# Orbital Angular Momentum in Quantum Mechanics

- Sections† G, H, I, J, K form a "short chapter" on the Quantum Theory of orbital angular momentum
- Many ideas can be carried over to another topic called spin angular momentum (see later chapter)

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† The sectioning follows that in Ch. VIII of QMI class notes

<u>Names</u>: $Y_{\ell m_\ell}(\theta, \phi)$

$\ell$ = "orbital quantum number"

[related to magnitude of orbital angular momentum $|\vec{L}|$]

$m_\ell$ = "magnetic quantum number"

[related to one component ($z$-component) of orbital angular momentum $L_z$]

Recall: Orbital Angular Momentum $\vec{L} = \vec{r} \times \vec{p}$

$\therefore$ We need to discuss Angular Momentum in QM.

# G. Orbital Angular Momentum

- "Orbital": To prepare for other angular momenta in QM, e.g. spin
- "Think Classical" $\vec{L} = \vec{r} \times \vec{p}$ [1D problems: Don't need it]

"Go Quantum"

$$\hat{L}_x = \hat{y}\hat{p}_z - \hat{z}\hat{p}_y = \frac{\hbar}{i}\left(y\frac{\partial}{\partial z} - z\frac{\partial}{\partial y}\right)$$

$$\hat{L}_y = \hat{z}\hat{p}_x - \hat{x}\hat{p}_z = \frac{\hbar}{i}\left(z\frac{\partial}{\partial x} - x\frac{\partial}{\partial z}\right) \quad (16)$$

$$\hat{L}_z = \underbrace{\hat{x}\hat{p}_y - \hat{y}\hat{p}_x}_{\text{general}} = \underbrace{\frac{\hbar}{i}\left(x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x}\right)}_{\text{using Schrödinger's way of imposing } [\hat{x},\hat{p}_x]=i\hbar \text{, etc.}}$$

$$\hat{L}^2 = \hat{L}_x^2 + \hat{L}_y^2 + \hat{L}_z^2$$

magnitude squared of orbital angular momentum

Commutators:

$$\boxed{\begin{array}{l} [\hat{L}^2, \hat{L}_x] = [\hat{L}^2, \hat{L}_y] = [\hat{L}^2, \hat{L}_z] = 0 \\ [\hat{L}_x, \hat{L}_y] = i\hbar\hat{L}_z \; ; \; [\hat{L}_y, \hat{L}_z] = i\hbar\hat{L}_x \; ; \; [\hat{L}_z, \hat{L}_x] = i\hbar\hat{L}_y \end{array}} \quad (17)$$

## H. Physical Meaning of $\ell$ in $Y_{\ell m_\ell}(\theta, \phi)$

$\boxed{\text{Ans: For a state with quantum number } \ell \text{, the magnitude of orbital angular momentum is } L = \sqrt{\ell(\ell+1)}\,\hbar \text{. Since } \ell = 0, 1, 2, \cdots \Rightarrow L \text{ takes on discrete/quantized values}}$ (18)

- Let's see Why.
  - Need $\hat{L}^2$ in spherical coordinates
  - From Eq.(16), go from $(x, y, z)$ to $(r, \theta, \phi)$

(Ex.)

$$\boxed{\begin{aligned} \hat{L}_x &= i\hbar\left(\sin\phi \frac{\partial}{\partial\theta} + \cot\theta \cos\phi \frac{\partial}{\partial\phi}\right) \\ \hat{L}_y &= i\hbar\left(-\cos\phi \frac{\partial}{\partial\theta} + \cot\theta \sin\phi \frac{\partial}{\partial\phi}\right) \\ \hat{L}_z &= -i\hbar \frac{\partial}{\partial\phi} \qquad [\hat{L}_z \text{ is simplest}] \end{aligned}} \tag{19}$$

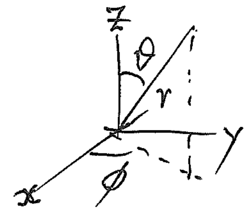
Example: $\hat{L}_z = \frac{\hbar}{i}\left(x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x}\right) = ?$ in spherical coordinates

Consider an arbitrary function $f$: $\frac{\partial f}{\partial \phi} = \frac{\partial f}{\partial x}\frac{\partial x}{\partial \phi} + \frac{\partial f}{\partial y}\frac{\partial y}{\partial \phi} + \frac{\partial f}{\partial z}\frac{\partial z}{\partial \phi}$

$$\frac{\partial x}{\partial \phi} = \frac{\partial}{\partial \phi}(r\sin\theta\cos\phi) = -r\sin\theta\sin\phi = -y$$

