

Operator

① What is an operator?

It is represented as \hat{H}, \hat{O}, \dots

It acts on the function written to the right of the operator and gives a change.

action

$$\hat{H}f = g$$

Examples of operators

1. Differentiations

$$\hat{H} = \frac{d}{dx}, \frac{\partial}{\partial x}, \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} = \nabla^2$$

2. Simple numbers

$$\hat{H} = 1, 100, \dots$$

3. Multiplying a function

$$\hat{H} = \frac{1}{2}kx^2, \frac{1}{\sqrt{x^2 + y^2 + z^2}}, \dots$$

② Acting $\hat{H} = \frac{d^2}{dx^2}$ on $f(x) = x^2$,

$$\frac{d^2}{dx^2}(x^2) = \frac{d}{dx}(2x) = 2$$

③ Act $\hat{H} = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2}$ on

$$f(x, y) = 4x^3y^2 + 5x^2 + 1,$$

$$\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} \right) [4x^3y^2 + 5x^2 + 1]$$

$$= \frac{\partial^2}{\partial x^2} [4x^3y^2 + 5x^2 + 1] + \frac{\partial^2}{\partial y^2} [4x^3y^2 + 5x^2 + 1]$$

$$= \frac{\partial}{\partial x} [12x^2y^2 + 10x] + \frac{\partial}{\partial y} [8x^3y]$$

$$= 24xy^2 + 10 + 8x^3$$

Basic Quantum Chemistry

Rachel Sandford



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