

Operator

① What is an operator?

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

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

$$\overset{\text{action}}{\hat{H}}f = g$$

Examples of operators

1. Differentiations

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

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

Rosina Ehmman



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Table of Contents Basic Quantum Chemistry

1. Understanding the eBook Basic Quantum Chemistry
 - The Rise of Digital Reading Basic Quantum Chemistry
 - Advantages of eBooks Over Traditional Books
2. Identifying Basic Quantum Chemistry
 - Exploring Different Genres
 - Considering Fiction vs. Non-Fiction
 - Determining Your Reading Goals
3. Choosing the Right eBook Platform
 - Popular eBook Platforms
 - Features to Look for in an Basic Quantum Chemistry
 - User-Friendly Interface
4. Exploring eBook Recommendations from Basic Quantum Chemistry
 - Personalized Recommendations
 - Basic Quantum Chemistry User Reviews and Ratings
 - Basic Quantum Chemistry and Bestseller Lists
5. Accessing Basic Quantum Chemistry Free and Paid eBooks
 - Basic Quantum Chemistry Public Domain eBooks
 - Basic Quantum Chemistry eBook Subscription Services
 - Basic Quantum Chemistry Budget-Friendly Options

6. Navigating Basic Quantum Chemistry eBook Formats
 - ePub, PDF, MOBI, and More
 - Basic Quantum Chemistry Compatibility with Devices
 - Basic Quantum Chemistry Enhanced eBook Features
7. Enhancing Your Reading Experience
 - Adjustable Fonts and Text Sizes of Basic Quantum Chemistry
 - Highlighting and Note-Taking Basic Quantum Chemistry
 - Interactive Elements Basic Quantum Chemistry
8. Staying Engaged with Basic Quantum Chemistry
 - Joining Online Reading Communities
 - Participating in Virtual Book Clubs
 - Following Authors and Publishers Basic Quantum Chemistry
9. Balancing eBooks and Physical Books Basic Quantum Chemistry
 - Benefits of a Digital Library
 - Creating a Diverse Reading Collection Basic Quantum Chemistry
10. Overcoming Reading Challenges
 - Dealing with Digital Eye Strain
 - Minimizing Distractions
 - Managing Screen Time
11. Cultivating a Reading Routine Basic Quantum Chemistry
 - Setting Reading Goals Basic Quantum Chemistry
 - Carving Out Dedicated Reading Time
12. Sourcing Reliable Information of Basic Quantum Chemistry
 - Fact-Checking eBook Content of Basic Quantum Chemistry
 - Distinguishing Credible Sources
13. Promoting Lifelong Learning
 - Utilizing eBooks for Skill Development
 - Exploring Educational eBooks
14. Embracing eBook Trends
 - Integration of Multimedia Elements

- Interactive and Gamified eBooks

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