Rigid rotor and angular momentum

Note Title 26-10-2009

Quiz II

November 4, 1715 hrs, WS204, 209, 213 (primarily post-Minor II)

Quantum Tutorial 2

Available on the web

Bring a copy to the tutorial. No excuses!

Test yourself!

1. What is the energy of a harmonic oscillator that is found in a state with a wavefunction
(64 y^6 - 480 y^4 + 720 y^2 - 120)exp(-y^2)?

2. If 1 amu is 1.66 x 10^(-27) kg, the reduced mass of 1H35Cl is approximately =

3. If the force constant of HCl is approximately 16.6*36 N m^(-1) the vibrational spectrum of HCl shows a line at a ω =

$$\omega = \sqrt{\frac{k}{\mu}} = \sqrt{\frac{16.6 \times 36}{16.6 \times 10^{-28}}}$$

$k_{HCl} = 517\ N/m$

$$= 6 \times 10^{14} /s$$

$$\bar{\nu} = cm^{-1}$$

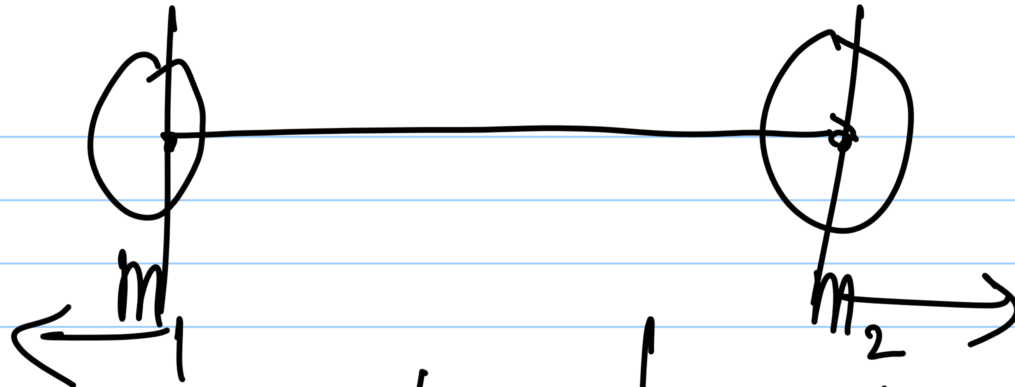
IR $\left\{ \begin{array}{l} 400 - \\ 4000\ cm^{-1} \end{array} \right.$