[math of partial derivatives]

$$\frac{\partial y}{\partial \phi} = \frac{\partial}{\partial \phi}(r\sin\theta\sin\phi) = r\sin\theta\cos\phi = x$$




$$\frac{\partial z}{\partial \phi} = \frac{\partial}{\partial \phi}(r\cos\theta) = 0$$

$$\frac{\partial f}{\partial \phi} = \left[-y\frac{\partial}{\partial x} + x\frac{\partial}{\partial y}\right] f \quad \text{for arbitrary } f$$

$$\Rightarrow \frac{\partial}{\partial \phi} = x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x} \quad \text{OR} \quad \boxed{\hat{L}_z = \frac{\hbar}{i}\frac{\partial}{\partial \phi} = -i\hbar\frac{\partial}{\partial \phi}} \qquad (19)$$

[c.f. $\hat{p}_x = \frac{\hbar}{i}\frac{\partial}{\partial x}$]  $\phi$ : coordinate, $L_z$ : conjugate momentum

Ex: How about $\hat{L}_x$, $\hat{L}_y$, $\hat{L}^2$?

- Construct $\hat{L}^2 = \hat{L}_x^2 + \hat{L}_y^2 + \hat{L}_z^2$ in spherical coordinates

Key Result

$$\boxed{\hat{L}^2 = -\hbar^2 \underbrace{\left[\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right) + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2}\right]}_{\text{looks familiar}}} \quad (20)$$

looks familiar [See $\theta$-$\phi$ eq. in Eq. (P2) on p. Atoms Prep. 2]
[See also $\theta$ & $\phi$ parts in $\nabla^2$]

## Eigenvalues / Eigenstates of $\hat{L}^2$?

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

$$= -\hbar^2\cdot[-\ell(\ell+1)]Y_{\ell m_\ell} \quad (\text{using Eq. (P2)})$$

$$= \ell(\ell+1)\hbar^2\, Y_{\ell m_\ell}(\theta,\phi) \quad (21)$$

Solved eigenvalue problem of $\hat{L}^2$ without effort!

$\therefore$ $\boxed{Y_{\ell m_\ell}(\theta,\phi) \text{ is an eigenstate of } \hat{L}^2 \text{ with eigenvalue } \ell(\ell+1)\hbar^2}$

$\therefore$ For state $\psi_{n\ell m_\ell} \sim R_{n\ell}(r)\, Y_{\ell m_\ell}(\theta,\phi)$ [energy $E_{n\ell}$] (General $U(r)$)

$$\hat{L}^2 \psi_{n\ell m_\ell} = R_{n\ell}(r)\, \hat{L}^2 Y_{\ell m_\ell}(\theta,\phi) = [\ell(\ell+1)\hbar^2]\, \psi_{n\ell m_\ell}$$

$$\Rightarrow \boxed{L = |\vec{L}| = \text{magnitude of orbital angular momentum} = \sqrt{\ell(\ell+1)}\,\hbar}$$

<u>Meaning:</u>

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| $\ell$ | 0 , | 1 , | 2 , | 3 , | 4 , | ... | quantized! |
| $L=\lvert\vec{L}\rvert$ | 0 , | $\sqrt{2}\hbar$ , | $\sqrt{6}\hbar$ , | $\sqrt{12}\hbar$ , | $\sqrt{20}\hbar$ , | ... | [Can't take on other values] |
| Symbol: (stands for $\ell$) | s , | p , | d , | f , | g , | ... | [convention] historical (from atomic spectrum) |

**Observation:** $\psi_{n\ell m_\ell}$ is an eigenstate of $\hat{H}$ with energy eigenvalue $E_{n\ell}$ **AND** an eigenstate of $\hat{L}^2$ with eigenvalue $\ell(\ell+1)\hbar^2$ [more later...]

