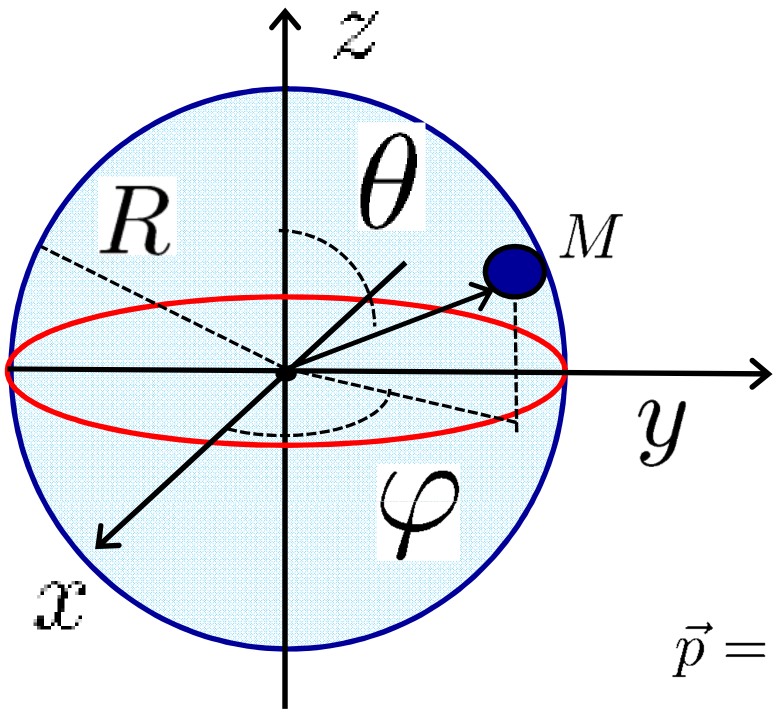
Momento angular orbital em MQ



Momento angular orbital

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

Operador Momento: coordenadas retangulares

$$\boxed{\vec{p} = \frac{\hbar}{i}\nabla = \frac{\hbar}{i}\left(\frac{\partial}{\partial x}\mathbf{i} + \frac{\partial}{\partial y}\mathbf{j} + \frac{\partial}{\partial z}\mathbf{z}\right)}$$

Operador Momento: coordenadas esféricas

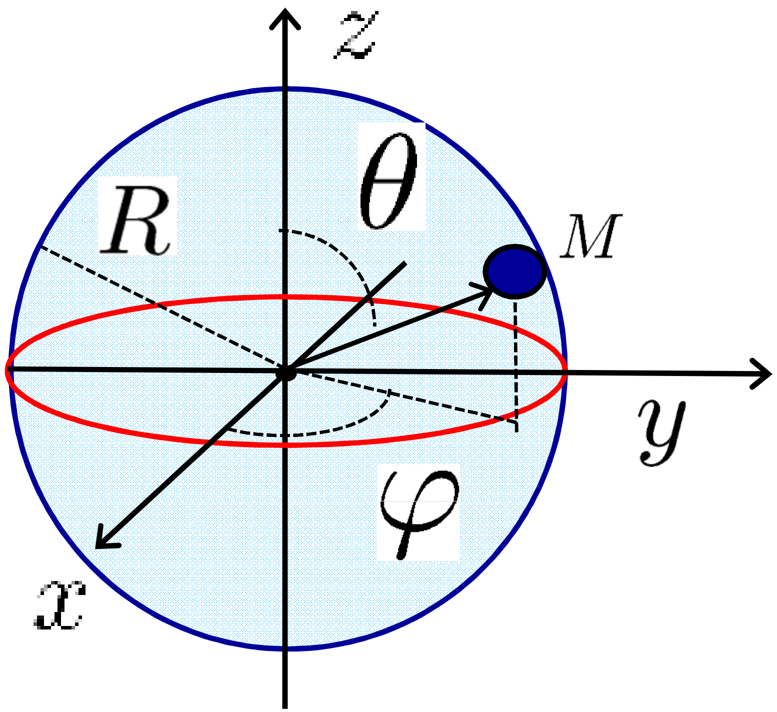
$$\vec{p} = \frac{\hbar}{i}\nabla = \frac{\hbar}{i}\left(\hat{r}\frac{\partial}{\partial r} + \hat{\theta}\frac{1}{r}\frac{\partial}{\partial \theta} + \hat{\varphi}\frac{1}{r\mathrm{sen}\theta}\frac{\partial}{\partial \varphi}\right)$$

$$\begin{aligned}
\hat{x} &= \hat{r}\sin\theta\cos\varphi + \hat{\theta}\cos\theta\cos\varphi - \hat{\varphi}\sin\varphi \\
\hat{y} &= \hat{r}\sin\theta\sin\varphi + \hat{\theta}\cos\theta\sin\varphi + \hat{\varphi}\cos\varphi, \\
\hat{z} &= \hat{r}\cos\theta - \hat{\theta}\sin\theta.
\end{aligned}$$

