Q. M.  Particle Superposition of Momentum Eigenstates

Partially localized Wave Packet $\xrightarrow{\Delta x \Delta p \geq \hbar/2}$

Photon – Electron

Photon wave packet description of light same as wave packet description of electron.

Electron and Photon can act like waves – diffract or act like particles – hit target.

Wave – Particle duality of both light and matter.
Commutators and the Correspondence Principle

Formal Connection

Q.M. ↔ Classical Mechanics

Correspondence between

Classical Poisson bracket of

functions \( f(x, p) \) and \( g(x, p) \)

And

Q.M. Commutator of

operators \( f \) and \( g \).
Commutator of Linear Operators

\[ [A, B] = AB - BA \]  (This implies operating on an arbitrary ket.)

If \( A \) and \( B \) numbers = 0

 Operators don’t necessarily commute.

\[
AB |C\rangle = A[B |C\rangle] \\
= A|Q\rangle \\
= |Z\rangle
\]

\[
BA |C\rangle = B[A |C\rangle] \\
= B|S\rangle \\
= |T\rangle
\]

In General

\[ |Z\rangle \neq |T\rangle \]  \( A \) and \( B \) do not commute.
Classical Poisson Bracket

\[ \{ f, g \} = \frac{\partial f}{\partial x} \frac{\partial g}{\partial p} - \frac{\partial f}{\partial x} \frac{\partial g}{\partial p} \]

\[ f = f(x, p) \quad \text{These are functions representing classical} \]
\[ g = g(x, p) \quad \text{dynamical variables \quad not operators.} \]

Consider position and momentum, classical.

\[ x \quad \text{and} \quad p \]

Poisson Bracket

\[ \{ x, p \} = \frac{\partial x}{\partial x} \frac{\partial p}{\partial p} - \frac{\partial x}{\partial p} \frac{\partial p}{\partial x} \]

\[ \{ x, p \} = 1 \quad \text{zero} \]
Dirac’s Quantum Condition

"The quantum-mechanical operators $\hat{f}$ and $\hat{g}$, which in quantum theory replace the classically defined functions $f$ and $g$, must always be such that the commutator of $\hat{f}$ and $\hat{g}$ corresponds to the Poisson bracket of $f$ and $g$ according to
\[
i\hbar \{f, g\} \rightarrow [\hat{f}, \hat{g}].\]"

Dirac
This means

\[ i\hbar \{ f(x, p), g(x, p) \} \Rightarrow [f, g] \]  

(commutator operates on a ket)

Poisson bracket of classical functions

Commutator of quantum operators

\textbf{Q.M. commutator of }x\textbf{ and }p. \]

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

Commutator \hspace{1cm} Poisson bracket

Therefore,

\[ [x, p] = i\hbar \]

\{x, p\} = 1

\textbf{Remember, the relation implies operating on an arbitrary ket.}

\textbf{This means that if you select operators for }x\textbf{ and }p\textbf{ such that they obey this relation, they are acceptable operators.}

\textbf{The particular choice} a representation of Q.M.
Schrödinger Representation

\[ p \rightarrow P = -i \hbar \frac{\partial}{\partial x} \]

momentum operator, \(-i\hbar\) times derivative with respect to \(x\)

\[ x \rightarrow x = x \]

position operator, simply \(x\)

Operate commutator on arbitrary ket \(|S\rangle\).

\[ [x, P] |S\rangle = \]

\[ (xP - Px) |S\rangle = \]

\[ x \left( -i \hbar \frac{\partial}{\partial x} \right) |S\rangle + i \hbar \frac{\partial}{\partial x} x |S\rangle \]

Using the product rule

\[ = i \hbar \left( -x \frac{\partial}{\partial x} |S\rangle + |S\rangle + x \frac{\partial}{\partial x} |S\rangle \right) \]

\[ = i \hbar |S\rangle \]

Therefore,

\[ [x, P] |S\rangle = i \hbar |S\rangle \]

and

\[ [x, P] = i \hbar \]

because the two sides have the same result when operating on an arbitrary ket.

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Another set of operators – Momentum Representation

\[ x \rightarrow x = i \hbar \frac{\partial}{\partial p} \] position operator, \( i\hbar \) times derivative with respect to \( p \)

\[ p \rightarrow p \] momentum operator, simply \( p \)

A different set of operators, a different representation.

In Momentum Representation, solve position eigenvalue problem. Get \( |x\rangle \), states of definite position.

They are waves in \( p \) space. All values of momentum.
Commutators and Simultaneous Eigenvectors

\[ A |S\rangle = \alpha |S\rangle \quad \quad \quad B |S\rangle = \beta |S\rangle \]

\[ |S\rangle \] are simultaneous Eigenvectors of operators \( A \) and \( B \) with eigenvalues \( \alpha \) and \( \beta \).

