CHM 325: Quiz 1 SOLUTIONS

1. $$\vec{L} = m\,\vec{r}\times\vec{v}$$

$$\vec{v} = \vec{\omega}\times\vec{r}$$

$$\Rightarrow \vec{L} = m\left(\vec{r}\times\vec{v}\right)\times\vec{r}$$

$$= m\left[\vec{v}\,(\vec{r}\cdot\vec{r}) - \vec{r}\,(\vec{r}\cdot\vec{v})\right]$$ (2)

$\left(\because\ \vec{A}\times\vec{B}\times\vec{C} = \vec{B}\,(\vec{A}\cdot\vec{C}) - \vec{C}\,(\vec{A}\cdot\vec{B})\right)$

$$= m\left[r^2\vec{v} - r^2\,\hat{r}\,(\hat{r}\cdot\vec{v})\right]$$ (using $\vec{r} = r\hat{r}$)

$$= mr^2\left[\vec{v} - \hat{r}\,(\hat{r}\cdot\vec{v})\right]$$ (2)

2. $$T = \int_{\text{all space}} \psi(\vec{r})\left(\frac{-\hbar^2}{2m}\nabla^2\psi(\vec{r})\right)d\tau$$

$$= \left(\frac{-\hbar^2}{2m}\right)\int_{\text{all space}} \psi(\vec{r})\,\nabla^2\psi(\vec{r})\,d\tau.$$

$$= \left(\frac{-\hbar^2}{2m}\right)\int_{\text{all space}} \left[\vec{\nabla}\cdot(\psi\nabla\psi) - (\vec{\nabla}\psi)^2\right]d\tau$$

(using $\vec{\nabla}\cdot(f\vec{v}) = \vec{\nabla}f\cdot\vec{v} + f\,\vec{\nabla}\cdot\vec{v}$ w/ $\vec{v} = \vec{\nabla}\psi$, $f = \psi$.)

(2)

$$= \left(\frac{-\hbar^2}{2m}\right)\left\{\int_{\text{all space}} \vec{\nabla}\cdot(\psi\nabla\psi)\,d\tau - \int_{\text{all space}} (\nabla\psi)^2\,d\tau\right\}$$

$$= \left(\frac{-\hbar^2}{2m}\right)\left\{ \int_{\substack{\text{Surface}\\ \text{at infinity}}} (\psi \vec{\nabla}\cdot\psi)\cdot d\vec{\sigma} - \int_{\text{all space}} (\nabla\psi)^2 d\tau \right\}$$

$1\frac{1}{2}$ (using Gauss theorem for the first term considering a surface ~~boun~~ bounding the integration space. ~~At~~ Note that as the integration volume extends to infinity, the all points on this surface will have $r \to \infty$).

$$= \left(\frac{-\hbar^2}{2m}\right)\left(-\int_{\text{all space}} (\nabla\psi)^2 d\tau\right) = \frac{\hbar^2}{2m}\int_{\text{all space}} (\nabla\psi)^2 d\tau \geq 0$$

$\frac{1}{2}$ The first term involving the surface integral goes to zero as $\psi(\vec{r}) \to 0$ for $r \to \infty$ $\Rightarrow$ $\psi\vec{\nabla}\psi$ evaluated on the surface would also be 0.

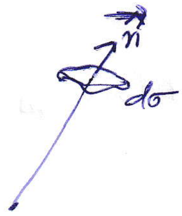
3. ψ satisfies Laplace's equation. This means:

$$\nabla^2 \psi(\vec{r}) = 0 \qquad \cdots 0 \cdots$$

(1)

Consider a region R lying within the volume V, with volume Ω_R & closed surface S_R. Let us consider the integral

$$I_R = \int_{S_R} \vec{\nabla}\psi \cdot d\vec{\sigma}$$



(1)

$$= \int_{S_R} (\vec{\nabla}\psi \cdot \vec{n})\, d\sigma \qquad \cdots 1 \cdots$$

where $d\vec{\sigma} = \vec{n}\, d\sigma$

$\vec{n} \rightarrow$ unit normal to the differential area $d\sigma$.

Let $\vec{f}(\vec{r}) = \vec{\nabla}\psi$

(2) Using Gauss' Theorem,

$$\int_{S_R} \vec{f}(\vec{r}) \cdot d\vec{\sigma} = \int_{\Omega_R} \vec{\nabla} \cdot \vec{f}(\vec{r})\, d\tau. \qquad \cdots 2 \cdots$$

Using ..2.. in ..1.. we get that

$$I_R = \int_{S_R} (\vec{\nabla}\psi \cdot \vec{n})\, d\sigma = \int_{S_R} \vec{\nabla}\psi \cdot d\vec{\sigma} = \int_{\Omega_R} \vec{\nabla} \cdot (\vec{\nabla}\psi)\, d\tau$$

(2)

$$= \int_{\Omega_R} \nabla^2 \psi\, d\tau = 0 \quad \text{using} \cdots 0 \cdots$$

4. $\hat{\vec{L}} = -i\hbar\, \vec{r} \times \vec{\nabla}$ ...0...

Position vector is spherical polar coordinates is

$\vec{r} = r\hat{r}$ ...1...

(1)

Gradient can be obtained by using the general formula

$$\vec{\nabla}\psi = \sum_{l=1}^{3} (\vec{e}_l \cdot \vec{\nabla}\psi)\, \vec{e}_l$$

(1)

$$= \sum_{l=1}^{3} \frac{1}{h_l}\frac{\partial \psi}{\partial q_l}\, \vec{e}_l \quad \text{...2...}$$

where $\vec{e}_l$ are unit vectors along the new coordinates,

& h_l is the scaling factor.

For spherical coordinates these are $\vec{e}_1 = \hat{r}$, $\vec{e}_2 = \hat{\theta}$, $\vec{e}_3 = \hat{\varphi}$

$h_1 = 1$, $h_2 = r$, $h_3 = r\sin\theta$.

(1/2)

∴ In spherical polar coordinates

$$\vec{\nabla}\psi = \frac{\partial \psi}{\partial r}\hat{r} + \frac{1}{r}\frac{\partial \psi}{\partial \theta}\hat{\theta} + \frac{1}{r\sin\theta}\frac{\partial \psi}{\partial \varphi}\hat{\varphi}$$

...3...

(1½)

In other words, $\vec{\nabla} = \hat{r}\frac{\partial}{\partial r} + \hat{\theta}\frac{1}{r}\frac{\partial}{\partial \theta} + \hat{\varphi}\frac{1}{r\sin\theta}\frac{\partial}{\partial \varphi}$ ...4...

Now, using ...1... & ...4...,

$$\vec{r} \times \vec{\nabla} = \begin{vmatrix} \hat{r} & \hat{\theta} & \hat{\varphi} \\ r & 0 & 0 \\ \frac{\partial}{\partial r} & \frac{1}{r}\frac{\partial}{\partial \theta} & \frac{1}{r\sin\theta}\frac{\partial}{\partial \varphi} \end{vmatrix} = \hat{\theta}\left(-\frac{1}{\sin\theta}\frac{\partial}{\partial \varphi}\right) + \hat{\varphi}\frac{\partial}{\partial \theta}$$

(2)

$$\Rightarrow \vec{L} = i\hbar\left[\hat{\theta}\frac{1}{\sin\theta}\frac{\partial}{\partial \varphi} - \hat{\varphi}\frac{\partial}{\partial \theta}\right]$$

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