Angular Momentum

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Introduction

Quantum Numbers

- the stationary states of the hydrogen atom are given by three numbers, n, ℓ, and m
- n is the principal quantum number, and determines the energy of the state
- ℓ and m are related to the orbital angular momentum

Angular Momentum

- classically, a particle's angular momentum is given by

$$\mathbf{L} = \mathbf{r} \times \mathbf{p} = \begin{bmatrix} yp_z - zp_y \\ zp_x - xp_z \\ xp_y - yp_x \end{bmatrix}$$

- now we simply replace classical momentum with the quantum momentum operator

$$\mathbf{L} = \frac{\imath}{\hbar} \begin{bmatrix} y\,\partial/\partial z - z\,\partial/\partial y \\ z\,\partial/\partial x - x\,\partial/\partial z \\ x\,\partial/\partial y - y\,\partial/\partial x \end{bmatrix} = \frac{\imath}{\hbar}(\mathbf{r} \times \boldsymbol{\nabla})$$

Eigenvalues

Fundamental Commutation Relations

- L_x and L_y do not commute

$$\begin{aligned}[L_x, L_y] &= [yp_z - zp_y, zp_x - xp_z] \\ &= [yp_z, zp_x] - [yp_z, xp_z] - [zp_y, zp_x] + [zp_y, xp_z]\end{aligned}$$

- the only terms which fail to commute are $[x, p_x]$, $[y, p_y]$, and $[z, p_z]$

$$[L_x, L_y] = yp_x[p_z, z] + xp_y[z, p_z] = \imath\hbar(xp_y - yp_x) = \imath\hbar L_z$$

$$[L_x, L_y] = \imath\hbar L_z; \quad [L_y, L_z] = \imath\hbar L_x; \quad [L_z, L_x] = \imath\hbar L_y$$

Uncertainty Principle

$$\sigma_A^2 \sigma_B^2 \geq \left(\frac{1}{2\imath} \left\langle [A, B] \right\rangle \right)^2$$

$$\sigma_{L_x}^2 \sigma_{L_y}^2 \geq \left(\frac{1}{2\imath} \left\langle \imath \hbar L_z \right\rangle \right)^2 = \frac{\hbar^2}{4} \left\langle L_z \right\rangle^2$$

$$\sigma_{L_x} \sigma_{L_y} \geq \frac{\hbar}{2} |\left\langle L_z \right\rangle|$$

Total Angular Momentum

- since L_x and L_y do not commute, there are no eigenfunctions of *both* L_x and L_y
- however, the square of the total angular momentum *does* commute with L_x

$$L^2 = \mathbf{L} \cdot \mathbf{L} = L_x^2 + L_y^2 + L_z^2$$

$$[L^2, L_x] = 0; \quad [L^2, L_y] = 0; \quad [L^2, L_z] = 0$$

or

$$[L^2, \mathbf{L}] = \mathbf{0}$$

Ladder Operator

- since L^2 is compatible with each component of $\mathbf{L}$, we can hope to find simultaneous eigenstates of L^2 and any given component, say L_z

$$L^2 f = \lambda f \quad \text{and} \quad L_z f = \mu f$$

- we define the ladder operator

$$L_\pm \equiv L_x \pm \imath L_y$$

$$[L_z, L_\pm] = [L_z, L_x] \pm \imath [L_z, L_y] = \imath\hbar L_y \pm \imath(-\imath\hbar L_x) = \pm\hbar(L_x \pm \imath L_y)$$

$$[L_z, L_\pm] = \pm\hbar L_\pm \quad \text{and} \quad [L^2, L_\pm] = 0$$

Ladder Operator and Eigenfunctions

- if f is an eigenfunction of L^2 and L_z, so too is $L_\pm f$
- since L^2 and $L_\pm$ commute,

$$L^2(L_\pm f) = L_\pm(L^2 f) = L_\pm(\lambda f) = \lambda(L_\pm f)$$

- $L_\pm f$ is an eigenfunction of L^2 with eigenvalue λ
- since $[L_z, L_\pm] = \pm\hbar L_\pm$,

$$\begin{aligned} L_z(L_\pm f) &= (L_z L_\pm - L_\pm L_z)f + L_\pm L_z f = \pm\hbar L_\pm f + L_\pm(\mu f) \\ &= (\mu \pm \hbar)(L_\pm f) \end{aligned}$$

- so $L_\pm f$ is an eigenfunction of L_z with eigenvalue $\mu \pm \hbar$

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Raising and Lowering Operators

- $L_{\pm}f$ is an eigenfunction of L_z with eigenvalue $\mu \pm \hbar$
- L_+ is the "raising" operator, since it increases the eigenvalue of L_z by $\hbar$
- L_- is the "lowering" operator, since it decreases the eigenvalue of L_z by $\hbar$
- for a given λ, we obtain a "ladder" of states, with each "rung" separated from its neighbors by $\hbar$ in the eigenvalue of L_z

