

Operators

→ An operator is a mapping between functions in its domain (input) and functions (output) in its range

◆ Examples:

- Multiplication operator
- Differentiation operator
- Integral operator

◆ Classes:

◆ Linear operators: If A and B are linear operators, f and g functions, and k a constant, then $(A+B)f = Af + Bf$, $A(f+g) = Af + Ag$, $Ak = kA$

◆ Differential Operators: include differentiation of the functions to which they are applied

$$\hat{A} (\psi) = \varphi$$

Figure 1. \hat{A} is an operator, acting on a function (ψ). Therefore, \hat{A} will map one state vector into another one.

Source: [Quantum Mechanical Operators - Quantum Chemistry - PSIBERG](#).

For every parameter that we can measure in physical systems, a quantum mechanical operator exists.

Quantum Mechanical Operators

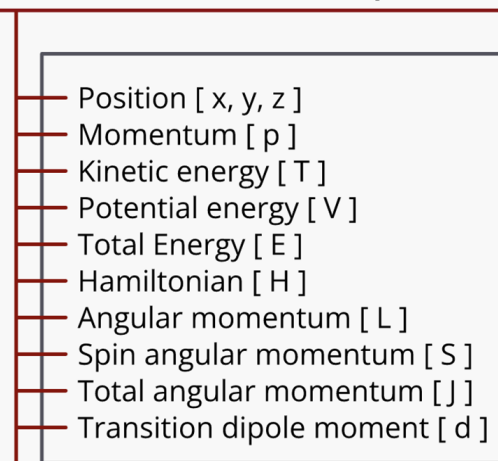


Figure. Examples of quantum mechanical operators. Source: [Quantum Mechanical Operators - Quantum Chemistry - PSIBERG](#)

Commutation of Operators

Differential operators act on the function(s) to their right, they do not necessarily commute with other operators containing the same independent variable. The commutator of operators A and B is therefore useful: $[A, B] = AB - BA$. Let's do an example: We will evaluate the commutator $[x, p]$ where $p = -i\hbar d/dx$. We apply $[x, p]$ to an arbitrary function $f(x)$.

$$\begin{aligned}
 [x, p]f(x) &= (xp - px)f(x) \\
 &= -i\hbar x df(x)/dx - (-i\hbar d/dx)(xf(x)) \\
 &= -i\hbar xf'(x) + i\hbar(f(x) + xf'(x)) = i\hbar f(x)
 \end{aligned}$$

Therefore, we see that $[x, p] = i\hbar$. This also indicates that $[x, p]f(x) = i\hbar f(x)$ for all f.

In general, if A, B, and C are operators and k is a constant, we have the following properties:

$$\begin{aligned}
[A, B] &= -[B, A] \\
[A, B + C] &= [A, B] + [A, C] \\
k[A, B] &= [kA, B] = [A, kB]
\end{aligned}$$

Identity, Inverse, Adjoint

The identity is an operator that leaves a function unchanged. It is generally denoted by I .

Some operators have an inverse, which is an operator that will “undo” its effect. Let A denote an operator, then A^{-1} will denote the inverse of A . Furthermore, the inverse will have the following property: $A^{-1}A = AA^{-1} = I$.

Associated with many operators will be another one called its adjoint. This operator is denoted: A^+ . For all functions f and g in Hilbert space, we have the following: $\langle f|Ag \rangle = \langle A^+f|g \rangle$. We can see that if we apply A to the right of any scalar product produces the same result as if we apply A^+ to the left of any scalar product. If we have the case that $A = A^+$, then the operator A is defined as self-adjoint or Hermitian. If we have that $A^+ = -A$ then A is called anti-Hermitian.

In addition, if the adjoint of an operator is equal to its inverse, $A^{-1} = A^+$, then the operator A is called unitary. [275-277]

Sources:

Mathematical Methods for Physicists by Arfken, George B. & Webber. Pages 275-277.

[Quantum Mechanical Operators - Quantum Chemistry - PSIBERG](#)