$$\psi_n = H_n(y)\, e^{-y^2}$$

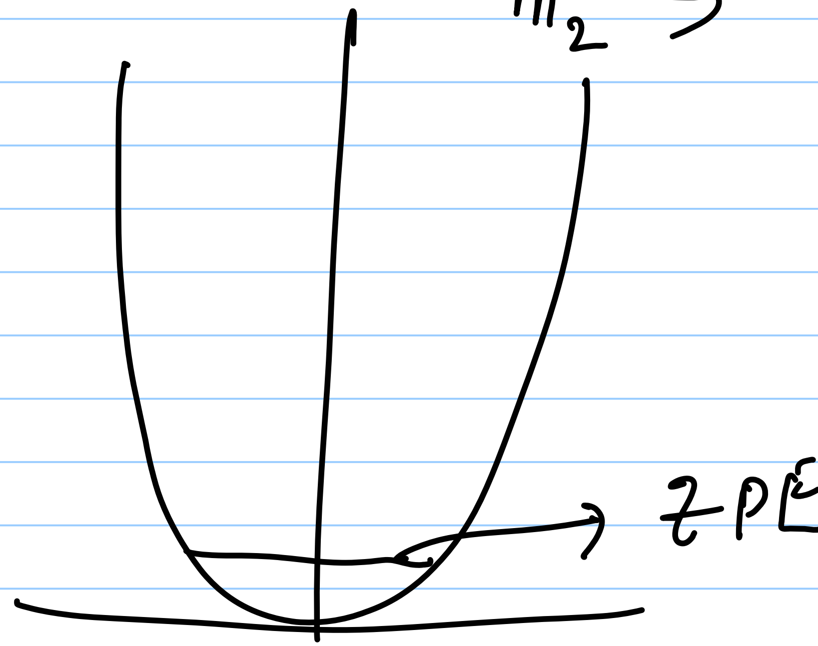
n is obtained

$$E = \left(n + \tfrac{1}{2}\right)\hbar\omega$$

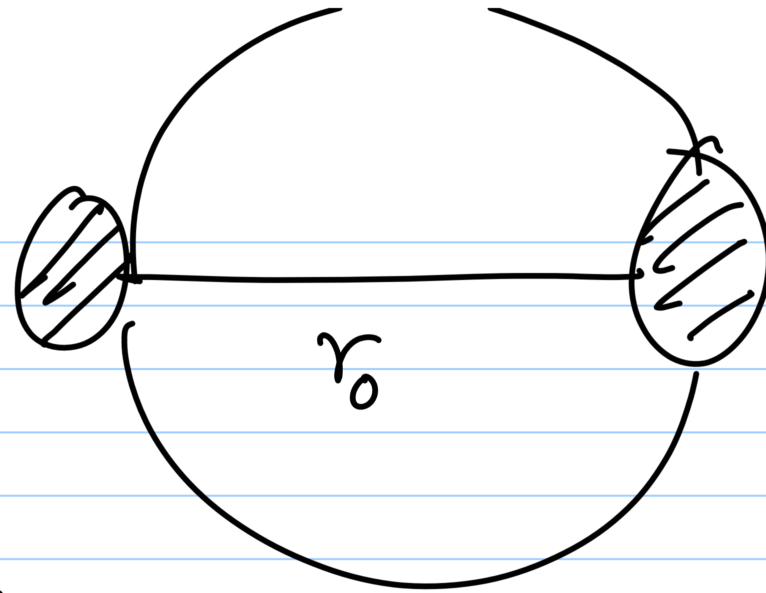
H—Cl



$\mu = er$



$V = 0$



Two body motion

$\downarrow$

Two one body motion

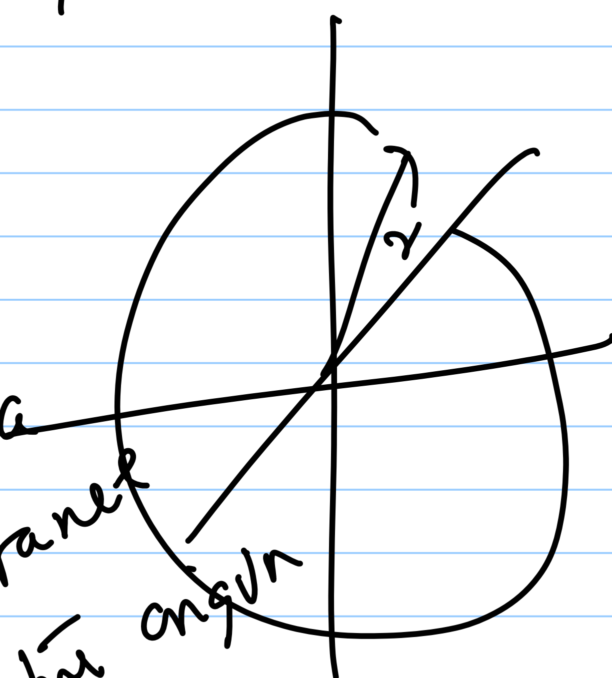
Motion of the centre of mass

$m_1 + m_2 = M$

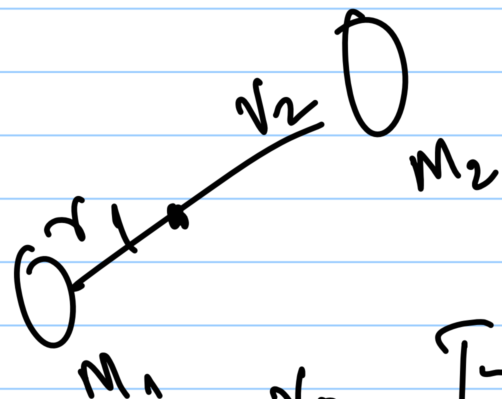
$$\frac{1}{\mu} = \frac{1}{m_1} + \frac{1}{m_2}$$

