LABORATORIUM KIMIA FISIKA
Jurusan Kimia - FMIPA
Universitas Gadjah Mada (UGM)

MATEMATIKA KIMIA
Operator

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

Drs. Iqmal Tahir, M.Si.

Laboratorium Kimia Fisika, Jurusan Kimia
Fakultas Matematika dan Ilmu Pengetahuan Alam
Universitas Gadjah Mada, Yogyakarta, 55281

Tel : 0857 868 77886; Fax : 0274-545188
Email :
iqmal@ugm.ac.id atau iqmal.tahir@yahoo.com

Website :
http://iqmal.staff.ugm.ac.id
http://iqmaltahir.wordpress.com

LATIHAN

1. Perform the following operations:

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

(c) ΔE

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

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

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

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

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

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

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

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

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

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

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

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 $\nabla(\psi\phi) = \psi \nabla \phi + \phi \nabla \psi$.

LATIHAN

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

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

(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

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

and show that it does not equal zero. (*Hint:* Apply the operators $\hat{\mathbf{x}}$ and $\hat{\mathbf{p}}_x$ 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

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

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

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

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

LATIHAN

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

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

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 $\mathbf{C}_3$ 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

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

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

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

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

LATIHAN

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

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

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) $3x^2 y$
(e) $2y^3$
(f) $12x^3 y^2$
(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
(b) commute
(c) commute
(d) do not commute

7. eigenvalues $= m\hbar$

9. eigenvalues $= a^2$

10. (a) (0.732, 2.732)
(b) (2.121, 3.535)
(c) (4, 3)
(d) (−0.232, 3.598)
(e) (−3.098, 0.634)

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. $\hat{M}^2 = -\frac{h^2}{4\pi^2}\left(\frac{\partial^2}{\partial\theta^2} + \cot\theta\frac{\partial}{\partial\theta} + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2}\right)$