



LABORATORIUM KIMIA FISIKA

Jurusan Kimia - FMIPA

Universitas Gadjah Mada (UGM)

MATEMATIKA KIMIA

Operator

(Sumber : Barrante, Applied Mathematics fo Physical Chemistry, Bab 10)

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1. Perform the following operations:

(a) $\sum_{n=0}^5 x^n$

(c) ΔE

(b) $\sum_{n=0}^5 (-1)^n x^n$

(d) $\hat{\mathbf{D}}_x(x^3y), \hat{\mathbf{D}}_x = \frac{\partial}{\partial x}$

(e) $\hat{\mathbf{D}}_x^2(x^2y^3)$

(h) $\hat{\mathbf{D}}_x \sum_{n=0}^5 x^n$

(f) $\hat{\mathbf{D}}_y \hat{\mathbf{D}}_x(x^4y^3)$

(i) $\prod_{n=0}^4 x_n!$

(g) $\hat{\mathbf{D}}_z \hat{\mathbf{D}}_y \hat{\mathbf{D}}_x(x^2y^2z^2)$

(j) $\begin{pmatrix} -1 & 0 \\ 0 & -1 \end{pmatrix} \begin{pmatrix} a \\ b \end{pmatrix}$

2. Determine whether the following pairs of operators commute:

(a) $[\hat{\mathbf{D}}_y, \hat{\mathbf{D}}_z]$

(c) $[\hat{\mathbf{D}}_x, \Delta]$

(b) $[\hat{\mathbf{D}}_x, \sum]$

(d) $[\sum, \sqrt{\quad}]$

3. Show that $\nabla \cdot \nabla \phi = \frac{\partial^2 \phi}{\partial x^2} + \frac{\partial^2 \phi}{\partial y^2} + \frac{\partial^2 \phi}{\partial z^2}$.

4. Show that $\nabla(\psi\phi) = \psi \nabla \phi + \phi \nabla \psi$.



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5. An interpretation of the *Heisenberg uncertainty principle* is that the operator for linear momentum in the x -direction does not commute with the operator for position along the x -axis. If

$$\hat{p}_x = -i\hbar \frac{\partial}{\partial x} \quad \text{and} \quad \hat{x} = x$$

(where $\hbar = h/2\pi$ is a constant and $i = \sqrt{-1}$) represent operators for linear momentum and position along the x -axis, evaluate the commutator

$$[\hat{p}_x \hat{x} - \hat{x} \hat{p}_x]$$

and show that it does not equal zero. (*Hint:* Apply the operators \hat{x} and \hat{p}_x to an arbitrary function $\phi(x)$, keeping in mind that $x\phi(x)$ must be differentiated as a product.)

6. Show that $y = \sin ax$ is not an eigenfunction of the operator d/dx , but is an eigenfunction of d^2/dx^2 .
7. Show that the functions $\Phi = Ae^{im\phi}$, where A , i , and m are constants, are eigenfunctions of the operator

$$\hat{M}_z = -i\hbar \frac{\partial}{\partial \phi}$$

What are the eigenvalues? Take $\hbar = h/2\pi$ to be constant and $i = \sqrt{-1}$.

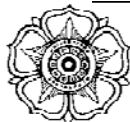
8. Show that the function

$$\psi = \sqrt{\frac{2}{a}} \sin \frac{n\pi x}{a}$$

where n and a are constants, is an eigenfunction of the Hamiltonian operator in one dimension

$$\hat{H} = -\frac{\hbar^2}{2m} \frac{d^2}{dx^2}$$

What are the eigenvalues? Take $\hbar = h/2\pi$ and m to be constants.



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9. Show that the function $\phi = xe^{ax}$ is an eigenfunction of the operator

$$\hat{O} = \frac{d^2}{dx^2} - \frac{2a}{x}$$

where a is a constant. What are the eigenvalues?