Top Rung

$$L^2 = L_x^2 + L_y^2 + L_z^2$$

- if we allowed the raising operator to be applied forever, eventually we would reach a point where $L_z > L^2$, which cannot be
- there must exist a "top rung" of the ladder, f_t, such that

$$L_+ f_t = 0$$

- let $\hbar\ell$ be the eigenvalue of L_z at this top rung

$$L_z f_t = \hbar\ell f_t; \quad L^2 f_t = \lambda f_t$$

Top Rung

- now we investigate what happens when one ladder operator is applied to its inverse

$$L_\pm L_\mp = (L_x \pm \imath L_y)(L_x \mp \imath L_y) = L_x^2 + L_y^2 \mp \imath(L_x L_y - L_y L_x)$$
$$= L^2 - L_z^2 \mp \imath(\imath\hbar L_z)$$

- solving for L^2 gives

$$L^2 = L_\pm L_\mp + L_z^2 \mp \hbar L_z$$

Top Rung

- we use the bottom of the $\pm$, and find that

$$L^2 f_t = (L_- L_+ + L_z^2 + \hbar L_z) f_t = (0 + \hbar^2 \ell^2 + \hbar^2 \ell) f_t = \hbar^2 \ell(\ell + 1) f_t$$

$$L^2 f_t = \hbar^2 \ell(\ell + 1) f_t = \lambda f_t \implies \lambda = \hbar^2 \ell(\ell + 1)$$

- so we have found the eigenvalue of L^2 in terms of the maximum eigenvalue of L_z

Bottom Rung

$$L^2 = L_x^2 + L_y^2 + L_z^2$$

- for the same reasons, there must exist a bottom rung, f_b, such that

$$L_- f_b = 0$$

- let $\hbar\bar{\ell}$ be the eigenvalue of L_z at this bottom rung

$$L_z f_b = \hbar\bar{\ell} f_b; \quad L^2 f_b = \lambda f_b$$

Bottom Rung

- we now use the top of the $\pm$, where we had previously used the bottom, and find that

$$L^2 f_b = (L_+ L_- + L_z^2 - \hbar L_z) f_b = (0 + \hbar^2 \bar{\ell}^2 - \hbar^2 \bar{\ell}) f_b = \hbar^2 \bar{\ell}(\bar{\ell} - 1) f_b$$

$$L^2 f_b = \hbar^2 \bar{\ell}(\bar{\ell} - 1) f_b = \lambda f_b \implies \lambda = \hbar^2 \bar{\ell}(\bar{\ell} - 1)$$

Combining the Top and Bottom

- we see that

$$\lambda = \hbar^2 \ell(\ell + 1) = \hbar^2 \bar{\ell}(\bar{\ell} - 1) \implies \ell(\ell + 1) = \bar{\ell}(\bar{\ell} - 1)$$

- there are two possibilities here

1. $\bar{\ell} = \ell + 1$
   - that would mean the bottom rung is higher than the top!
2. $\bar{\ell} = -\ell$

Eigenvalues of Angular Momentum

- we have just shown that the eigenvalues of L_z are $m\hbar$, where $m = -\ell, -\ell + 1, \ldots, 1 + \ell, +\ell$
- if we let the number of eigenvalues be N, then $\ell = -\ell + N$

$$\ell = N/2$$

- ℓ must be an integer, or a half-integer

$$\ell = 0, 1/2, 1, 3/2, \ldots$$

- the eigenfunctions are characterized by ℓ and m

$$L^2 f_\ell^m = \hbar^2 \ell(\ell + 1) f_\ell^m; \quad L_z f_\ell^m = \hbar m f_\ell^m$$

Eigenfunctions

Angular Momentum in Spherical Coordinates

- the angular momentum operator is

$$\mathbf{L} = \frac{\imath}{\hbar}(\mathbf{r} \times \boldsymbol{\nabla})$$

- in spherical coordinates, the gradient is given by

$$\boldsymbol{\nabla} = \hat{r}\frac{\partial}{\partial r} + \hat{\theta}\frac{1}{r}\frac{\partial}{\partial \theta} + \hat{\phi}\frac{1}{r\sin\theta}\frac{\partial}{\partial \phi}$$

- $\mathbf{r}$ is simply $r\hat{r}$

Angular Momentum in Spherical Coordinates

$$\mathbf{L} = \frac{\hbar}{\imath}\left[r(\hat{r} \times \hat{r})\frac{\partial}{\partial r} + (\hat{r} \times \hat{\theta})\frac{\partial}{\partial \theta} + (\hat{r} \times \hat{\phi})\frac{1}{\sin\theta}\frac{\partial}{\partial \phi}\right]$$

- $(\hat{r} \times \hat{r}) = 0$, $(\hat{r} \times \hat{\theta}) = \hat{\phi}$, and $(\hat{r} \times \hat{\phi}) = -\hat{\theta}$

$$\mathbf{L} = \frac{\hbar}{\imath}\left(\hat{\phi}\frac{\partial}{\partial \theta} - \hat{\theta}\frac{1}{\sin\theta}\frac{\partial}{\partial \phi}\right)$$

