b\rangle \) such that
  \[
  A |a,b\rangle = a |a,b\rangle \\
  B |a,b\rangle = b |a,b\rangle
  \]
- Operate on \( |a,b\rangle \) with \( M := [A,B] \)
  \[
  M(a,b) = AB|a,b\rangle - BA|a,b\rangle \\
  = bA|a,b\rangle - aB|a,b\rangle \\
  = (ba-ab)|a,b\rangle 
  \]
  \[\Rightarrow M|a,b\rangle = 0\]

- Either \( \det |M| = 0 \) or \( |a,b\rangle = 0 \)

- If \( \det |M| \neq 0 \) then \( |a,b\rangle \) does not exist
  - Then \( A \) and \( B \) are compatible

- If \( \langle A,b| = 0 \), then \( M = 0 \), \( |a,b\rangle \) do exist
  - Then \( A \) and \( B \) are incompatible
Coordinate Eigenstates

- Clearly $X$ and $P$ are incompatible, thus a particle cannot simultaneously have a well-defined position and momentum.

- Since $X$ is a Hermitian operator, it follows that its eigenstates form a complete set of unit vectors:

  - Eigenvalue equation: $X|\psi\rangle = \lambda |\psi\rangle$ $\forall \lambda \in \mathbb{R}$
  - Orthonormality: $\langle \psi | \psi' \rangle = \delta(\psi - \psi')$
  - Closure: $\int_{-\infty}^{\infty} \psi \psi^* d\psi = 1$

  - A state in Hilbert space is completely specified by its components in a 'physical' basis:
    $c_\psi = \langle \psi | \psi \rangle \Rightarrow \psi(x) = \langle x | \psi \rangle$

\[ \Psi : \mathbb{R} \rightarrow \mathbb{C} \text{ unit vector labels} \]
Momentum Representation

• The same logic applies also to momentum eigenstates:

\[ P|p\rangle = p|p\rangle \quad \forall p \in \mathbb{R} \]
\[ \langle p'|p\rangle = \delta(p-p') \]
\[ \int dp\langle p'|p\rangle = I \]
\[ \psi(p) = \langle p|\psi\rangle \]

• In order to move fluidly between coordinate and momentum basis, we need to know the transformation coefficients \( \langle x|p\rangle \) and \( \langle p|x\rangle \):

\[ \psi(x) = \langle x|\psi\rangle = \int dp \delta(x-p) \psi(p) \]
\[ \psi(p) = \langle p|\psi\rangle = \int dx \delta(x-p) \psi(x) \]
Deriving $\langle x | p \rangle$

- This is the direct derivation
  - Most textbooks use a round-about approach to avoid mathematical subtleties
  - We will just tackle them head on

- Start from $P | p \rangle = p | p \rangle$

- Hit with $\langle x | \rangle$ $\langle x | P | p \rangle = p \langle x | p \rangle$

- Insert $I$: $\int dx' \langle x | P | x' \rangle \langle x' | p \rangle = p \langle x | p \rangle$

- Thus we need to know $\langle x | P | x' \rangle$
  - i.e., the matrix elements of $P$ in basis $\{ | x \rangle \}$
Derivation of $\langle x|P|x' \rangle$

- All properties of $X$ and $P$ follow from: $[X,P] = i\hbar I$

- sandwich with $\langle x'|\psi\rangle$ and $\psi(x')$
  
  $\langle x'|P|x'\rangle - \langle x|P|x'\rangle = i\hbar \langle x|\psi\rangle$

  $(x-x') \langle x|P|x'\rangle = i\hbar \langle x|\psi\rangle$

  $\langle x|P|x'\rangle = i\hbar \frac{\langle x|\psi\rangle}{(x-x')}$

\[ \langle x|P|x' \rangle = i\hbar \frac{\delta(x-x')}{(x-x')} \]

- At first glance this looks like a monstrosity, it is zero for $x \neq x'$, but at $x = x'$, it is infinity divided by zero
  - By treating the delta-distribution correctly, we will see that we can easily understand the meaning of this result
Distribution Theory

• Q: is $\delta(x)$ a function?
  – A: no, technically it is a ‘distribution’
  – A ‘function’ is a mapping from one space onto another:
    
    $$y = f(x)$$
  – A ‘distribution’ is more general than a function
  – A distribution is defined only under integration

    $$y = \int dx F(x) f(x)$$

    • Here, $F(x)$ is the distribution and $f(x)$ is an ordinary function
  – For example, the delta-distribution is defined by:

    $$\int dx \delta(x - x_0) f(x) = f(x_0)$$

  – A distribution can also be defined as the limit of a sequence of functions. All properties of the distribution are by definition, the limiting properties of the sequence
  • Example:

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

    • Properties of $\delta(x)$ are well defined
  – sequence is not unique
\[ \langle x | P | x' \rangle \text{ is a Distribution} \]

- Our previous result can be written as:
  \[
  \langle x | p | x' \rangle = \frac{1}{\pi \sigma^2} e^{-\frac{(x-x')^2}{\sigma^2}}
  \]
  - This is well-behaved for any finite \( \sigma \)
  - This proves that it has a clear meaning.

- Insert result into original equation:
  
  \[
  (\text{For } \langle x | p \rangle)
  \int dx' \ i \hbar \delta(x-x') \langle x' | p \rangle = p \langle x | p \rangle
  \]

- Expand \( \langle x | p \rangle \) around \( x_0 = x \):

  \[
  \langle x' | p \rangle = \langle x | p \rangle + (x'-x) \frac{\partial}{\partial x} \langle x | p \rangle + \frac{(x'-x)^2}{2} \frac{\partial^2}{\partial x^2} \langle x | p \rangle + \ldots
  \]
\[
\int dx' \frac{\delta(x-x')}{(x-x')} \left[ \langle x' | \hat{p} | x \rangle + (x'-x) \frac{d}{dx} \langle x' | \hat{p} | x \rangle + \frac{(x'-x)^2}{2} \frac{d^2}{dx^2} \langle x' | \hat{p} | x \rangle + \ldots \right] = -i \frac{\dot{\hat{p}}}{\hbar} \langle x' | \hat{p} | x \rangle
\]

\[
\langle x | \hat{p} | x \rangle \int dx' \frac{\delta(x-x')}{(x-x')} - \frac{d}{dx} \langle x | \hat{p} | x \rangle \int dx' \frac{\delta(x-x')}{(x-x')}
\]

\[
+ \frac{d^2}{dx^2} \langle x | \hat{p} | x \rangle \int dx' \frac{\delta(x-x')}{(x-x')} + \ldots = \frac{i}{\hbar} \langle x | \hat{p} | x \rangle
\]

\[
\int dx' \frac{\delta(x-x')}{(x-x')} = \lim_{\sigma \to 0} \frac{1}{\sqrt{\pi \sigma^2}} \int dx' e^{-\frac{(x-x')^2}{2\sigma^2}}
\]

\[
= \lim_{\sigma \to 0} \frac{1}{\sqrt{\pi \sigma^2}} \int dx e^{-\frac{\sigma^2}{\sigma^2}}
\]

\[
= 0 \text{ by parity (odd function)}
\]

\[
\int dx' \frac{\delta(x-x')}{(x-x')} = 0
\]