10. Using the two-dimensional rotational operator

$$\begin{pmatrix} \cos \theta & -\sin \theta \\ \sin \theta & \cos \theta \end{pmatrix}$$

find the new coordinates of the point after rotation through the angle

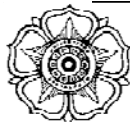
- (a) (2, 2) through 30° .
 - (b) (4, 1) through 45° .
 - (c) (-4, -3) through 180° .
 - (d) (3, 2) through 60° .
 - (e) (1, -3) through 240° .
11. The BF_3 molecule is a planar molecule, the fluorine atoms lying at the corners of an equilateral triangle. By assigning x - and y -coordinates to each fluorine atom (the boron atom being placed at the origin), show that a two-dimensional C_3 operation perpendicular to the x - y plane and through the boron atom will transform the molecule into itself. (*Hint: Place one B-F bond along the y -axis.*)
12. The differential operator for angular momentum is given by the expression

$$\hat{M} = -i\hbar(\mathbf{r} \times \nabla)$$

where \hbar is a constant, $\mathbf{r} = i\mathbf{x} + \mathbf{j}y + \mathbf{k}z$ and

$$\nabla = i\frac{\partial}{\partial x} + \mathbf{j}\frac{\partial}{\partial y} + \mathbf{k}\frac{\partial}{\partial z}$$

Assuming $\hat{M} = i\hat{M}_x + \mathbf{j}\hat{M}_y + \mathbf{k}\hat{M}_z$, find the components of this operator \hat{M}_x , \hat{M}_y , and \hat{M}_z .

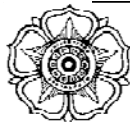


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13. Transform the components of angular momentum \hat{M}_x , \hat{M}_y , and \hat{M}_z found in Problem 12, to spherical polar coordinates.
14. Derive an expression for the total squared angular momentum operator

$$\hat{M}^2 = \hat{M}_x^2 + \hat{M}_y^2 + \hat{M}_z^2$$

using the expressions found in Problem 13. Remember that the operator \hat{M}_x^2 is \hat{M}_x operating on \hat{M}_x , and is not found by merely squaring \hat{M}_x (see Section 10-1).



KUNCI JAWABAN

1. (a) $1 + x + x^2 + x^3 + x^4 + x^5$
 (b) $1 - x + x^2 - x^3 + x^4 - x^5$
 (c) $\Delta E = E_2 - E_1$
 (d) $3x^2y$
 (e) $2y^3$
 (f) $12x^3y^2$
 (g) $8xyz$
 (h) $1 + 2x + 3x^2 + 4x^3 + 5x^4$
 (i) $x_0! \cdot x_1! \cdot x_2! \cdot x_3! \cdot x_4!$
 (j) $\begin{pmatrix} -1 & 0 \\ 0 & -1 \end{pmatrix} \begin{pmatrix} a \\ b \end{pmatrix} = \begin{pmatrix} -a \\ -b \end{pmatrix}$
2. (a) commute (c) commute
 (b) commute (d) do not commute
7. eigenvalues = $m\hbar$
9. eigenvalues = a^2
10. (a) (0.732, 2.732) (d) (-0.232, 3.598)
 (b) (2.121, 3.535) (e) (-3.098, 0.634)
 (c) (4, 3)
11. $\hat{M}_x = -i\hbar \left(y \frac{\partial}{\partial z} - z \frac{\partial}{\partial y} \right)$
 $\hat{M}_y = -i\hbar \left(z \frac{\partial}{\partial x} - x \frac{\partial}{\partial z} \right)$
 $\hat{M}_z = -i\hbar \left(x \frac{\partial}{\partial y} - y \frac{\partial}{\partial x} \right)$
12. $\hat{M}_x = i\hbar \left(\sin\phi \frac{\partial}{\partial\theta} + \cot\theta \cos\phi \frac{\partial}{\partial\phi} \right)$
 $\hat{M}_y = i\hbar \left(-\cos\phi \frac{\partial}{\partial\theta} + \cot\theta \sin\phi \frac{\partial}{\partial\phi} \right)$
 $\hat{M}_z = -i\hbar \frac{\partial}{\partial\phi}$
13. $\hat{M}^2 = -\frac{\hbar^2}{4\pi^2} \left(\frac{\partial^2}{\partial\theta^2} + \cot\theta \frac{\partial}{\partial\theta} + \frac{1}{\sin^2\theta} \frac{\partial^2}{\partial\phi^2} \right)$