Operador Momento angular

$$\boxed{\vec{L} = \frac{\hbar}{i}\left(\hat{\varphi}\frac{\partial}{\partial \theta} - \hat{\theta}\frac{1}{\mathrm{sen}\theta}\frac{\partial}{\partial \varphi}\right)}$$

Operadores L_z e L^2 :



Operador Momento angular

$$\boxed{\vec{L} = \frac{\hbar}{i}\left(\hat{\varphi}\frac{\partial}{\partial\theta} - \hat{\theta}\frac{1}{\mathrm{sen}\theta}\frac{\partial}{\partial\varphi}\right)}$$

Componente z:

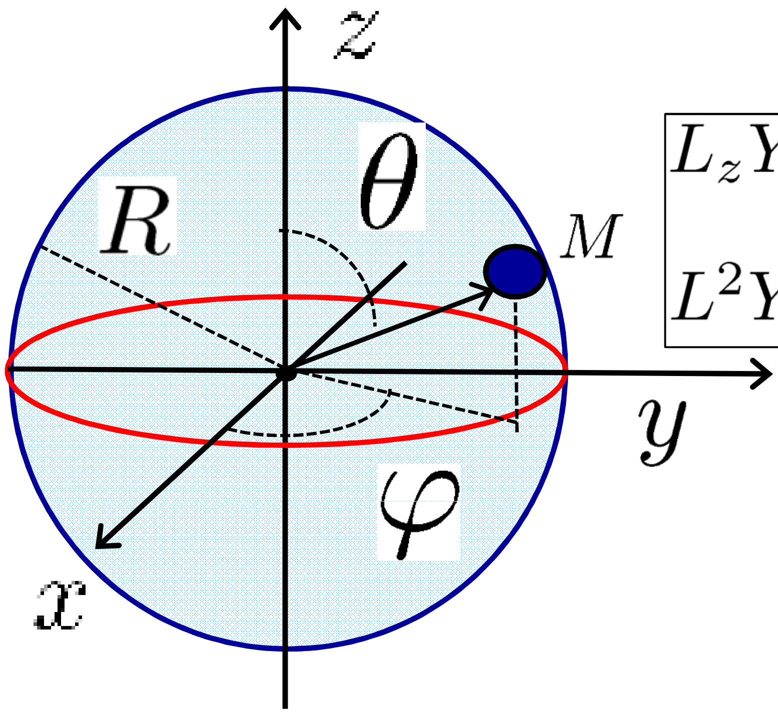
$$\mathbf{k} = \hat{r}\cos\theta - \hat{\theta}\mathrm{sen}\theta$$

$$\boxed{L_z = \mathbf{k}\cdot\vec{L} = \frac{\hbar}{i}\left(\frac{\partial}{\partial\varphi}\right)}$$

Operador L^2:

$$\boxed{\vec{L}\cdot\vec{L} = L^2 = -\hbar^2\left[\frac{1}{\mathrm{sen}\theta}\frac{\partial}{\partial\theta}\left(\mathrm{sen}\theta\frac{\partial}{\partial\theta}\right) + \frac{1}{\mathrm{sen}^2\theta}\frac{\partial^2}{\partial\varphi^2}\right]}$$

Autofunções de L_z e L^2 :



Operador Momento angular:

$$\boxed{\begin{aligned} L_z Y_l^{m_l}(\theta,\varphi) &= \hbar m_l Y_l^{m_l}(\theta,\varphi) \\ L^2 Y_l^{m_l}(\theta,\varphi) &= \hbar^2 l(l+1) Y_l^{m_l}(\theta,\varphi) \end{aligned}}$$

Quantização do momento angular:

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

$$m_l = -l, -l+1, \ldots, l-1, l$$

Harmônicos Esféricos (funções especiais)

