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 functions.

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.**

So, consider:

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

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

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

$$
\begin{aligned}
-i\hbar\frac{d}{dx}\left(-\frac{h^2}{2m}\frac{d^2}{dx^2}\right)f(x)-\left(-\frac{h^2}{2m}\frac{d^2}{dx^2}\right)\left(-i\hbar\frac{d}{dx}\right)f(x) \\
\left(i\frac{h^3}{2m}\frac{d^3}{dx^3}\right)f(x)-\left(i\frac{h^3}{2m}\frac{d^3}{dx^3}\right)f(x) \\
0
\end{aligned}
$$

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

-

$$
-i\hbar\frac{d}{dx}\left(-\frac{h^2}{2m}\frac{d^2}{dx^2}+V(x)\right)f(x)-\left(-\frac{h^2}{2m}\frac{d^2}{dx^2}+V(x)\right)\left(-i\hbar\frac{d}{dx}\right)f(x) \tag{1}
$$

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

$$
\begin{aligned}
-i\hbar\frac{d}{dx}\left(V(x)f(x)\right)+i\hbar V(x)\ \frac{d}{dx}f(x) \\
-i\hbar V(x)\frac{d}{dx}f(x)-i\hbar f(x)\frac{d}{dx}V(x)+i\hbar V(x)\ \frac{d}{dx}f(x) \\
-i\hbar f(x)\frac{d}{dx}V(x)
\end{aligned} \tag{2}
$$

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:

- Given an initial velocity, the **momentum is defined exactly**.
- Since energy is conserved, the momentum does not change with time
- The probability of finding the one-dimensional quantum mechanical free particle in an interval dx at x is given as (Equation 15.6, Engell and Reid):

$$P(x)dx = \frac{dx}{2L} \tag{3}$$

  This is based on a **plane-wave** form of the wavefunction which cannot be normalized over an infinite interval; thus the interval for consideration is taken to be 2L.

- We see that if we consider an extremely large interval ($vis{-}a{-}vis, L \rightarrow \infty$), the probabililty becomes vanishingly small, but it is equivalent **everywhere**. Thus, we lose any information on the **exact** location(position) of the free particle.

If we further consider the commutator of the momentum and position operators, we will find that (derivation left for individual pursuit)

$$[\hat{x}, \hat{p_x}] \neq 0$$

We see that if we knew **exactly** the momentum ($k = \frac{p}{\hbar}$), then the position is essentially unknown (particularly if we consider an infinite extent for the particle motion). Conversely, though we have not shown it rigorously, if one knows the location exactly, then the momentum becomes uncertain. This relation between the uncertainties in momentum and position is embodied in the **Heisenberg Uncertainty Principle**, 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.

Note: On a more fundamental level, the Heisenberg principle is related to properties of Fourier Transforms via the Cauchy inequality. This is a topic for an advanced discussion, but one should take note here of the interplay between the results of pure mathematics and the physical interpretation a physics-based analysis confers on them; this is non-trivial.

Wave Packets

Here we present a very coarse discussion on the origins of the uncertainty relations.

- The free particle plane-wave function is

$$\Psi(x,t) = A\ e^{i(kx-\omega t-\alpha)}$$

Consider the wavefunction at time $t = 0$ and ignore the phase shift for the present purpose.

- Let's expand the particle wavefunction representation around a wavevector k_0

$$\psi(x) = \frac{1}{2}Ae^{ik_o x} + \frac{1}{2}A\sum_{n=-m}^{n=+m} e^{i(k_o+n\Delta k)x}$$

with $\Delta k <<< k$.

- As shown in Figure 17.4 in Engell and Reid, as we add more and more plane-waves of slightly different wave-vectors (hence momenta), the **superposition** wavefunction in position space becomes more and more **localized**. The probability density of the particle becomes more narrow and highly peaked about some reference position.

- However, as the uncertainty in the position of the particle has **decreased**, the uncertainty in the momentum has **increased**.

- For the contrived problem we are considering here, we can propose a bound on the values of the momentum we measure since we have expanded about some reference wave-vector k_0:

$$\hbar\,(k_0 - m\Delta k) \leq p \leq \hbar\,(k_0 + m\Delta k)$$

- As a result of the superposition of many plane waves, the position of the particle is no longer completely unknown (we have reduced the uncertainty in position), and the momentum of the particle is no longer exactly known (we have increased the uncertainty in momentum).

- **Both momentum and position cannot be known exactly and simultaneously in quantum mechanics. We must accept a trade off**.

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:

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