

FAQs & their solutions for Module 5: **Angular Momentum-I**

Question1: The operator representation of L_z is given by:

$$L_z = -i\hbar \frac{\partial}{\partial \phi} \quad (1)$$

(a) Solve the eigen value equation for L_z ; determine the eigen values and normalized eigen functions.

(b) Write the orthonormality condition.

Solution1:

The operator representation of L_z is given by:

$$L_z = -i\hbar \frac{\partial}{\partial \phi} \quad (2)$$

We write the eigenvalue equation for L_z :

$$L_z \Phi = m\hbar \Phi \quad (3)$$

where $m\hbar$ represents the eigenvalues of L_z ; we have introduced the Planck's constant \hbar for the sake of convenience. Replacing L_z by its operator representation we get

$$-i\hbar \frac{\partial \Phi}{\partial \phi} = m\hbar \Phi$$

or

$$\frac{\partial \Phi}{\partial \phi} = im\Phi \quad (4)$$

The solution of the above equation is given by

$$\Phi(\phi) \sim e^{im\phi}$$

For the wave function to be a single-valued, we must have

$$\Phi(\phi + 2\pi) = \Phi(\phi)$$

or

$$e^{2\pi mi} = 1$$

giving

$$m = 0, \pm 1, \pm 2, \dots$$

Thus we get the result that the eigenvalues of L_z are $0, \pm \hbar, \pm 2\hbar, \dots$. The above result implies that if we measure L_z we will *only* get one of the discrete eigenvalues which is an integral multiple of \hbar .

This is the quantization of angular momentum and since z can be in any arbitrary direction, the above result implies that if we measure *any* Cartesian component of the angular momentum we will get one of the following values : $0, \pm \hbar, \pm 2\hbar, \dots$. We label the corresponding functions by the subscript m

$$\Phi_m(\phi) = \frac{1}{\sqrt{2\pi}} e^{im\phi} ; m = 0, \pm 1, \pm 2, \dots \quad (5)$$

where the factor $1/\sqrt{2\pi}$ ensures that

$$\int_0^{2\pi} |\Phi(\phi)|^2 d\phi = 1 \quad (6)$$

which is the normalization condition. Thus, the eigenvalue equation can be written as

$$L_z \left[\frac{1}{\sqrt{2\pi}} e^{im\phi} \right] = m\hbar \left[\frac{1}{\sqrt{2\pi}} e^{im\phi} \right] ; m = 0, \pm 1, \pm 2, \dots \quad (7)$$

Further,

$$\int_0^{2\pi} \Phi_{m'}^*(\phi) \Phi_m(\phi) d\phi = \delta_{mm'} \quad (8)$$

which represents the orthonormality condition for $\Phi_m(\phi)$.

Question2: Solve the eigen value equation for L_z^2 .

Solution 2: Now, the square of an operator is defined by the following equation:

$$\alpha^2 = \alpha\alpha$$

Thus

$$L_z^2 \Phi = L_z L_z \Phi = (-i\hbar)^2 \frac{\partial}{\partial \phi} \frac{\partial \Phi}{\partial \phi} = -\hbar^2 \frac{\partial^2 \Phi}{\partial \phi^2}$$

The solution of the eigenvalue equation

$$L_z^2 \Phi = \lambda \Phi \quad (9)$$

will immediately give

$$\lambda = m^2 \hbar^2 ; m = 0, \pm 1, \pm 2, \dots \quad (10)$$

as the eigenvalues with

$$\Phi_m(\phi) = \frac{1}{\sqrt{2\pi}} e^{im\phi}$$

as the corresponding (normalized) eigenfunction. Thus we see that the functions $\Phi_m(\phi)$ are simultaneous eigenfunctions of L_z and L_z^2 :

$$L_z \Phi_m(\phi) = m\hbar \Phi_m(\phi) \quad (11)$$

and

$$L_z^2 \Phi_m(\phi) = m^2 \hbar^2 \Phi_m(\phi) \quad (12)$$

Question3: Using spherical polar coordinates one can show that

$$L^2 \psi = -\hbar^2 \left[\frac{1}{\sin \theta} \frac{\partial}{\partial \theta} \left(\sin \theta \frac{\partial \psi}{\partial \theta} \right) + \frac{1}{\sin^2 \theta} \frac{\partial^2 \psi}{\partial \phi^2} \right] \quad (13)$$

We write the eigenvalue equation

$$L^2 Y(\theta, \phi) = \lambda \hbar^2 Y(\theta, \phi) \quad (14)$$

Show that

$$Y(\theta, \phi) = F(\theta) \left[\frac{1}{\sqrt{2\pi}} e^{im\phi} \right] \quad (15)$$

Solution3: The eigen value equation is

$$L^2 \psi(\theta, \phi) = \lambda \hbar^2 \psi(\theta, \phi)$$

$$\text{Since } L^2 \psi = -\hbar^2 \left[\frac{1}{\sin \theta} \frac{\partial}{\partial \theta} \left(\sin \theta \frac{\partial \psi}{\partial \theta} \right) + \frac{1}{\sin^2 \theta} \frac{\partial^2 \psi}{\partial \phi^2} \right]$$

we get

$$-\hbar^2 \left[\frac{1}{\sin \theta} \frac{\partial}{\partial \theta} \left(\sin \theta \frac{\partial \psi}{\partial \theta} \right) + \frac{1}{\sin^2 \theta} \frac{\partial^2 \psi}{\partial \phi^2} \right] = \lambda \hbar^2 \psi(\theta, \phi)$$