- $\psi_{n\ell m_\ell}$ is a simultaneous eigenstate [共同本徵態] of $\hat{H}$ and $\hat{L}^2$
  (a QM concept)

Inspect:

$$\hat{H} = -\frac{\hbar^2}{2m}\nabla^2 + U(r) \qquad (\text{general } U(r))$$

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

$$= -\frac{\hbar^2}{2m}\left[\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right) + U(r)\right] + \frac{\hat{L}^2}{2mr^2} \qquad (22)$$

$$\therefore [\hat{H}, \hat{L}^2] = 0 \quad (\text{commute}) \qquad (\text{Why? Ex.})$$

$[\hat{A}, \hat{B}] = 0$ then $\hat{A}$ and $\hat{B}$ share simultaneous eigenstates

- Apply previous knowledge: $\psi_{n\ell m_\ell}(r,\theta,\phi)$
  - Measure energy? Outcome: 100% certain to be $E_{n\ell} \Rightarrow \Delta E = 0$
    [even do it for 1M copies]
  - Measure $L^2$? Outcome: 100% certain to be $\ell(\ell+1)\hbar^2 \Rightarrow (\Delta L^2) = 0$

$\therefore \quad (\Delta E)\cdot(\Delta L^2) = 0 \quad$ [can possibly be zero as the case here]

Key idea! → [No uncertainty relation between commute quantities] (23)

- Contrast: $[\hat{x}, \hat{p}] = i\hbar \neq 0$ CANNOT find simultaneous eigenstates
  e.g. $\psi_p \sim e^{ikx}$ has definite momentum ($\hbar k$)
  but $\psi_p$ does not have definite position
  and $\Delta x \cdot \Delta p \geq \hbar/2$ [never zero] (for any state)

# I. Physical Meaning of $m_\ell$ : What does it specify?

Recall: $\hat{L}_z = \frac{\hbar}{i}\frac{\partial}{\partial\phi} = -i\hbar\frac{\partial}{\partial\phi}$ (see (19))

$$\hat{L}_z Y_{\ell m_\ell}(\theta,\phi) = -i\hbar\,(A\,P_\ell^{|m_\ell|}(\cos\theta))\frac{\partial}{\partial\phi}e^{im_\ell\phi} = \overbrace{m_\ell\hbar}^{\text{eigenvalue}}\,Y_{\ell m_\ell}(\theta,\phi) \qquad (24)^{+}$$

$\therefore$ $\boxed{Y_{\ell m_\ell}(\theta,\phi) \text{ is an eigenstate of } \hat{L}_z \text{ with eigenvalue } m_\ell\hbar}$

$\therefore$ $Y_{\ell m_\ell}$ is a simultaneous eigenstate of $\hat{L}^2$ and $\hat{L}_z$

[Note: $[\hat{L}^2, \hat{L}_z] = 0$, they share simultaneous eigenstates]

It follows that $\hat{L}_z\psi_{n\ell m_\ell} = m\hbar\,\psi_{n\ell m_\ell}$

$\therefore$ $\psi_{n\ell m_\ell}$ (OR $Y_{\ell m_\ell}$) is a state of definite $L_z$ giving ($m_\ell\hbar$)

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$^+$ Solved eigenvalue problem of $\hat{L}_z$ without effort!

Putting together: Any $U(r)$

TISE Solutions: $\psi_{n\ell m_\ell}(r,\theta,\phi) = R_{n\ell}(r)\cdot Y_{\ell m_\ell}(\theta,\phi)$

$$\left.\begin{array}{l} \text{Energy Eigenvalue} = E_{n\ell} \\ L^2 \text{ eigenvalue} = \ell(\ell+1)\hbar^2 \\ L_z \text{ eigenvalue} = m_\ell \hbar \end{array}\right\} \text{all 100\% certain}$$

Key Concept

i.e. $\boxed{\psi_{n\ell m_\ell}(r,\theta,\phi) \text{ is a simultaneous eigenstate of } \underset{E_{n\ell}}{\underset{\uparrow}{\hat{H}}},\ \underset{\ell(\ell+1)\hbar^2}{\underset{\uparrow}{\hat{L}^2}},\ \underset{m_\ell\hbar}{\underset{\uparrow}{\hat{L}_z}}}$ (25)

<u>Note</u>: $\hat{H}$, $\hat{L}^2$, $\hat{L}_z$ are mutually commuting operators

Up to now, we don't need to invoke explicit form of $U(r)$, but we already know much about TISE solutions. [Only used symmetry of $U(r)$]

## J. Unusual Features of QM Orbital Angular Momentum

$[\hat{L}^2, \hat{L}_z] = 0 \quad \Rightarrow$ Can find simultaneous eigenstates of $\hat{L}^2$ and $\hat{L}_z$ (which are $Y_{\ell m_\ell}$)

