Advanced Mathematical Methods for Chemistry

QUIZ 1 - SOLUTIONS

1. ∞ $f(x)$ can be arbitrary so it is not possible to write all $f(x)$ as a linear combination of a finite number of basis functions.

2. $r = \sqrt{x^2+y^2+z^2}$

$$\vec{\nabla} r = \frac{\partial r}{\partial x}\hat{i} + \frac{\partial r}{\partial y}\hat{j} + \frac{\partial r}{\partial z}\hat{k}$$

$$\frac{\partial r}{\partial x} = \frac{1}{2\sqrt{x^2+y^2+z^2}} \times 2x = \frac{x}{r}$$

$$\vec{\nabla} r = (x\hat{i} + y\hat{j} + z\hat{k})/r = \vec{r}/r$$

3. (b) and (c) are not linearly independent sets, since Z-coordinate $= 0$ for all vectors in (b) and (c).

(a) is a L.I. set since

$$\begin{vmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 1 & 1 & 1 \end{vmatrix} = 1 \neq 0$$

4. $$\vec{\nabla}\cdot\vec{r} = \frac{\partial x}{\partial x} + \frac{\partial y}{\partial y} + \frac{\partial z}{\partial z} = 3$$

5. ~~So~~ Two functions $f_1(x)$ and $f_2(x)$ are LD if $f_2(x) = a f_1(x)$ where a is a constant.

Clearly, none of the sets are linearly dependent.

6. $\vec{\omega} = \vec{\nabla} \times \vec{v}$

$$= \begin{vmatrix} i & j & k \\ \frac{\partial}{\partial x} & \frac{\partial}{\partial y} & \frac{\partial}{\partial z} \\ y & x & 0 \end{vmatrix} = \hat{i}(0-0) + j(0-0) + \hat{k}(1-1)$$

$$= 0$$

7. $\vec{F}(\vec{r}) = -\vec{\nabla} V(\vec{r})$

$$\vec{F}(\vec{r}) = -\vec{\nabla} . \frac{A}{\sqrt{x^2+y^2+z^2}}$$

$$= -A \left[\frac{\partial}{\partial x} \frac{1}{\sqrt{x^2+y^2+z^2}} \hat{i} + \frac{\partial}{\partial y} \frac{1}{\sqrt{x^2+y^2+z^2}} + \frac{\partial}{\partial z} \frac{1}{\sqrt{x^2+y^2+z^2}} \right]$$

$$= +A \frac{(x\hat{i} + y\hat{j} + z\hat{k})}{r^3} = \frac{A\vec{r}}{r^3}$$

At $r \equiv (1,0,0)$ $\quad \vec{F} = A\hat{i}$

8. $A^2 \int_0^2 \sin^2(2\pi x)\,dx \int_0^4 \sin^2\left(\frac{\pi y}{2}\right) dy \int_0^1 \sin^2 \pi z \,dz = 1$

$$\Rightarrow A^2 . \left(\frac{2}{2} \times \frac{4}{2} \times \frac{1}{2} \right) = 1$$

$$\Rightarrow A = 1$$

9. $W = \int \vec{f} . d\vec{r} = \int f_x\,dx + \int f_y\,dy$

Along straight line from $(1,1)$ to $(2,2)$, $x=y$

$$W = \int_1^2 \frac{2dx}{2x^2} = \frac{1}{2}$$

10. Consider $\underbrace{5x^2}_{A}\hat{i} + \underbrace{5x^2}_{B}\hat{j}$

$$\frac{\partial A}{\partial y} = 0 \neq \frac{\partial B}{\partial x} = 10x$$

$$\underbrace{5y^2}_{A}\hat{i} + \underbrace{5x^2}_{B}\hat{j}$$

$$\frac{\partial A}{\partial y} = 10y \neq \frac{\partial B}{\partial x} = 10x$$

$$\underbrace{5xy^2}_{A}\hat{i} + \underbrace{5yx^2}_{B}\hat{j}$$

$$\frac{\partial A}{\partial y} = 10xy = \frac{\partial B}{\partial x}$$ Path Independent