We try the method of separation of variables:

$$\psi(\theta, \phi) = F(\theta) \Phi(\phi)$$

to obtain

$$-\frac{\Phi(\phi)}{\sin \theta} \frac{d}{d\theta} \left(\sin \theta \frac{dF}{d\theta} \right) - \frac{F(\theta)}{\sin^2 \theta} \frac{d^2 \Phi}{d\phi^2} = \lambda F(\theta) \Phi(\phi)$$

Simple rearrangement gives us

$$-\frac{1}{F(\theta)} \sin \theta \frac{d}{d\theta} \left(\sin \theta \frac{dF}{d\theta} \right) + \lambda \sin^2 \theta = \frac{1}{\Phi(\phi)} \frac{d^2 \Phi}{d\phi^2} = -m^2$$

The variables are indeed separated out and $\Phi(\phi)$ is given by

$$\Phi_m(\phi) = \frac{1}{\sqrt{2\pi}} e^{im\phi}$$

For the wave function to be a single-valued, we must again have

$$m = 0, \pm 1, \pm 2, \dots$$

Thus we have

$$\psi(\theta, \phi) = F(\theta)\Phi(\phi) = F(\theta) \left(\frac{1}{\sqrt{2\pi}} e^{im\phi} \right); m = 0, \pm 1, \pm 2, \dots$$

Question4: In the simplest model of a rotating diatomic molecule, it is assumed to be a rigid rotator, i.e., the distance between the two atoms is assumed to be fixed. Show from classical considerations, that the rotational energy of such a rigid rotator is given by

$$H = \frac{L^2}{2\mu r_e^2}$$

where μ represents the reduced mass, r_e the distance between the two atoms (assumed to be fixed) and L represents the angular momentum of the molecule about the axis passing through the centre of mass.

Solution4: The rotational kinetic energy is $\frac{1}{2}I\omega^2$, where $I (= \mu r_e^2)$ is the moment of inertia about the axis passing through the centre of mass and μ being the reduced mass. Further the angular momentum $L = I\omega$. Thus

$$\text{Rotational Kinetic Energy} = \frac{L^2}{2I} = \frac{L^2}{2\mu r_e^2} \quad (16)$$

Question5: Determine the eigenvalues and eigenfunctions of the rotational energy of a rigid rotator given by

$$H = \frac{L^2}{2\mu r_e^2}$$

Solution5: The eigenvalues of L^2 are $l(l+1)\hbar^2$ [with $l = 0, 1, 2, \dots$] and the corresponding eigenfunctions are known as the spherical harmonics and are denoted by $Y_{lm}(\theta, \phi)$. Thus

$$L^2 Y_{lm}(\theta, \phi) = l(l+1)\hbar^2 Y_{lm}(\theta, \phi) \quad (17)$$

$$l = 0, 1, 2, \dots$$

$$m = -l, -l+1, \dots, l-1, l$$

Thus, we get the following expression for the rotational energy levels

$$E = \frac{J(J+1)\hbar^2}{2\mu r_e^2} \quad (18)$$

where $J(=0,1,2,\dots)$ is known as the rotational quantum number; we have written $J(J+1)$ instead of $l(l+1)$ so as to be consistent with the spectroscopic notation.

Question6: Molecules like HCl, HF, LiH can be considered as rigid rotators and because these molecules have permanent dipole moments, transitions take place only between adjacent rotational energy levels (this is the selection rule). Show that this leads to equally spaced lines in the emission as well as in the absorption spectra.

Solution6: For emission $J_f = J_i - 1$ (f and i refer to the final and initial states) and the wave number of the emitted radiation is given by

$$\nu(\text{cm}^{-1}) = \frac{E_i - E_f}{hc} = 2J_i B \quad (19)$$

where

$$B = \frac{h}{8\pi^2 \mu r_e^2 c} \quad (20)$$

is known as the rotational constant. Thus the lines are equally spaced. Similarly for absorption $J_f = J_i + 1$ and

$$\nu(\text{cm}^{-1}) = \frac{E_f - E_i}{hc} = 2(J_i + 1)B \quad (21)$$

Question7: The rotational absorption spectrum of HCl appears at wave numbers 21.18, 42.36, 63.54, 84.72 and 105.91 cm^{-1} . Assuming $M_{Cl} \approx 35 M_H$ and $M_H \approx 1.86 \times 10^{-24}$ g, calculate the value of r_e .

Solution7: The absorption spectra should therefore appear at $2B, 4B, 6B, 8B, \dots$ Corresponding to $J_i = 0, 1, 2, 3, \dots$ respectively. From the data given one readily finds $B \approx 10.59 \text{ cm}^{-1}$. Thus

$$B = \frac{h}{8\pi^2 \mu r_e^2 c} \approx 10.59 \text{ cm}^{-1}$$

Since

$$\begin{aligned} \mu &\approx \frac{M_H M_{Cl}}{M_H + M_{Cl}} \\ &\approx \frac{35}{36} M_H \approx \frac{35}{36} \times 1.68 \times 10^{-24} \text{ g} \end{aligned}$$

we get

$$r_e \approx 1.27 \text{ \AA}$$