## **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 ( $\psi$ ). Therefore,  $\hat{A}$  will map one state vector into another one. Source: Quantum Mechanical Operators - Quantum Chemistry - PSIBERG.

Classical observables have an associated quantum mechanical operator. In other words, for every parameter that we can measure in physical systems, a quantum mechanical operator exists.

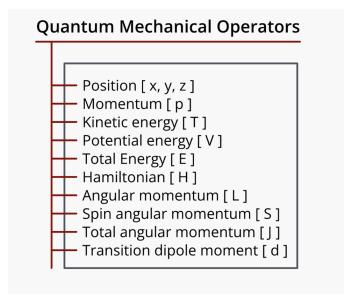


Figure. Examples of quantum mechanical operators. Source: Quantum Mechanical Operators - Quantum Chemistry - PSIBERG

## 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 = -id/dx. We apply [x, p] to an arbitrary function f(x).

$$[x, p]f(x) = (xp - px)f(x) =- ixdf(x)/dx - (-id/dx)(xf(x)) =- ixf'(x) + i(f(x) + xf'(x)) = if(x)$$

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

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

$$[A, B] = -[B, A]$$
  
 $[A, B + C] = [A, B] + [A, C]$   
 $k[A, B] = [kA, B] = [A, kB]$ 

## 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 donte 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 aint-Hermitian.

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

## Sources:

Mathematical Methods for Physicists by Arfken, George B. & Webber Quantum Mechanical Operators - Quantum Chemistry - PSIBERG