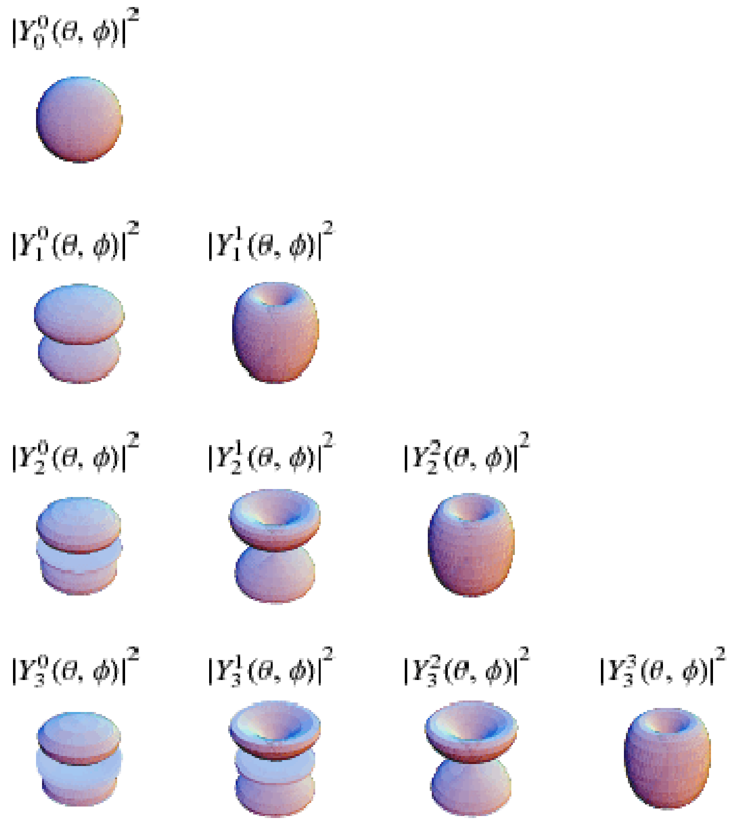
$$\boxed{Y_l^m(\theta,\varphi) = \left(\frac{2l+1}{2} \frac{(l-|m|)!}{(l+|m|)!} \right)^{1/2} P_l^{|m|}(\cos\theta) \frac{1}{\sqrt{2\pi}} e^{im\varphi}}$$

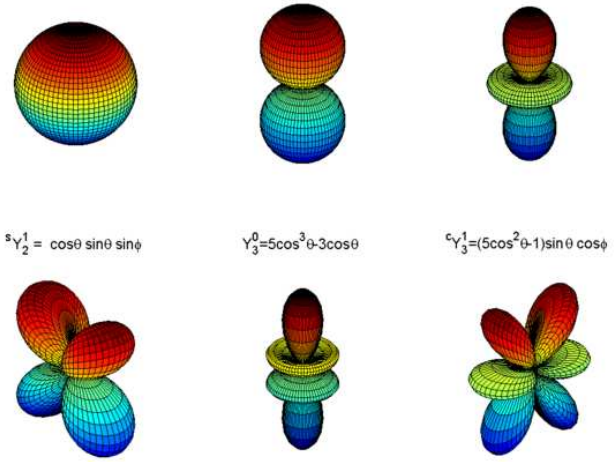
Harmônicos Esféricos

TABLE 3.7
Some Spherical Harmonics

Symbol	Polar	Cartesian	Normalization Constant
Y_{00}	1	1	$\frac{1}{2}(1/\pi)^{1/2}$
Y_{10}	$\cos\theta$	z/r	$\frac{1}{2}(3/\pi)^{1/2}$
$Y_{1\pm1}$	$\mp(\sin\theta)e^{\pm i\phi}$	$\mp(x \pm iy)/r$	$\frac{1}{2}(3/2\pi)^{1/2}$
Y_{20}	$(3\cos^2\theta - 1)$	$(3z^2 - r^2)/r^2$	$\frac{1}{4}(5/\pi)^{1/2}$
$Y_{2\pm1}$	$\mp(\sin\theta)(\cos\theta)e^{\pm i\phi}$	$\mp z(x \pm iy)r^2$	$\frac{1}{2}(15/2\pi)^{1/2}$
$Y_{2\pm2}$	$(\sin^2\theta)e^{\pm 2i\phi}$	$(x \pm iy)^2/r^2$	$\frac{1}{4}(15/2\pi)^{1/2}$
Y_{30}	$(5\cos^3\theta - 3\cos\theta)$	$z(5z^2 - 3r^2)/r^3$	$\frac{1}{4}(7/\pi)^{1/2}$
$Y_{3\pm1}$	$\mp\sin\theta(5\cos^2\theta - 1)e^{\pm i\phi}$	$\mp(x \pm iy)(5z^2 - r^2)/r^3$	$\frac{1}{8}(21/\pi)^{1/2}$
$Y_{3\pm2}$	$(\sin^2\theta)(\cos\theta)e^{\pm 2i\phi}$	$z(x \pm iy)^2/r^3$	$\frac{1}{4}(105/2\pi)^{1/2}$
$Y_{3\pm3}$	$\mp(\sin^3\theta)e^{\pm 3i\phi}$	$\mp(x \pm iy)^3/r^3$	$\frac{1}{8}(35/\pi)^{1/2}$

Douglas, Bodie E. and Hollingsworth, Charles A. *Symmetry in Bonding and Spectra – An Introduction* (Orlando, Florida: Academic Press, Inc., 1985) p. 88.



