Hermitian Operators

In QM we use three types of mathematical objects.

(1) complex numbers : c
(2) state vectors (kets) : $|arb\rangle$
(3) Operators : $\hat{A}$

For (1) & (2), we have "partner" or "dual" objects:
(1) $c \rightarrow c^*$ complex conjugation
(2) bra vectors : $\langle arb|$

There is also a "partner" object for operators. It is called the "Hermitian Conjugate Operator", and written as $\hat{A}^+$. So we have

	Mathematical object	"partner"
number:	c	c^*
vector:	$\|arb\rangle$	$\langle arb\|$
operator:	$\hat{A}$	$\hat{A}^+$

these are the objects we use in QM.

We can write the laws of QM in terms of the "objects" or their "partners". They both describe the same thing. For example, the TDSE is

$$i\hbar \frac{\partial \Psi(x,t)}{\partial t} = \hat{H}\,\Psi(x,t)$$

but we could also write

$$-i\hbar \frac{\partial \Psi^{*}(x,t)}{\partial t} = \hat{H}^{\dagger} \Psi^{*}(x,t)$$ ← this describes the same physics.

~~We will define the meaning of $\hat{A}^{+}$ in a minute, but first let's discuss why it is important. Basically,~~

When an operator is equal to it's Hermitian conjugate, we say that the operator is "Hermitian".

$\boxed{\text{If } \hat{A} = \hat{A}^{+}, \text{ we say } \hat{A} \text{ is Hermitian".}}$

This situation is the moral equivalent of a real number, except for the case of an operator.

"Hermitian Operators" are important for two reasons.

(1) They always have real eigenvalues. Since observable quantities must be real, we modify Postulate I:

Postulate I For every observable A, there is a Hermitian operator $\hat{A}$ for which $\underbrace{\hat{A}|n\rangle = a_n|n\rangle}_{\text{Eigenvalue Eq. in Dirac Notation}}$

(2) Hermitian Operators have eigenfunctions which are orthogonal. ⇒ If $\{|n\rangle\}$ are eigenvectors of $\hat{A}$, and $\hat{A} = \hat{A}^{+}$, then $\langle m|n\rangle = \delta_{mn}$.

The meaning of A^+

Loosely speaking, if $\hat{A}$ is an operator which can be applied to a |ket vector⟩, then A^+ is the equivalent operator which should be applied to the partner ⟨bra vector| :

$$\hat{A}\,|arb\rangle \overset{\text{partners}}{\Longleftrightarrow} \langle arb|\,\hat{A}^+$$

applied to the right — applied to the left

Strict definition: if ~~$|\alpha\rangle$ and $|\beta\rangle$ are two ket vectors, and $\hat{A}$ can operate on them,~~ $\hat{A}^+$ is the operator which satisfies

$$\left(\langle\alpha|\hat{A}^+\right)|\beta\rangle \overset{\text{definition}}{\equiv} \langle\alpha|\hat{A}|\beta\rangle$$

to the right

For all $|\alpha\rangle$ & $|\beta\rangle$

The def. is confusing because it is legal to apply a Hermitian conjugate to a ket state: $A^+|\beta\rangle$ is legal. But the def. of A^+, it gets applied to the bra $\langle\alpha|A^+$

Example 1 Let $\hat{D}$ be $\frac{d}{dx}$ in position space. What is $\hat{D}^+$?

Evaluate $\langle\alpha|\left(\hat{D}|\beta\rangle\right)$ in position space:

$$\langle\alpha|\left(\hat{D}|\beta\rangle\right) = \int_{-\infty}^{\infty}\psi_\alpha^*(x)\,\frac{d}{dx}\,\psi_\beta(x)\,dx = \underbrace{\left(\psi_\alpha^*(x)\,\psi_\beta(x)\right)_{-\infty}^{\infty}}_{0-0\text{, if }\psi_\alpha\ \&\ \psi_\beta\text{ are normalizable.}} - \int_{-\infty}^{\infty}\left(\frac{d}{dx}\psi_\alpha^*(x)\right)\psi_\beta \ldots$$

$$= \int_{-\infty}^{\infty}\left(-\frac{d}{dx}\psi_\alpha^*(x)\right)\psi_\beta(x)\,dx$$

$$\equiv \left(\langle\alpha|\hat{D}^+\right)|\beta\rangle \text{ by definition of } \hat{D}^+$$