But $[\hat{L}_x, \hat{L}_y] \neq 0$, $[\hat{L}_y, \hat{L}_z] \neq 0$, $[\hat{L}_z, \hat{L}_x] \neq 0$ [c.f. $[\hat{x}, \hat{p}_x] \neq 0$]

$\Rightarrow$ If we know one component definitely (say $L_z$), we cannot know $L_x$ and $L_y$

$\therefore$ $\boxed{\text{At best, we can find simultaneous eigenstates of } \underline{\hat{L}^2 \text{ and one component}}}$ [+]

- Which component? Any one will do!
- Why $z$-component $L_z$? $\hat{L}_z = \frac{\hbar}{i}\frac{\partial}{\partial\phi}$ (simple!) and it is <u>completely general</u>!

  $U(r)$ has no sense of direction. You pick a direction, then call it $\hat{z}$-direction.

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[+] In <u>classical mechanics</u>, $\vec{L} = \vec{r} \times \vec{p}$. In central force problems, $\vec{L}$ is conserved. We know its direction and its magnitude (and thus <u>all</u> components). Not so in QM!

$Y_{\ell m_\ell}(\theta,\phi)$

- $\ell = 0\,(s),\ 1\,(p),\ 2\,(d),\ 3\,(f),\ 4\,(g),\ \cdots$
- Given $\ell$: $m_\ell = \underbrace{-\ell, -\ell+1, \cdots, 0, \cdots, \ell-1, \ell}_{(2\ell+1)\text{ values}}$

Example: $\ell = 2$ (d)

$L = \sqrt{2(2+1)}\,\hbar = \sqrt{6}\,\hbar$ [length of $\vec{L}$]

$L_z = \underbrace{-2\hbar, -\hbar, 0, +\hbar, +2\hbar}_{[m_\ell = -2,\ -1,\ 0,\ 1,\ 2]}$ [z-component of $\vec{L}$] (quantized)

Inspect: Biggest $L_z = 2\hbar$ ["Biggest" $\Rightarrow$ Largest projection of $\vec{L}$ onto z-direction]

Length of $\vec{L}$ is $L = \sqrt{6}\,\hbar \approx 2.45\hbar > 2\hbar$ [Generally, $\sqrt{\ell(\ell+1)} > \ell$]

$\boxed{\text{length of vector} > \text{biggest projection onto } z\text{-direction!}}$

(any direction)

- Once a direction (called $\hat{z}$-direction) is chosen, $\vec{L}$ cannot point in that direction ($\because L_z^{max} < L$)

$\therefore$ $\boxed{\vec{L} \text{ can never point in any specific direction}}$ (24) (Quantum)

Here, we try to "visualize QM quantity ($\vec{L}$ here, operators) classically."

- We could take results $\hat{L}^2 Y_{\ell m_\ell} = (\ell(\ell+1)\hbar^2) Y_{\ell m_\ell}$ ; $\hat{L}_z Y_{\ell m_\ell} = (m_\ell \hbar) Y_{\ell m_\ell}$ and move on. No problem. Don't interpret results classically.
- OR find a way $\underbrace{\text{to picture the QM results}^{+}}_{\text{just help visualize results}^{+}}$

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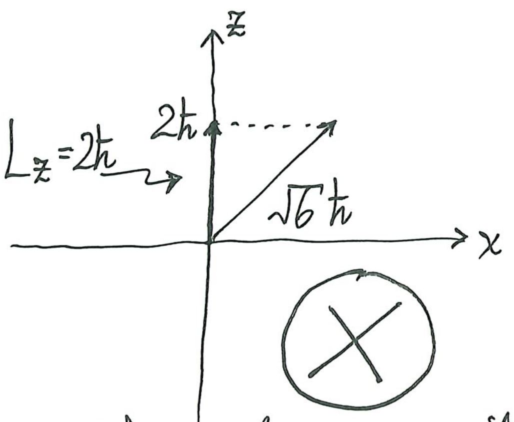
$^{+}$ Picture that helps further visualize other topics such as Zeeman effect (spectroscopy), NMR (chemistry/medical physics), spintronics, without being too theoretical.

