PROBLEM SET SOLUTIONS

Chapter 5, *Quantum Chemistry*, 5th Ed., Levine

5.9 Let **A** have the components (3, -2, 6) & let **B** have the components (-1, 4 ,4). Find |**A**|, |**B**|, **A** + **B**, **A - B**, **A** · **B**, **A** x **B**. Find the angle between **A** and **B.**

A = **i** (3) + **j** (-2) + **k** (6)   **B** = **i** (-1) + **j** (4) + **k** (4)

|**A**| $= (A_x^2 + A_y^2 + A_z^2)^{1/2} = (9 + 4 + 36)^{1/2} = (49)^{1/2} = 7$
SCALAR

|**B**| $= (B_x^2 + B_y^2 + B_z^2)^{1/2} = (1 + 16 + 16)^{1/2} = (33)^{1/2} = 5.74$
SCALAR

A + **B** = **i** (3-1) + **j** (-2+4) + **k** (6+4) = **i** (2) + **j** (2) + **k** (10)
VECTOR

A - B = **i** (3+1) + **j** (-2-4) + **k** (6-4) = **i** (4) + **j** (-6) + **k** (2)
VECTOR

A • B $= A_xB_x + A_yB_y + A_zB_z = (3)(-1) + (-2)(4) + (6)(4) = 13$
SCALAR

A x **B** = **i** (-8-24) + **j** (-1) (12+6) + **k**(12-2) = **i** (-32) + **j** (-18) + **k**(10) VECTOR

$$|\mathbf{A} \times \mathbf{B}| = |\mathbf{A}|\,|\mathbf{B}| \sin\theta = (|\mathbf{A} \times \mathbf{B}| \bullet |\mathbf{A} \times \mathbf{B}|)^{1/2}$$

$$= ((-32)^2 + (-18)^2 + (-10)^2)^{1/2} = 38.05$$

$$\sin\theta = |\mathbf{A} \times \mathbf{B}| / (|\mathbf{A}|\,|\mathbf{B}|) = 38.05/(7 \times 5.7) = 0.947$$

$$\theta = \sin^{-1}(0.947) = 71.26^{o}$$

5.14(b) The divergence of a vector function **A** is given by

$$\text{div}\,\mathbf{A} = \nabla \bullet \mathbf{A}$$

$$= (\mathbf{i}\,\partial/\partial x + \mathbf{j}\,\partial/\partial y + \mathbf{k}\,\partial/\partial z) \bullet (\mathbf{i}\,A_x + \mathbf{j}\,A_y + \mathbf{k}\,A_z)$$

$$= \partial A_x/\partial x + \partial A_y/\partial y + \partial A_z/\partial z.$$

Find $\nabla \bullet \mathbf{r}$, where $\mathbf{r} = \mathbf{i}x + \mathbf{j}y + \mathbf{k}z$.

$$\nabla \bullet \mathbf{r} = \partial x/\partial x + \partial y/\partial y + \partial z/\partial z = 1 + 1 + 1 = 3$$

5.24 Calculate the possible angles between **L** and the z-axis for l = 2.

l = 2, m= -2, -1, 0 , 1, 2

$|\mathbf{L}|$ = SQRT (l (l + 1)) $\hbar$ = SQRT(2x3) $\hbar$ = SQRT(6) $\hbar$

$|\mathbf{L_z}|$ = m $\hbar$

l = 2, m = 2: cos θ = 2 $\hbar$ / SQRT(6) $\hbar$ = 2/SQRT(6) = 0.816, $\theta = 35.2^o$

l = 2, m = 1: cos θ = 1 $\hbar$ / SQRT(6) $\hbar$ = 1/SQRT(6) = 0.408, $\theta = 65.9^o$

l = 2, m = 0:, $\theta = 90.0^o$

l = 2, m = -1: $\theta = (180 - 65.9)^o = 114^o$

l = 2, m = -2: $\theta = (180 - 35.2)^o = 144.8^o$

5.25 Show that the spherical harmonics are eigenfunctions of the operator

L_{xL}