To keep track of which way the operator is applied, we sometimes move the operator inside the bra or ket symbol:

$A^+|\beta\rangle \equiv |A^+\beta\rangle$ $\quad\langle\alpha|A^+ = \langle A^+\alpha|$

partners

$$\therefore \quad \boxed{\hat{D}^\dagger = -\frac{d}{dx} \iff \hat{D} = \frac{d}{dx}}$$

Since $\hat{D}^\dagger \neq \hat{D}$, $\hat{D}$ is not Hermitian, and it cannot represent an observable.

~~This is both~~

The momentum operator $\hat{p}$ includes a factor of (i) so it will be Hermitian. $\hat{p} = -i\hbar\frac{d}{dx} = \hat{p}^\dagger$.

<u>Example 2</u> IF $\hat{A}$ = multiplication by a number c,

Then $\hat{A}^\dagger$ = multiplication by c^*.

Proof: $\langle\alpha|\left(\hat{A}|\beta\rangle\right) = \langle\alpha|\left(c|\beta\rangle\right) = c\langle\alpha|\beta\rangle$

$$= c\int_{-\infty}^{\infty}\psi_\alpha^*(x)\psi_\beta(x)\,dx$$

$$= \int_{-\infty}^{\infty}\left(c^*\psi_\alpha(x)\right)^*\psi_\beta(x)\,dx$$

by def. of $\hat{A}^\dagger$

$$= \left(\langle\alpha|\hat{A}^\dagger\right)|\beta\rangle = \int_{-\infty}^{\infty}\left(\psi_\alpha(x)\hat{A}^\dagger\right)^*\psi_\beta(x)\,dx$$

$\therefore$ $\hat{A}^\dagger$ = multiplication by c^*.

Now we prove the two important consequences of an operator being Hermitian:

<u>Important Property</u> (1) IF $\hat{A} = \hat{A}^\dagger$, then the eigenvalues of $\hat{A}$ are real: $\hat{A}|n\rangle = a_n|n\rangle$, where $a_n = a_n^*$, and $|n\rangle$ = eigenvector of $\hat{A}$

<u>Proof</u>

Evaluate $\langle n|\left(\hat{A}|n\rangle\right) = \langle n|a_n|n\rangle = a_n\langle n|n\rangle$

||| by def of $A^\dagger$ b/c $\hat{A}=\hat{A}^\dagger$

$$\left(\langle n|\hat{A}^\dagger\right)|n\rangle = \int\left(\psi_n^*(x)\hat{A}^\dagger\right)^*\psi_n\,dx = \int\left(\hat{A}\psi_n(x)\right)^*\psi_n(x)\,dx = \int a_n^*\psi_n^*(x)\psi_n(x)\,dx = a_n^*\langle n|n\rangle$$

$\therefore \quad a_n = a_n^*$, and a_n = real number.

~~Pr~~

Important Property ②

If $|n\rangle$ & $|m\rangle$ are eigenvectors of $\hat{A}$, and $\hat{A} = \hat{A}^\dagger$ then

$\langle m|n\rangle = \delta_{mn}$ ← the eigenvectors are orthogonal.

Proof: $\hat{A}|n\rangle = a_n|n\rangle$ and $\langle n|\hat{A} = a_n\langle n|$ by I.P. ①.

$\hat{A}|m\rangle = a_m|m\rangle$ and $\langle m|\hat{A} = a_m\langle m|$

Therefor $\langle m|\hat{A}|n\rangle = \langle m|(\hat{A}|n\rangle) = a_n\langle m|n\rangle$

$$\begin{gathered} \parallel \\ (\langle m|\hat{A})|n\rangle = a_m\langle m|n\rangle \end{gathered}$$

$$\therefore \quad a_m\langle m|n\rangle = a_n\langle m|n\rangle$$

$$(a_m - a_n)\langle m|n\rangle = \emptyset.$$

Three ~~two~~ cases ~~① $a_m \neq a_n$. Then $\langle m|n\rangle = \emptyset$.~~

~~② $a_m = a_n$:~~

① $m = n$. Thus we have $\overbrace{(a_m - a_m)}^{\emptyset}\langle m|m\rangle = \emptyset$

If $|m\rangle$ is normalized, $\langle m|m\rangle = 1$.