Eigenvalues of linear operators \( A \) and \( B \) are different operators that represent different observables, e. g., energy and angular momentum.

If \( |S\rangle \) are simultaneous eigenvectors of two or more linear operators representing observables, then these observables can be simultaneously measured.
\[
A|S\rangle = \alpha |S\rangle \quad B|S\rangle = \beta |S\rangle
\]
\[
BA|S\rangle = B\alpha |S\rangle \quad AB|S\rangle = A\beta |S\rangle
\]
\[
= \alpha B|S\rangle \quad = \beta A|S\rangle
\]
\[
= \alpha \beta |S\rangle \quad = \beta \alpha |S\rangle
\]

Therefore, \[AB|S\rangle = BA|S\rangle\]

Rearranging \[ (AB - BA)|S\rangle = 0 \]

\( (AB - BA) \) is the commutator of \( A \) and \( B \), and since in general \(|S\rangle \neq 0\), \[ [A, B] = 0 \]

since operating on an arbitrary ket gives 0.

The operators \( A \) and \( B \) commute.

Operators having simultaneous eigenvectors commute.

The eigenvectors of commuting operators can always be constructed in such a way that they are simultaneous eigenvectors.
There are always enough Commuting Operators (observables) to completely define a system.

Example: Energy operator, $\hat{H}$, may give degenerate states.

$\text{H atom 2s and 2p states have same energy.}$

$\hat{J}^2 \Rightarrow \text{square of angular momentum operator}$

$\begin{align*}
  j & \Rightarrow 1 \quad \text{for p orbital} \\
  j & \Rightarrow 0 \quad \text{for s orbital}
\end{align*}$

But $p_x, p_y, p_z$

$\hat{J}_z \Rightarrow \text{angular momentum projection operator}$

$\hat{H}, \hat{J}^2, \hat{J}_z \text{ all commute.}$
Commutator Rules

\[
[A, B] = -[B, A]
\]

\[
[A, BC] = [A, B]C + B[A, C]
\]

\[
[AB, C] = [A, C]B + A[B, C]
\]

\[
[A, [B, C]] + [B, [C, A]] + [C, [A, B]] = 0
\]

\[
[A, B + C] = [A, B] + [A, C]
\]
Expectation Value and Averages

\[ A |a\rangle = \alpha |a\rangle \quad \text{normalized} \]

eigenvector    eigenvalue

If make measurement of observable \( A \) on state \(|a\rangle\) will observe \( \alpha \).

What if measure observable \( A \) on state not an eigenvector of operator \( A \).

\[ A |b\rangle \Rightarrow ? \]

normalized

Expand \(|b\rangle\) in complete set of eigenkets \(|a\rangle\) \(\Rightarrow\) Superposition principle.

Eigenkets – complete set. One for each state. Spans state space.
\[ |b\rangle = c_1|a_1\rangle + c_2|a_2\rangle + c_3|a_3\rangle + \cdots \] (If continuous range \rightarrow integral)

\[ |b\rangle = \sum_i c_i|a_i\rangle \]

Consider only two states (normalized and orthogonal).

\[ |b\rangle = c_1|a_1\rangle + c_2|a_2\rangle \]

\[ A|b\rangle = A(c_1|a_1\rangle + c_2|a_2\rangle) \]

\[ = c_1A|a_1\rangle + c_2A|a_2\rangle \]

\[ = \alpha_1c_1|a_1\rangle + \alpha_2c_2|a_2\rangle \]

Left multiply by \langle b | .

\[ \langle b | \bar{A} | b \rangle = (c_1^* \langle a_1 | + c_2^* \langle a_2 |)(\alpha_1c_1|a_1\rangle + \alpha_2c_2|a_2\rangle) \]

\[ = \alpha_1c_1^*c_1 + \alpha_2c_2^*c_2 \]

\[ = \alpha_1|c_1|^2 + \alpha_2|c_2|^2 \]
The absolute square of the coefficient $c_i$, $|c_i|^2$, in the expansion of $|b\rangle$ in terms of the eigenvectors $|a_i\rangle$ of the operator (observable) $A$ is the probability that a measurement of $A$ on the state $|b\rangle$ will yield the eigenvalue $\alpha_i$.

If there are more than two states in the expansion

$$|b\rangle = \sum_i c_i |a_i\rangle$$

$$\langle b | A | b \rangle = \sum_i \alpha_i |c_i|^2$$

eigenvalue probability of eigenvalue
Definition: The average is the value of a particular outcome times its probability, summed over all possible outcomes.

Then

$$\langle b | A | b \rangle = \sum_{i} |c_{i}|^{2} \alpha_{i}$$

is the average value of the observable when many measurements are made.

