Mathematics for Chemistry

ASSIGNMENT 3: SOLUTIONS

$\boxed{1}$ $\vec{F} = -\dfrac{\hat{r}}{r^2} = -\dfrac{(x\hat{i} + y\hat{j} + z\hat{k})}{r^3}$

$\vec{F}.d\vec{r} = -\left(\dfrac{x\,dx + y\,dy + z\,dz}{r^3}\right)$

$= -\dfrac{(x\,dx + y\,dy + z\,dz)}{(x^2+y^2+z^2)^{3/2}}$

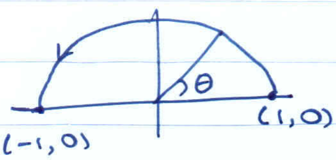
Let $t = x^2+y^2+z^2$ $\quad dt = 2(x\,dx + y\,dy + z\,dz)$

$\vec{F}.d\vec{r} = -\dfrac{1\,dt}{2\,t^{3/2}}$

$\displaystyle\int_{(1,1,1)}^{(2,2,2)} \vec{F}.d\vec{r} = \left[\frac{1}{t^{1/2}}\right]_{(1,1,1)}^{(2,2,2)} = \frac{1}{\sqrt{12}} - \frac{1}{\sqrt{3}} = -\frac{1}{2\sqrt{3}}$

Work done by force $= -\dfrac{1}{2\sqrt{3}} = -0.29$

$\boxed{2}$ $\vec{F}.d\vec{r} = 3\dfrac{x\,dx}{y} + (x^2+y^2)\,dy$



along path

$x = \cos\theta$; $dx = -\sin\theta\,d\theta$

$y = \sin\theta$; $dy = \cos\theta\,d\theta$

$\vec{F}.d\vec{r} = (-3\cos\theta + \cos\theta)\,d\theta$

$= -2\cos\theta\,d\theta$

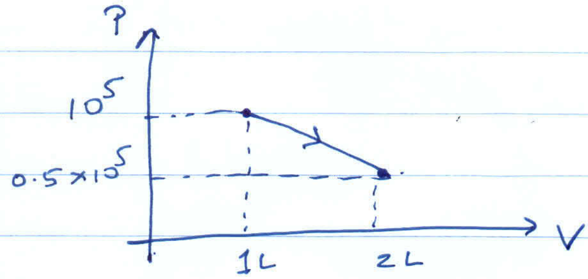
$W = \displaystyle\int_0^{\pi} -2\cos\theta\,d\theta = \left[-2\sin\theta\right]_0^{\pi} = 0$

3. For a conservative force $dW = \bar{F}.d\bar{r}$ is independent of path

$dW = F_x\,dx + F_y\,dy$ is exact

$\Rightarrow \frac{\partial F_x}{\partial y} = \frac{\partial F_y}{\partial x}$. Holds only for (B)

4. $dW = -P\,dV$



Along path

$P = 1.5\times10^5 - 0.5\times10^5\,V$

$dW = -1.5\times10^5\,dV + 0.5\times10^5\,V\,dV$

$W = \int_1^2 -1.5\times10^5\,dV + 0.5\times10^5\,V\,dV$

$= -1.5\times10^5 + 0.5\times10^5 \times \frac{3}{2}$

$= -0.75\times10^5$ Pa L

$= -0.75 \times 100$ J

$= -75$ J

5. $dG = V\,dP - S\,dT$

Condition for exact $\Rightarrow \frac{\partial V}{\partial T} = -\frac{\partial S}{\partial P}$

6. We have $\frac{\partial S}{\partial P} = -\frac{\partial V}{\partial T} = -\frac{R}{P}$

$\Rightarrow S(P,T) = -R\ln P + \underline{\underline{f(T)}}$

Integration constant

$\boxed{7}$

$$dA = -\frac{RT}{V}\,dV - \left(R\ln V + \frac{3R}{2T}\right) dT$$

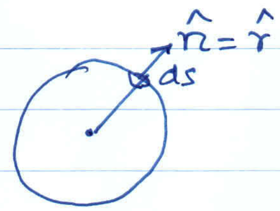
$$\Delta A = -RT\int \frac{dV}{V} - \int\left(R\ln V + \frac{3R}{2T}\right) dT$$

$$= \left[-RT\ln V - RT\ln V - \frac{3R}{2}\ln T\right]_{(1,1)}^{(2,2)}$$

$$= -2R\ln 2 - \frac{3}{2}R\ln 2$$

$$= -\frac{7}{2}R\ln 2$$

$\boxed{8}$



$$\vec{V} = x\hat{i} + y\hat{j} + z\hat{k} = \vec{r} = r\hat{r}$$

$$d\vec{S} = \hat{r}\,dS$$

$$= \hat{r}\sin\theta\,d\theta\,d\phi \qquad (r = 1 \text{ on surface})$$

$$\vec{V}\cdot d\vec{S} = \sin\theta\,d\theta\,d\phi$$

$$\int_S \vec{V}\cdot d\vec{S} = \int_0^{2\pi}\int_0^{\pi}\sin\theta\,d\theta\,d\phi = 4\pi$$

$\boxed{9}$

$$\psi(x,y,z) = \sin\pi x \;\sin(\pi y/2)\;\sin(\pi z/2)$$

$$\psi^2(x,y,z) = \sin^2(\pi x)\;\sin^2(\pi y/2)\;\sin^2(\pi z/2)$$

$$\int \psi^2(x,y,z)\,dV = \int_0^1 \sin^2\pi x\,dx \int_0^2 \sin^2\left(\frac{\pi y}{2}\right)dy \int_0^2 \sin^2\left(\frac{\pi z}{2}\right)dz$$

$$= \frac{1}{2}\cdot 1\cdot 1$$

$$= 0.5$$

$\boxed{10}$

$$\int_0^{2\pi}\int_0^{\pi}\int_0^{\infty}\cos^2\theta\left(\frac{r}{a_0}\right)^2 e^{-r/a_0}\cdot r^2\sin\theta\,dr\,d\theta\,d\phi$$

$$= 2\pi \times \frac{2}{3}\times a_0^3\int\left(\frac{r}{a_0}\right)^4 e^{-(r/a_0)}\,d\left(\frac{r}{a_0}\right) = 32\pi a_0^3$$