② $m \neq n$, $a_m \neq a_n$. Thus

$$\underset{\neq 0}{(a_m - a_n)}\underbrace{\langle m|n\rangle}_{\emptyset} = \emptyset$$

$$\langle m|n\rangle = \emptyset$$

③ $m \neq n$, but $a_m = a_n$.

In this case two different states $|m\rangle$ & $|n\rangle$ have the same eigenvalue. We call this situation "degenerate eigenstates"

In the case of degenerate eigenstates, it turns out that we can make linear combinations of the states which are orthogonal. We'll ignore this detail and jump straight to the conclusion.

$\boxed{\langle m|n\rangle = \delta_{mn}}$ For ~~ortho~~ the eigenstates of a Hermitian operator

The Uncertainty Principle

In Quantum Mechanics, we have compatible observables & incompatible observables.

Compatible Observables can have eigenstates in common. Measuring the eigenvalues for these states does not ~~observe~~ disturb them.

Ex: Momentum & Energy of the free particle

If $\psi(x) = \frac{1}{\sqrt{2\pi}} e^{ikx}$, then $p = \hbar k$ & $E = \frac{(\hbar k)^2}{2m}$

no uncertainty

Algebraically, it doesn't matter which operator we apply first:

$$\hat{p}\,\hat{H}_{free}|k\rangle = pE|k\rangle = \hat{H}_{free}\hat{p}\,|k\rangle$$

If we define the Commutator

$$\hat{p}\hat{H} - \hat{H}\hat{p} \equiv [\hat{p}, \hat{H}_{free}], \quad \text{then } [\hat{p}, \hat{H}_{free}]|k\rangle = \emptyset$$

In fact, on Exam #1 you proved that

$$[\hat{p}, \hat{H}_{free}] = \emptyset \text{ always}$$

Incompatible Observables can never have an eigenfunction in common.

Ex: position & momentum.

If we measure x, p becomes infinitely uncertain

$$\psi(x) = \delta(x - x'), \quad \phi(k) = \frac{1}{\sqrt{2\pi}} e^{ikx'}$$

all k.

If we measure p, x becomes infinitely uncertain:

$$\phi(k) = \delta(k-k') \quad , \quad \psi(x) = \frac{1}{\sqrt{2\pi}} e^{ik'x}$$

all x from $-\infty$ to $+\infty$.

(This is Homework #4 Question #1)

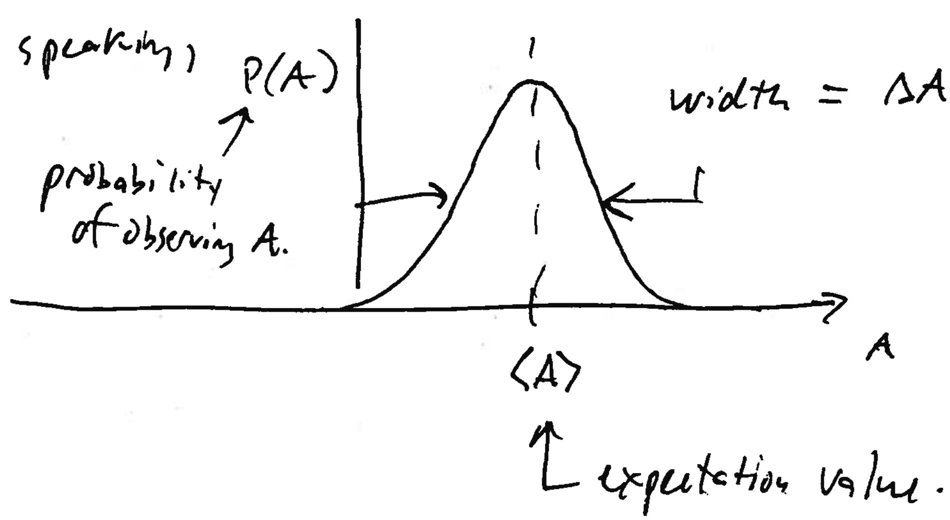
Algebraically, applying $\hat{x}$ to a function followed by $\hat{p}$ is not the same as $\hat{p}$ followed by $\hat{x}$:

$$[\hat{x}, \hat{p}] = \hat{x}\hat{p} - \hat{p}\hat{x} = i\hbar \neq 0.$$ from Homework #

For any two incompatible observables, there will be an uncertainty relation in QM which states how well you can minimize the ~~an~~ combined "spread" in the two variables.

<u>Notation</u> Recall that we use σ_A or ΔA to represent the RMS spread in variable A.

Roughly speaking,



$$\Delta A = \sqrt{\langle A^2 \rangle - \langle A \rangle^2}$$

In QM, For a state $|\psi\rangle$, $\langle A \rangle = \langle \psi | \hat{A} | \psi \rangle$ by postulate II

Similarly, $\langle A^2 \rangle = \langle \psi | \hat{A}^2 | \psi \rangle$

So $\Delta A = \sqrt{\langle \psi | \hat{A}^2 | \psi \rangle - \left(\langle \psi | \hat{A} | \psi \rangle \right)^2}$ in QM.

Similarly, for a second ~~variable~~ observable B,

$$\Delta B = \sqrt{\langle \psi | \hat{B}^2 | \psi \rangle - \langle \psi | \hat{B} | \psi \rangle^2}$$

Multiply ΔA & ΔB and you will get

"Generalized Uncertainty Principle" $\boxed{\Delta A \, \Delta B \geq \frac{1}{2} |\langle C \rangle|,}$ where $\hat{C} = [\hat{A}, \hat{B}]$

For position & momentum, this says $\cancel{\Delta x \Delta p \geq \hbar/2}$
Recall $[\hat{X}, \hat{P}] = i\hbar$ $\cancel{\langle \psi | i\hbar | \psi \rangle}$

$$(\Delta x)(\Delta p) \geq \frac{1}{2} \left| \langle \psi | i\hbar | \psi \rangle \right| = \frac{1}{2} |i\hbar| = \frac{\hbar}{2}$$

$$\boxed{\Delta x \Delta p \geq \frac{\hbar}{2}}$$

Comments

1. The uncertainty principle says that $(\Delta A)(\Delta B)$ cannot be smaller than some value, given by $\frac{1}{2} |\langle [\hat{A}, \hat{B}] \rangle|$.

For a typical ~~wavefunction~~, $(\Delta A)(\Delta B)$ will be larger than the minimal value.

For the x-p uncertainty principle, only the Gaussian Wavefunction satisfies the minimum uncertainty between x & p. All other wavefunctions will have $\Delta x \Delta p$ larger than $\hbar/2$.

(2) Mathematically, the "greater than" symbol in the uncertainty principle comes from the ~~Sc~~ "Cauchy-Schwartz" Inequality:

$$|\langle \alpha | \psi \rangle| \le ||\alpha|| \, ||\psi|| = \sqrt{|\langle \alpha|\alpha\rangle|^2 |\langle\psi|\psi\rangle|}$$

For ordinary three-vectors, this statement is:

$$|\vec{a}\cdot\vec{b}| \le |\vec{a}||\vec{b}|$$

This is true for ordinary vectors because
$$\vec{a}\cdot\vec{b} = |\vec{a}||\vec{b}|\cos\theta_{ab} \;\; \& \;\; \cos\theta_{ab} \le 1.$$

The Cauchy-Schwartz Inequality written above generalizes this to the bras & kets of QM.

(3) If two operators commutes, then $[\hat{A},\hat{B}] = 0$,

$$\& \;\; \Delta A \Delta B \ge \frac{1}{2}|\langle [A,B]\rangle| = \phi.$$

Thus the observables are compatible, and there is no uncertainty principle.