$$T = \frac{p^2}{2m}$$

Rotation of a mass μ at a fixed distance from the origin



$$T = \frac{1}{2} m v^2 = \frac{p^2}{2m}$$



$$v = r\omega$$

$$T = \frac{1}{2} m r^2 \omega^2 = \frac{L^2}{2I}$$

$$r_1 + r_2 = r_0$$

$$I = m r^2$$

$$T = \frac{1}{2} m_1 r_1^2 \omega^2 + \frac{1}{2} m_2 r_2^2 \omega^2$$

Express r_1 and r_2 in terms of r_0

$$T = \boxed{\frac{1}{2} M r_0^2 \omega^2} + \boxed{\frac{1}{2} \mu r_0^2 \omega^2}$$

Not concerned with

mass μ

$$T = \frac{L^2}{2I} = -\frac{\hbar^2}{2m} \nabla^2$$

$$\nabla^2 = \frac{1}{r^2} \cancel{\frac{\partial}{\partial r} r^2 \frac{\partial}{\partial r}} + \frac{1}{r^2 \sin\theta} \frac{\partial}{\partial \theta} \sin\theta \frac{\partial}{\partial \theta}$$

$$+ \frac{1}{r^2 \sin^2\theta} \frac{\partial^2}{\partial \varphi^2}$$

fixed distance from the origin

$$\hat{\mathcal{H}} = \hat{T} = -\frac{\hbar^2}{2\mu} \left\{ \frac{1}{r^2 \sin\theta} \frac{\partial}{\partial \theta} \sin\theta \frac{\partial}{\partial \theta} + \frac{1}{r^2 \sin^2\theta} \frac{\partial^2}{\partial \varphi^2} \right\}$$

$$\hat{H} = -\frac{\hbar^2}{2\mu r_0^2}\left\{ \boxed{\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\sin\theta\frac{\partial}{\partial\theta}} + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\varphi^2} \right\}$$

$$= \frac{L^2}{2I}$$

$$\hat{L}^2 = -\hbar^2 \left\{ \qquad\qquad \right\}$$

$$\hat{\mathcal{H}}_{PRR} = \boxed{-\frac{\hbar^2}{2I}\frac{\partial^2}{\partial\varphi^2}}$$