Angular Momentum in Spherical Coordinates

- write the unit vectors $\hat{\theta}$ and $\hat{\phi}$ in cartesian coordinates

$$\hat{\theta} = (\cos\theta\cos\phi)\hat{\imath} + (\cos\theta\sin\phi)\hat{\jmath} - (\sin\theta)\hat{k}$$
$$\hat{\phi} = -(\sin\phi)\hat{\imath} + (\cos\phi)\hat{\jmath}$$

$$\mathbf{L} = \frac{\hbar}{\imath}\Bigg[(-\sin\phi\hat{\imath} + \cos\phi\hat{\jmath})\frac{\partial}{\partial\theta} - (\cos\theta\cos\phi\hat{\imath} + \cos\theta\sin\phi\hat{\jmath} - \sin\theta\hat{k})\frac{1}{\sin\theta}\frac{\partial}{\partial\phi}\Bigg]$$

Angular Momentum in Spherical Coordinates

- separating the x, y, and z components, we find

$$L_x = \frac{\hbar}{\imath}\left(-\sin\phi\frac{\partial}{\partial\theta} - \cos\phi\cot\theta\frac{\partial}{\partial\phi}\right)$$
$$L_y = \frac{\hbar}{\imath}\left(+\cos\phi\frac{\partial}{\partial\theta} - \sin\phi\cot\theta\frac{\partial}{\partial\phi}\right)$$
$$L_z = \frac{\hbar}{\imath}\frac{\partial}{\partial\phi}$$

Ladder Operators in Spherical Coordinates

- now we consider the ladder operators

$$L_{\pm} = L_x \pm \imath L_y = \frac{\hbar}{\imath}\left[(-\sin\phi \pm \imath\cos\phi)\frac{\partial}{\partial\theta} - (\cos\phi \pm \imath\sin\phi)\cot\theta\frac{\partial}{\partial\phi}\right]$$

- by Euler's formula, $\cos\phi \pm \imath\sin\phi = \exp(\pm\imath\phi)$

$$L_{\pm} = \pm\hbar\exp(\pm\imath\phi)\left(\frac{\partial}{\partial\theta} \pm \imath\cot\theta\frac{\partial}{\partial\phi}\right)$$

Ladder Operators in Spherical Coordinates

$$L_+ L_- = -\hbar^2 \left(\frac{\partial^2}{\partial \theta^2} + \cot\theta \frac{\partial}{\partial \theta} + \cot^2\theta \frac{\partial^2}{\partial \phi^2} + \imath \frac{\partial}{\partial \phi} \right)$$

- recall $L^2 = L_\pm L_\mp + L_z^2 \mp \hbar L_z$

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

Eigenfunctions of L^2

- now we apply L^2 to its eigenfunction, $f_\ell^m(\theta, \phi)$, which has eigenvalue $\hbar^2 \ell(\ell+1)$

$$L^2 f_\ell^m = -\hbar^2 \left[\frac{1}{\sin\theta} \frac{\partial}{\partial\theta} \left(\sin\theta \frac{\partial}{\partial\theta} \right) + \frac{1}{\sin^2\theta} \frac{\partial^2}{\partial\phi^2} \right] f_\ell^m = \hbar^2 \ell(\ell+1) f_\ell^m$$

- this is simply the angular equation

$$\sin\theta \frac{\partial}{\partial\theta} \left(\sin\theta \frac{\partial y}{\partial\theta} \right) + \frac{\partial^2 Y}{\partial\phi^2} = -\ell(\ell+1) \sin^2\theta \, Y$$

Eigenfunctions of L_z

- f_ℓ^m is also an eigenfunction of L_z with eigenvalue $m\hbar$

$$L_z f_\ell^m = \frac{\hbar}{\imath} \frac{\partial}{\partial \phi} f_\ell^m = \hbar m f_\ell^m$$

- this is equivalent to the azimuthal equation

$$\frac{1}{\Phi} \frac{\mathrm{d}^2 \Phi}{\mathrm{d}\phi^2} = -m^2$$

Spherical Harmonics

- f_ℓ^m is simply $Y_\ell^m(\theta, \phi)$, the spherical harmonic (after normalization)
- spherical harmonics are eigenfunctions of L^2 and L_z
- when solving the Schrödinger equation by separation of variables, we "inadvertently" constructed eigenfunctions of the three commuting operators

$$H\psi = E\psi; \quad L^2\psi = \hbar^2\ell(\ell+1)\psi; \quad L_z\psi = \hbar m\psi$$

Schrödinger Equation

$$-\frac{\hbar^2}{2m}\left[\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial\psi}{\partial r}\right)+\frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial\psi}{\partial\theta}\right)+\frac{1}{r^2\sin^2\theta}\left(\frac{\partial^2\psi}{\partial\theta^2}\right)\right] + V\psi = E\psi$$

- we can now write the Schrödinger equation in this form

$$\frac{1}{2mr^2}\left[-\hbar^2\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right)+L^2\right]\psi + V\psi = E\psi$$

Thank You