If two operators commute then both quantities can be measured at the same time, if not then there is a tradeoff in the accuracy in the measurement for one quantity vs. the other.

**Introduction**

Operators are commonly used to perform a specific mathematical operation on another function. The operation can be to take the derivative or integrate with respect to a particular term, or to multiply, divide, add or subtract a number or term with regards to the initial function. Operators are commonly used in physics, mathematics and chemistry, often to simplify complicated equations such as the Hamiltonian operator, used to solve the Schrödinger equation.

**Operators**

Operators are generally characterized by a hat. Thus they generally appear like the following equation with \( \hat{E} \) being the operator operating on \( f(x) \)

\[
\hat{E} f(x) = g(x)
\]

For example if \( \hat{E} = \frac{d}{dx} \) then:

\[
g(x) = f'(x)
\]

**Commuting Operators**

One property of operators is that the order of operation matters. Thus:

\[
\hat{A}\hat{E}f(x) \neq \hat{E}\hat{A}f(x)
\]

unless the two operators commute. Two operators commute if the following equation is true:

\[
[\hat{A},\hat{E}] = \hat{A}\hat{E} - \hat{E}\hat{A} = 0
\]

To determine whether two operators commute first operate \( \hat{A}\hat{E} \) on a function \( f(x) \). Then operate \( \hat{E}\hat{A} \) the same function \( f(x) \). If the same answer is obtained subtracting the two functions will equal zero and the two operators will commute.

**Example 1**

Do \( \hat{A} \) and \( \hat{E} \) commute if \( \hat{A} = \frac{d}{dx} \) and \( \hat{E} = x^2 \)?

**SOLUTION**

This requires evaluating \( \left[\hat{A},\hat{E}\right] \).

\[
\hat{A}\hat{E} f(x) = \hat{A}\left[x^2 f(x)\right] = x^2 \frac{d}{dx} f(x) + \frac{d}{dx} x^2 f(x) = 2xf(x) + x^2 f'(x)
\]

\[
\hat{E}\hat{A} f(x) = \left[x^2 \frac{d}{dx}\right] f(x) = x^2 f'(x) + 2xf(x)
\]

Subtracting the two gives:

\[
2xf(x) + x^2 f'(x) - (x^2 f'(x) + 2xf(x)) = 0
\]

Thus \( \hat{A}\hat{E} = \hat{E}\hat{A} \) and the operators commute.
\[\hat{E}\hat{A}f(x) = \hat{E}\left[f'(x)\right] = x^2 f'(x)\]
\[\left[\hat{A},\hat{E}\right] = 2x f(x) + x^2 f'(x) - x^2 f'(x) = 2x f(x) \neq 0\]

Therefore the two operators do not commute.

Example 2

Do \(\hat{B}\) and \(\hat{C}\) commute if \(\hat{B} = \frac{h}{x}\) and \(\hat{C} = f(x) + 5\)?

**SOLUTION**

This requires evaluating \(\left[\hat{B},\hat{C}\right]\)

\[\hat{B}\hat{C}f(x) = \hat{B}f(x) + 3 = \frac{h}{x} (f(x) + 3) = \frac{h f(x)}{x} + \frac{3h}{x}\]
\[\hat{C}\hat{B}f(x) = \hat{C} \frac{h}{x} f(x) = \frac{h f(x)}{x} + 3\]

\[\left[\hat{B},\hat{C}\right] = \frac{h f(x)}{x} + \frac{3h}{x} - \frac{h f(x)}{x} - 3 \neq 0\]

The two operators do not commute.

Example 3

Do \(\hat{B}\) and \(\hat{C}\) commute if \(\hat{J} = 3x\) and \(\hat{O} = x^{-1}\)?

**SOLUTION**

This requires evaluating \(\left[\hat{J},\hat{O}\right]\)

\[\hat{J}\hat{O}f(x) = \hat{J}(f(x) 3x) = f(x) 3x/x = 3f(x)\]
\[\hat{O}\hat{J}f(x) = \hat{O}(f(x)/x) = f(x) 3x/x = 3f(x)\]

\[\left[\hat{J},\hat{O}\right] = 3f(x) - 3f(x) = 0\]

Because the difference is zero, the two operators commute.

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**Applications in Physical Chemistry**

Operators are very common in Physical Chemistry with a variety of purposes. They are used to figure out the energy of a wave function using the Schrödinger Equation.

\[\hat{H}\psi = E\psi\]

They also help to explain observations made in the experimentally. An example of this is the relationship between the magnitude of the angular momentum and the components.
\[
\left[\hat{L}^2, \hat{L}^2_x\right] = \left[\hat{L}^2, \hat{L}^2_y\right] = \left[\hat{L}^2, \hat{L}^2_z\right] = 0
\]

However the components do not commute themselves. An additional property of commutators that commute is that both quantities can be measured simultaneously. Thus, the magnitude of the angular momentum and ONE of the components (usually z) can be known at the same time however, NOTHING is known about the other components.

References


Problems

Determine whether the following combination of operators commute.

\[
\left[\hat{K}, \hat{H}\right]
\]

where \(\hat{K} = \alpha \int_{1}^{\infty} d[x]\) and \(\hat{H} = d/dx\)

\[
\left[\hat{I}, \hat{L}\right]
\]

where \(\hat{I} = 5\) and \(\hat{L} = \int_{1}^{\infty} d[x]\)

Show that the components of the angular momentum do not commute.

\[
\hat{L}_x = -i \hbar \left[-\sin \left(\phi \frac{\delta}{\delta \theta}\right) - \cot(\Theta) \cos \left(\phi \frac{\delta}{\delta \phi}\right)\right]
\]

\[
\hat{L}_y = -i \hbar \left[\cos \left(\phi \frac{\delta}{\delta \theta}\right) - \cot(\Theta) \cos \left(\phi \frac{\delta}{\delta \phi}\right)\right]
\]

\[
\hat{L}_z = -i \hbar \frac{\delta}{\delta \theta}
\]

Solution

\[
\left[\hat{L}_z, \hat{L}_x\right] = i \hbar \hat{L}_y
\]

\[
\left[\hat{L}_x, \hat{L}_y\right] = i \hbar \hat{L}_z
\]

\[
\left[\hat{L}_y, \hat{L}_z\right] = i \hbar \hat{L}_x
\]