$$\frac{2IE}{\hbar^2}$$

$$\hat{\mathcal{H}}\psi = E\psi$$

$$\psi =$$

$$-\frac{\hbar^2}{2I}\frac{d^2\psi}{d\varphi^2} = E\psi$$

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} = E\psi$$

I

$$\psi(\varphi) = ?? \boxed{A \sin k\varphi}$$

$$k = \sqrt{\frac{2IE}{\hbar^2}}$$

$$E_{PIB} = \frac{n^2h^2}{8ma^2}$$

$$= A e^{ik\varphi}$$

$$E_{HO} = (n+\tfrac{1}{2})\hbar\omega$$

$$\psi(\varphi) = \psi(\varphi + 2\pi)$$

$$\psi = A e^{\pm i m \varphi}$$

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

$$E = \frac{m^2 \hbar^2}{2I}$$

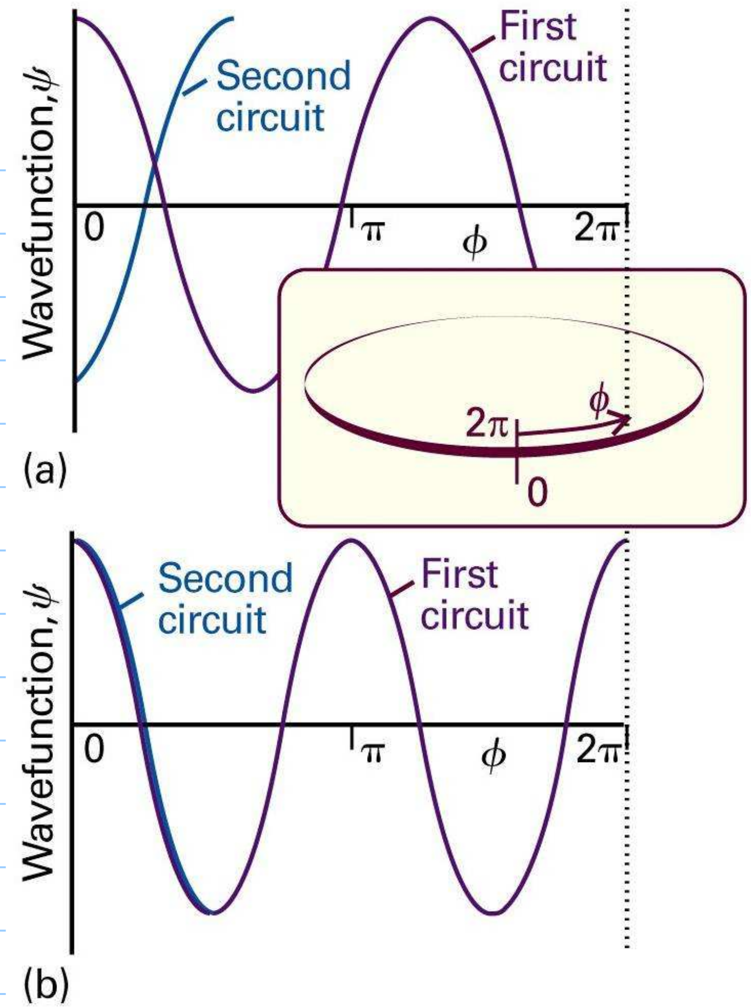


Figure 9-28
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$$E = \frac{m^2 \hbar^2}{2I}$$

$m = 0, \pm 1, \pm 2, \cdots \infty$

$$\psi = A e^{im\varphi}$$

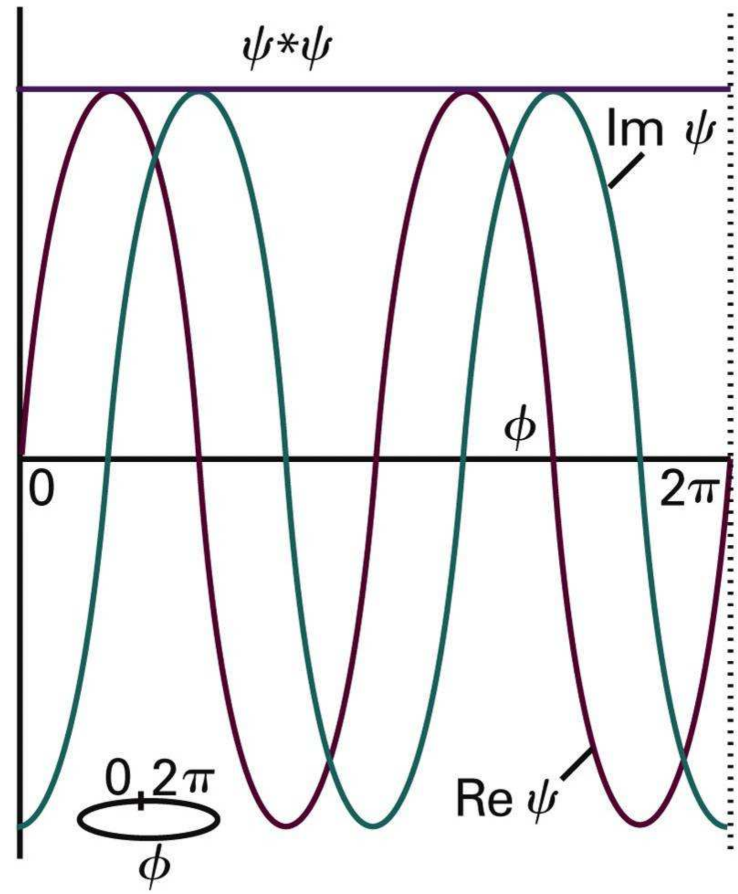

Figure 9-33
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$$\hat{\mathcal{H}}_{RR} = -\frac{\hbar^2}{2I}\left\{\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\sin\theta\frac{\partial}{\partial\theta} + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\varphi^2}\right\}$$

