Quantum Mechanics: Commutation

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I. Commutators: Measuring Several Properties Simultaneously

In classical mechanics, once we determine the dynamical state of a system, we can **simultaneously** obtain many different system properties (i.e., velocity, position, momentum, acceleration, angular/linear momentum, kinetic and potential energies, etc.). The uncertainty is governed by the resolution and precision of the instruments at our disposal.

In quantum mechanics, the situation is different. Consider the following:

1. We would like to measure **several properties** of a particle represented by a wavefunction.

2. Properties of a q.m. system can be measured experimentally. Theoretically, the measurement process corresponds to an **operator acting on the wavefunction.** The outcomes of the measurement are the eigenvalues that correspond to the operator. The operator is taken to be acting on a wavefunction that is either a pure eigenfunction of the operator of interest, or an expansion in the basis of eigenfunctions.

In order to measure, for instance, 2 properties *simultaneously*, the **wavefunction of the particle must be an eigenstate of the two operators that corespond to the properties we would like to measure simultaneously.** How do we formalize this mathematically?

Consider:

We have to operators, $\hat{A}$ and $\hat{B}$. Each operator acting on its eigenstate gives back the corresponding eigenvalues, A_i and B_j, respectively.

$$\hat{A}\ \psi_{A_i} \ =\ A_i\ \psi_{A_i}$$
$$\hat{B}\ \psi_{B_i} \ =\ B_i\ \psi_{B_i}$$

If we have a wavefunction that is an eigenstate of **both** operators, then:

$$\hat{A}\psi_{A_i,B_j} \ =\ A_i\psi_{A_i,B_j}$$

$$\hat{B}\psi_{A_i,B_j} \;=\; B_j\psi_{A_i,B_j}$$

Thus,

$$\hat{B}\hat{A}\psi_{A_i,B_j} \;=\; \hat{B}A_i\psi_{A_i,B_j}$$

$$\hat{A}\hat{B}\psi_{A_i,B_j} \;=\; \hat{A}B_j\psi_{A_i,B_j}$$

So, using the fact that ψ_{A_i,B_j} is an eigenfunction of $\hat{A}$ and $\hat{B}$:

$$\hat{B}\hat{A}\psi_{A_i,B_j} \;=\; B_jA_i\psi_{A_i,B_j}$$

$$\hat{A}\hat{B}\psi_{A_i,B_j} \;=\; A_iB_j\psi_{A_i,B_j}$$

Subtracting the equations, we realize a compact notation for defining what is called a **commutator**:

$$[A,B] \;=\; \hat{A}\hat{B} - \hat{B}\hat{A}$$

- The commutator is itself either **zero** or an **operator**
- The order of operations is important and will give unique commutators depending on this ordering

For two physical properties to be simultaneously observable, their operator representations must commute.
Thus,

$$\hat{A}\left[\hat{B}f(x)\right] - \hat{B}\left[\hat{A}f(x)\right] = 0 \quad \textit{2 operators that commute}$$

Example Problem 17.1: Determine whether the momentum operator commutes with the a) kinetic energy and b) total energy operators.
a). To determine whether the two operators commute (and importantly, to determine whether the two observables associated with those operators **can be known simultaneously**), one considers the following:

- momentum and kinetic energy

$$-i\hbar \frac{d}{dx}\left(-\frac{h^2}{2m}\frac{d^2}{dx^2}\right)f(x) - \left(-\frac{h^2}{2m}\frac{d^2}{dx^2}\right)\left(-i\hbar\frac{d}{dx}\right)f(x)$$

$$\left(i\frac{h^3}{2m}\frac{d^3}{dx^3}\right)f(x) - \left(i\frac{h^3}{2m}\frac{d^3}{dx^3}\right)f(x)$$

$$0$$

Thus, the momentum and kinetic energy operators commute
b). momentum and total energy

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$$-i\hbar\frac{d}{dx}\left(-\frac{h^2}{2m}\frac{d^2}{dx^2}+V(x)\right)f(x) - \left(-\frac{h^2}{2m}\frac{d^2}{dx^2}+V(x)\right)\left(-i\hbar\frac{d}{dx}\right)f(x)$$

$$(1)$$

- Since the momentum and kinetic energy operators commute from part a, we can write

$$-i\hbar\frac{d}{dx}\ V(x)f(x)) + i\hbar V(x)\ \frac{d}{dx}f(x)$$

$$-i\hbar V(x)\frac{d}{dx}f(x) - i\hbar f(x)\frac{d}{dx}V(x) + i\hbar V(x)\ \frac{d}{dx}f(x)$$

$$-i\hbar f(x)\frac{d}{dx}V(x)$$

$$(2)$$

Thus, the commutator for the momentum and total energy reduces as follows:

$$\left[\hat{H}, -i\hbar\frac{d}{dx}\right] = \left[V(x), -i\hbar\frac{d}{dx}\right] = -i\hbar\frac{d}{dx}V(x)$$

The last equation does not equal zero identically, and thus we see two things: 1. the momentum and total energy do not commute 2. the commutator reduces to a unique operation (we will see this again with respect to angular momentum)

Heisenberg Uncertainty Principle
Recall the discussion of the free particle. For that system, we determined that the energy (and momentum) spectrum is continuous since there were no boundary conditions imposed on the wavefunction (thus we arrive at plan-wave representations of the particle-wave entity).
The important point for the present dicussion is the relation between our knowledge of the momentum of the particle and its position. We note a few things:

- The Heisenberg Uncertainty principle is stated as:

$$\delta p \delta x \geq \frac{\hbar}{2}$$

For a quantum mechanical description of a particle's dynamics, we cannot know exactly and simultaneously both the particle's position and momentum. We must accept an uncertainty in measurements of these quantities as given by the inequality.

To relate the uncertainty principle to variances and statistical measures, the relation:

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

can be used in conjunction with wavefunctions and definitions of average properties:

$$\sigma_p^2 = <p^2> - <p>^2 \quad (likewise \ for \ \sigma_x)$$