## K. The "Vector Model": A Picture representing QM results

- $L_z = m_\ell \hbar$ $\quad (m_\ell = -\ell, \cdots, 0, \cdots + \ell)$ finite number of values (given $\ell$)
- $\vec{L}$ cannot point in any specific direction
- $\vec{L}$ is somewhere on a cone such that $L_z = m_\ell \hbar$

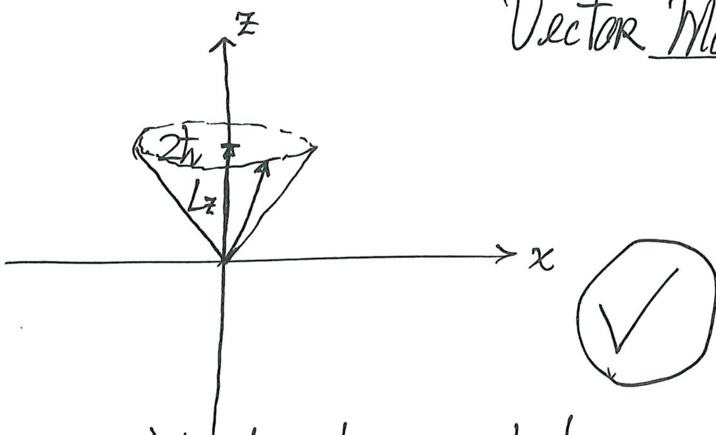
$m_\ell = 2 \quad (\ell = 2)$




- $\vec{L}$ points in specific direction
- $\underbrace{\text{Can know } L_x, L_y \text{ as well!}}_{\text{QM says No! } [\hat{L}_z, \hat{L}_x] \neq 0}$

$m_\ell = 2 \quad (\ell = 2)$

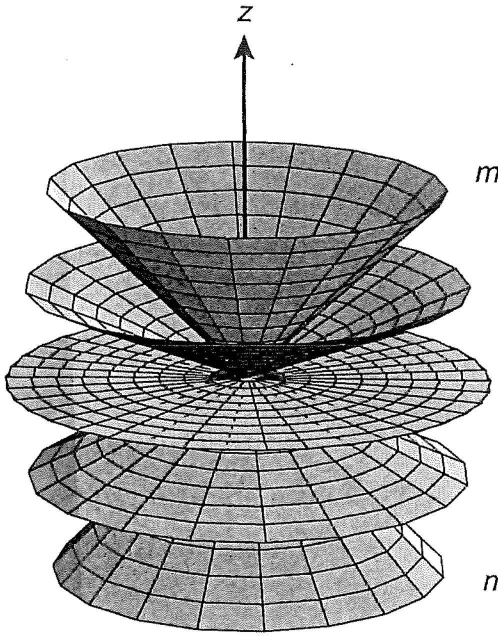
Vector Model/Picture




- $\vec{L}$'s direction not known (somewhere on cone)
- $L_z = 2\hbar$ [doesn't matter where on cone is $\vec{L}$]
- $L = \sqrt{6}\hbar$ [on cone]

[also means don't know definitely about $L_x$ and $L_y$]

- To display the five $m_\ell (= 2, 1, 0, -1, -2)$ values, there are 5 cones




All possible orientations of an angular momentum vector with $l = 2$. The $z$ component of the angular momentum is shown in units of $\hbar$.

- Projections $L_z = 2\hbar, \ \hbar, \ 0, \ -\hbar, \ -2\hbar$
- length $L = \sqrt{6}\hbar$ (all 5 cones)
- In books with jargons...
  - there are conical surfaces at specific angles on which $\vec{L}$ could lie

$\underbrace{\hphantom{there are conical surfaces at specific angles on which L could lie}}$

"spatial quantization"

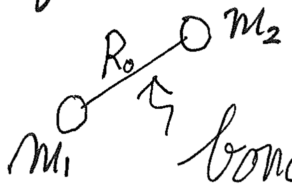
"Space quantization"

There are $(2\ell+1)$ conical surfaces for a given $\ell$.