Assume: One measurement on a large number of identically prepared non-interacting systems is the same as the average of many repeated measurements on one such system prepared each time in an identical manner.
\[ \langle b | A | b \rangle \Rightarrow \text{Expectation value of the operator } A. \]

In terms of particular wavefunctions

\[ \langle b | A | b \rangle = \int_{-\infty}^{\infty} \psi_b^* A \psi_b d\tau \]
The Uncertainty Principle - derivation

Have shown - \([x, P] \neq 0\)

and that \(\Delta x \Delta p \approx \hbar\)

Want to prove:

Given \(A\) and \(B\), Hermitian with

\([A, B] = iC\)

another Hermitian operator (could be number – special case of operator, identity operator).

Then

\[\Delta A \Delta B \geq \frac{1}{2} |\langle C \rangle|\]

with \(\langle C \rangle = \langle S | C | S \rangle\)

short hand for expectation value

\(\langle S \text{ and } | S \rangle\) arbitrary but normalized.
Consider operator

\[ D = A + \alpha B + i \beta B \]

arbitrary real numbers

\[ D |S\rangle = |Q\rangle \]

\[ \langle Q | Q \rangle = \langle S | DD | S \rangle \geq 0 \]

Since \( \langle Q | Q \rangle \) is the scalar product of vector with itself.

\[ \langle Q | Q \rangle = \langle S | DD | S \rangle = \langle A^2 \rangle + (\alpha^2 + \beta^2)\langle B^2 \rangle + \alpha \langle C' \rangle - \beta \langle C \rangle \geq 0 \]

(derive this in home work) \[ C' = AB + BA \]

is the anticommutator of \( A \) and \( B \).

\[ AB + BA = [A, B]_+ \]

anticommutator

\[ \langle A^2 \rangle = \langle S | A^2 | S \rangle = \langle S | AA | S \rangle \]
\[ \langle Q | Q \rangle = \langle S | \overline{D D} | S \rangle = \langle A^2 \rangle + (\alpha^2 + \beta^2) \langle B^2 \rangle + \alpha \langle C' \rangle - \beta \langle C \rangle \geq 0 \]

\[ \overline{B} | S \rangle \neq 0 \quad \text{for arbitrary ket } | S \rangle. \]

Can rearrange to give

\[ \langle A^2 \rangle + \langle B^2 \rangle \left( \alpha + \frac{1}{2} \frac{\langle C' \rangle}{\langle B^2 \rangle} \right)^2 + \langle B^2 \rangle \left( \beta - \frac{1}{2} \frac{\langle C \rangle}{\langle B^2 \rangle} \right)^2 - \frac{1}{4} \frac{\langle C' \rangle^2}{\langle B^2 \rangle} - \frac{1}{4} \frac{\langle C \rangle^2}{\langle B^2 \rangle} \geq 0 \]

Holds for any value of \( \alpha \) and \( \beta \).

Pick \( \alpha \) and \( \beta \) so terms in parentheses are zero. Multiplied through by \( \langle B^2 \rangle \) and transposed.

Then \( \langle A^2 \rangle \langle B^2 \rangle \geq \frac{1}{4} \left( \langle C' \rangle^2 + \langle C \rangle^2 \right) \geq \frac{1}{4} \langle C \rangle^2 \)

Positive numbers because square of real numbers.

Thus,

\[ \langle A^2 \rangle \langle B^2 \rangle \geq \frac{1}{4} \langle C \rangle^2 \]

The sum of two positive numbers is \( \geq \) one of them.
\[ \langle A^2 \rangle \langle B^2 \rangle \geq \frac{1}{4} \langle C \rangle^2 \]

\[ [A, B] = iC \]

\[ \Delta A \Delta B \geq \frac{1}{2} \left| \langle C \rangle \right| \]

Define

\[ (\Delta A)^2 = \langle A^2 \rangle - \langle A \rangle^2 \]

\[ (\Delta B)^2 = \langle B^2 \rangle - \langle B \rangle^2 \]

Second moment of distribution - for Gaussian standard deviation squared.

For special case

\[ \langle A \rangle = \langle B \rangle = 0 \]

Average value of the observables are zero.

\[ \Delta A \Delta B \geq \frac{1}{2} \left| \langle C \rangle \right| \]

\[ \left( \langle C \rangle^2 \right)^{\frac{1}{2}} = \left| \langle C \rangle \right| \]

Square root of the square of a number
Have proven that for $[A, B] = iC$

$$\Delta A \Delta B \geq \frac{1}{2} |\langle C \rangle|$$

$\langle A \rangle = \langle B \rangle = 0$  Average value of the observables are zero.

Example

$[x, P] = i\hbar$

Number, special case of an operator. Number is implicitly multiplied by the identity operator.

$\langle x \rangle = \langle P \rangle = 0$

Therefore

$$\Delta x \Delta p \geq \hbar / 2.$$ Uncertainty comes from superposition principle.

The more general case is discussed in the book.