$$\hat{\mathcal{H}}_{RR}\psi = E\psi(\theta,\varphi)$$

$$\psi(\theta,\varphi) = \Theta(\theta)\,\Phi(\varphi)$$

Table 9.3 The spherical harmonics

l	m_l	$Y_{l,m_l}(\theta,\varphi)$
0	0	$\left(\frac{1}{4\pi}\right)^{1/2}$
1	0	$\left(\frac{3}{4\pi}\right)^{1/2}\cos\theta$
	±1	$\mp\left(\frac{3}{8\pi}\right)^{1/2}\sin\theta\, e^{\pm i\phi}$
2	0	$\left(\frac{5}{16\pi}\right)^{1/2}(3\cos^2\theta-1)$
	±1	$\mp\left(\frac{15}{8\pi}\right)^{1/2}\cos\theta\sin\theta\, e^{\pm i\phi}$
	±2	$\left(\frac{15}{32\pi}\right)^{1/2}\sin^2\theta\, e^{\pm 2i\phi}$
3	0	$\left(\frac{7}{16\pi}\right)^{1/2}(5\cos^3\theta-3\cos\theta)$
	±1	$\mp\left(\frac{21}{64\pi}\right)^{1/2}(5\cos^2\theta-1)\sin\theta\, e^{\pm i\phi}$
	±2	$\left(\frac{105}{32\pi}\right)^{1/2}\sin^2\theta\cos\theta\, e^{\pm 2i\phi}$
	±3	$\mp\left(\frac{35}{64\pi}\right)^{1/2}\sin^3\theta\, e^{\pm 3i\phi}$

Table 9-3
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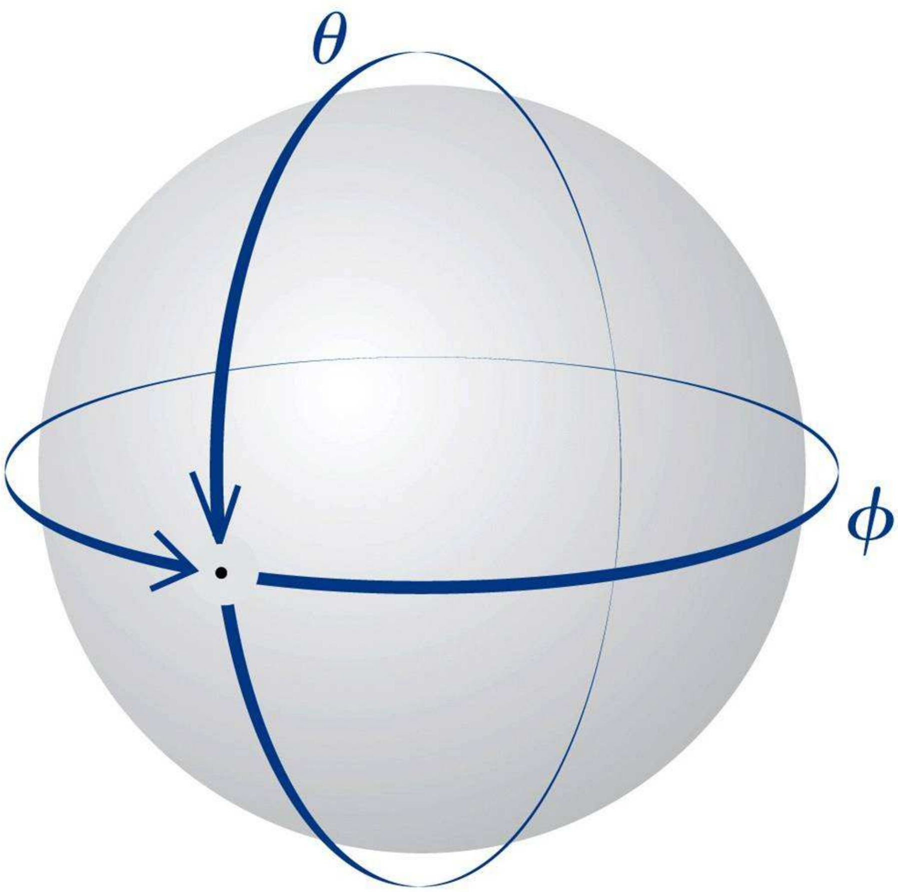