- Vector Model:
  - Just a picture
  - Useful for visualizing how angular momenta add

## L. Buy one get (at least) one free : 3D Rigid Rotor

Context : diatomic molecule




bond $\approx$ rigid rod
(i.e. ignore vibrations)

**Simple thought**

- One end fixed at origin + another end moves freely (on surface of sphere)
- freely $\Rightarrow$ $U=0$ but fixed $r = R_0$

**Careful thought**

- Center of Mass Motion [not our business] + relative motion
- one end fixed at origin + another end (mass $\mu$) moves freely

$$\frac{1}{\mu} = \frac{1}{m_1} + \frac{1}{m_2}$$

Either way $\Rightarrow$ Same problem

- $R_0$ fixed $\Rightarrow$ Only $\theta$ and $\phi$ angles

$$\hat{H} = -\frac{\hbar^2}{2\mu}\nabla^2 + \cancel{V}^{\to 0} \quad \text{freely moving}$$

- TISE: $$-\frac{\hbar^2}{2\mu}\left[\frac{1}{R_0^2 \sin\theta}\left(\frac{\partial}{\partial\theta}\sin\theta\frac{\partial}{\partial\theta}\right) + \frac{1}{R_0^2\sin^2\theta}\frac{\partial^2}{\partial\phi^2}\right]\psi(\theta,\phi) = E\,\psi(\theta,\phi)$$

$$\Rightarrow \left[\frac{1}{\sin\theta}\left(\frac{\partial}{\partial\theta}\sin\theta\frac{\partial}{\partial\theta}\right) + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2}\right]\psi(\theta,\phi) = \frac{-2\mu R_0^2 E}{\hbar^2}\psi(\theta,\phi) \qquad (24)$$

3D Rigid Rotor [Schrödinger called it rotator] problem (1926)

<u>Solutions?</u> No need to do anything!

$$\because \left[\frac{1}{\sin\theta}\left(\frac{\partial}{\partial\theta}\sin\theta\frac{\partial}{\partial\theta}\right) + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2}\right]Y_{\ell m_\ell}(\theta,\phi) = -\ell(\ell+1)\,Y_{\ell m_\ell}(\theta,\phi)$$

(Same equation) (See OAM-5 Eq.(21))

$\therefore$ Eigenstates are $Y_{\ell m_\ell}(\theta,\phi)$ with

energy eigenvalues $\frac{2\mu R_0^2 E}{\hbar^2} = \ell(\ell+1)$

$$\boxed{E_\ell^{(\text{rotor})} = \frac{\ell(\ell+1)\hbar^2}{2\mu R_0^2}} \quad (25)$$

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

Given $\ell$,
$(2\ell+1)$ values of $m_\ell$
$\Rightarrow$ degeneracy $= (2\ell+1)$

We need these <u>rotational levels</u> next term.

<u>Short Cut</u>

- Classical Physics $E^{\text{rotation}} = \frac{L^2}{2I} = \frac{L^2}{2\mu R_0^2}$ $\quad I =$ Moment of Inertia $= \mu R_0^2$
- QM $\quad L^2 \rightarrow \ell(\ell+1)\hbar^2$

Done!

Eigenstates: $Y_{\ell m_\ell}(\theta,\phi)$

Eigenvalues: $E_\ell^{\text{rotation}} = \frac{\ell(\ell+1)\hbar^2}{2\mu R_0^2}$

# Summary

- $\hat{L} = \hat{\vec{r}} \times \hat{\vec{p}}$ [due to motion "$\vec{p}$", thus "orbital"]
- $[\hat{L}^2, \hat{L}_i] = 0$ $(i = x, y, z)$; $[\hat{L}_x, \hat{L}_y] = i\hbar \hat{L}_z$, $[\hat{L}_y, \hat{L}_z] = i\hbar \hat{L}_x$, $[\hat{L}_z, \hat{L}_x] = i\hbar \hat{L}_y$
- In spherical coordinates, single-valuedness ($\phi$ & $\phi + 2\pi$ same value) gives $\hat{L}^2 Y_{\ell m_\ell} = \ell(\ell+1)\hbar^2 Y_{\ell m_\ell}$ and $\ell = 0, 1, 2, \cdots$ (+ve integers)

$$m_\ell = \ell, \cdots, 0, \cdots, -\ell \text{ for given } \ell$$

$$\hat{L}_z Y_{\ell m_\ell} = m_\ell \hbar \, Y_{\ell m_\ell}$$

- Can find simultaneous eigenstates of $\hat{L}^2$ and $\hat{L}_z$ (one component)
- $|L| > L_z^{max} \Rightarrow \vec{L}$ cannot point at any specific direction
- Vector model is a way to visualize QM results
- Application: $\underbrace{\text{3D rigid rotor}}_{\text{rotational spectrum of molecules}}$ $\hat{H}^{(3D)}_{rotor} = \dfrac{\hat{L}^2}{2\mu R_0^2}$ thus exactly solvable