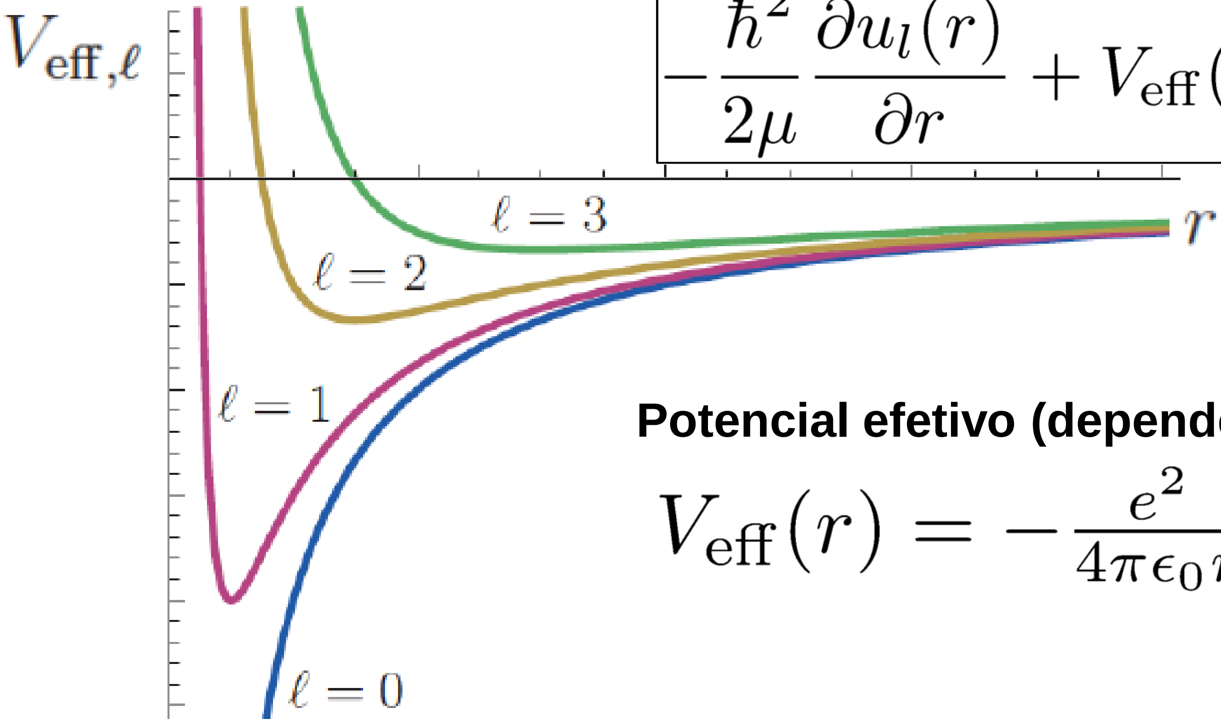


Átomo de H: Auto-funções

$$\boxed{\psi_{n,l,m}(r,\theta,\varphi) = A.\frac{u_{nl}(r)}{r}.Y_l^m(\theta,\varphi)}$$

O no. quântico n vem da solução da Equação radial:

$$\boxed{-\frac{\hbar^2}{2\mu}\frac{\partial u_l(r)}{\partial r} + V_{\text{eff}}(r)u_l(r) = -\epsilon_l u_l(r)}$$



Potencial efetivo (depende de l):

$$V_{\text{eff}}(r) = -\frac{e^2}{4\pi\epsilon_0 r} + \frac{\hbar^2 l(l+1)}{2\mu r^2}$$

Espectro do átomo de H

$$E_n = \frac{E_1}{n^2} = -\frac{13.6 \text{ eV}}{n^2}$$

$$n = 1, 2, \ldots$$

$$l = 0, 1, 2, \cdots, n-1$$

$$-l \leq m \leq l \qquad \boxed{2l+1 \text{ valores}}$$

$$\boxed{\text{Degenerescência em cada nível: } n^2}$$