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$$\hat{\mathcal{H}} = \frac{L^2}{2I}$$

$$\frac{L^2}{2I}\psi(\theta,\varphi) = \frac{L^2}{2I} Y_{lm}(\theta,\varphi)$$

$$= \frac{l(l+1)\hbar^2}{2I} Y_{lm}(\theta,\varphi)$$

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

$$-i\hbar\frac{\partial}{\partial\varphi} = L_z Y_{lm}(\theta,\varphi) = m\hbar Y_{lm}(\theta,\varphi)$$

$$L^2 Y_{10} = -\hbar^2 \left\{ \frac{1}{\sin\theta} \frac{\partial}{\partial\theta} \sin\theta \frac{\partial}{\partial\theta} + \frac{1}{\sin^2\theta} \frac{\partial^2}{\partial\varphi^2} \right\} \cos\theta$$

$$= 1 \times 2\hbar^2 \cos\theta$$

$$-i\hbar \frac{\partial}{\partial\varphi} \cos\theta = 0\hbar \cos\theta \qquad Y_{10}$$

$$L_z Y_{10} = 0\hbar \, Y_{10}$$

$$L^2 Y_{11} = \{ \quad \} \times \sin\theta \, e^{+i\varphi}$$

$$= 2\hbar^2 \sin\theta \, e^{i\varphi}$$

$$L_z Y_{11} = 1\hbar \sin\theta \, e^{i\varphi}$$

$$E_{RR} = \frac{\ell(\ell+1)\hbar^2}{2I} \rightarrow \frac{L^2}{2I}$$

$$\psi_{RR} = Y_{\ell m}(\theta, \varphi) : (\text{polynomial in } \cos\theta) \times e^{im\varphi}$$

Space quantization

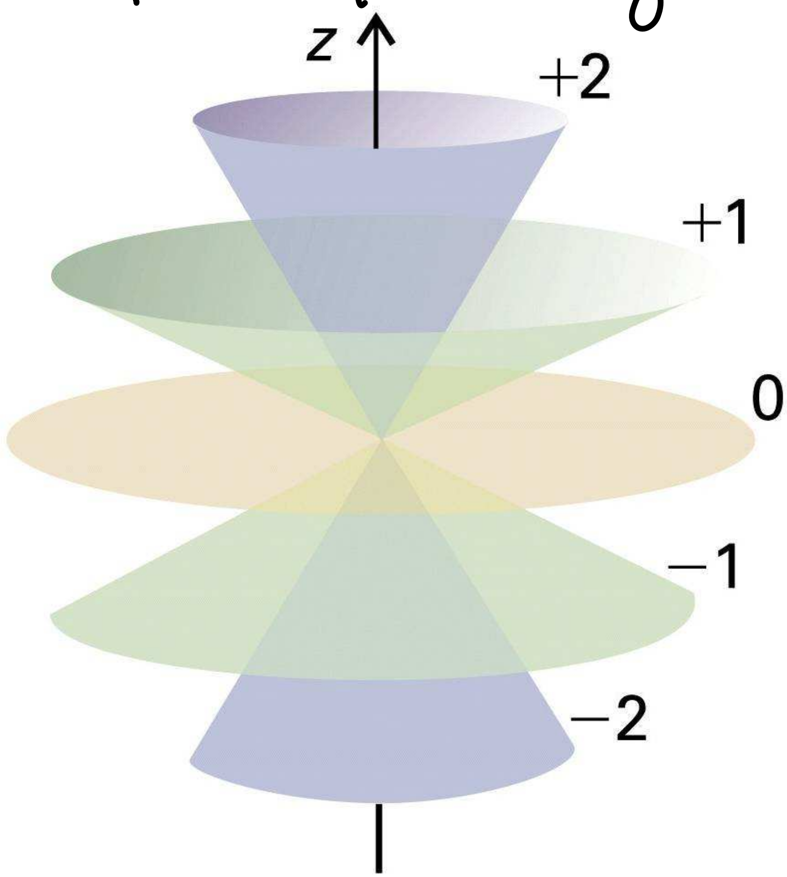

Figure 9-40b
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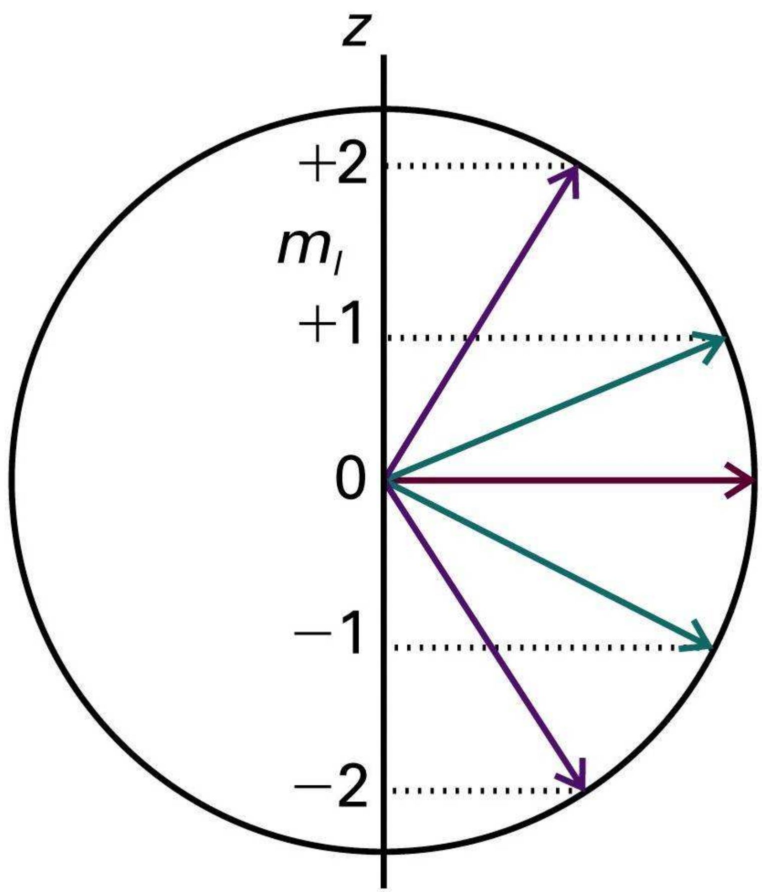

Figure 9-40a
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$$L^2 = -\hbar^2 \left\{ \frac{1}{\sin\theta} \frac{\partial}{\partial\theta} \sin\theta \frac{\partial}{\partial\theta} + \frac{1}{\sin^2\theta} \frac{\partial^2}{\partial\varphi^2} \right\}$$

$$\vec{L} = \vec{r} \times \vec{p}$$

$$\hat{\vec{L}} = \begin{vmatrix} \hat{i} & \hat{j} & \hat{k} \\ \hat{x} & \hat{y} & \hat{z} \\ -i\hbar\frac{\partial}{\partial x} & -i\hbar\frac{\partial}{\partial y} & -i\hbar\frac{\partial}{\partial z} \end{vmatrix}$$

$$= \hat{i}\left(y \left(-i\hbar\frac{\partial}{\partial z}\right) - z\left(-i\hbar\frac{\partial}{\partial y}\right)\right)$$

$$+ \hat{j} \; - \; - \; - \; -$$

$$\hat{L}_x = -i\hbar \left\{ y \frac{\partial}{\partial z} - z \frac{\partial}{\partial y} \right\}$$

$$\hat{L}_y = -i\hbar \left\{ \qquad \right\}$$

$$\left[[\hat{L}_x , \hat{L}_y] \neq 0 = i\hbar L_z \right]$$

$$[\hat{L}_y , \hat{L}_z] = i\hbar L_x$$

$$\vdots$$

$$[\hat{L}^2, \hat{L}_x] = [\hat{L}^2, \hat{L}_y] = [\hat{L}^2, \hat{L}_z] = 0$$

Rigid rotor

$$[\hat{L}_x, \hat{L}_y] = \hat{L}_z \qquad E = \frac{l(l+1)\hbar^2}{2I} \qquad l = 0, 1, 2, \ldots$$

$$[L^2, L_x] = 0$$

$$= [L^2, L_y]$$

$$= [L^2, L_z]$$

$$\psi = (\text{polynomial in } \cos\theta) \times e^{im\varphi}$$

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