Momento Angular

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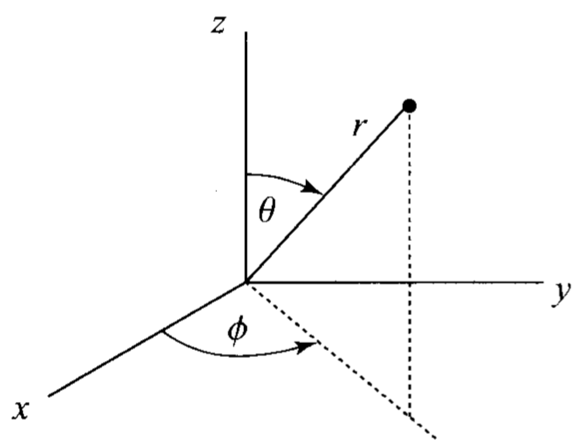
$$\hat{L}_x = -i\hbar\left(y\frac{\partial}{\partial z} - z\frac{\partial}{\partial y}\right)$$

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

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

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



$$x = r\,\mathrm{sen}\,\theta\cos\phi, \qquad y = r\,\mathrm{sen}\,\theta\,\mathrm{sen}\,\phi, \qquad z = r\cos\theta$$

$$r^2 = x^2 + y^2 + z^2, \qquad \cos\theta = \frac{z}{(x^2+y^2+z^2)^{1/2}}, \qquad \tan\phi = y/x$$

$$\hat{L}_x = i\hbar \left(\operatorname{sen}\phi \frac{\partial}{\partial \theta} + \cot\theta \cos\phi \frac{\partial}{\partial \phi} \right)$$

$$\hat{L}_y = -i\hbar \left(\cos\phi \frac{\partial}{\partial \theta} - \cot\phi \operatorname{sen}\phi \frac{\partial}{\partial \phi} \right)$$

$$\hat{L}_z = -i\hbar \frac{\partial}{\partial \phi}$$

$$\hat{L}^2 = -\hbar^2 \left(\frac{\partial^2}{\partial \theta^2} + \cot\theta \frac{\partial}{\partial \theta} + \frac{1}{\operatorname{sen}^2\theta} \frac{\partial^2}{\partial \phi^2} \right)$$

Autofunciones Y autovalores (Momento angular)

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

$$\hat{L}_z Y(\theta, \phi) = bY(\theta, \phi)$$

$$\hat{L}^2 Y(\theta, \phi) = cY(\theta, \phi)$$

$$-i\hbar\frac{\partial}{\partial\phi}Y(\theta,\phi)=bY(\theta,\phi)$$

$$Y(\theta,\phi)=S(\theta)T(\phi)$$

$$-i\hbar\frac{\partial}{\partial\phi}\left[S(\theta)T(\phi)\right]=bS(\theta)T(\phi)$$

$$-i\hbar S(\theta)\frac{dT(\phi)}{d\phi}=bS(\theta)T(\phi)$$

$$\frac{dT(\phi)}{T(\phi)}=\frac{ib}{\hbar}d\phi$$

$$T(\phi)=Ae^{ib\phi/\hbar}$$

Es admisible T como función propia?

$$T(\phi) = Ae^{ib\phi/\hbar}$$

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

$$Ae^{ib\phi/\hbar}e^{ib2\pi/\hbar} = Ae^{ib\phi/\hbar}$$

$$e^{ib2\pi/\hbar} = 1$$

$$e^{i\alpha} = \cos\alpha + i\,\mathrm{sen}\,\alpha = 1 \longrightarrow \alpha = 2\pi m \longrightarrow m = 0,\ \pm 1,\ \pm 2, \pm\cdots$$

$$2\pi b/\hbar = 2\pi m \longrightarrow b = m\hbar, \qquad m = \cdots -2,\ -1,\ 0,\ 1, \ldots$$

$$T(\phi) = Ae^{ib\phi/\hbar}$$

$$T(\phi) = Ae^{im\phi}, \qquad m = 0, \pm 1, \pm 2, \ldots$$

Normalizando la función encontramos el valor de A

$$\int_0^{2\pi} \left|T^2\right| d\phi = 1$$

$$|A| = (2\pi)^{-1/2}$$

$$T(\phi) = \frac{1}{\sqrt{2\pi}} e^{im\phi}, \qquad m = 0, \pm 1, \pm 2, \pm \ldots$$

$$\hat{L}^2 Y = cY \quad \left\{ \begin{array}{l} Y(\theta,\phi) = S(\theta)T(\phi) \\ T(\phi) = \dfrac{1}{\sqrt{2\pi}} e^{im\phi}, \qquad m = 0, \pm 1, \pm 2, \pm \ldots \end{array} \right.$$

$$\hat{L}^2 = -\hbar^2 \left(\frac{\partial^2}{\partial\theta^2} + \cot\theta \frac{\partial}{\partial\theta} + \frac{1}{\operatorname{sen}^2\theta} \frac{\partial^2}{\partial\phi^2} \right)$$

$$-\hbar^2 \left(\frac{\partial^2}{\partial\theta^2} + \cot\theta \frac{\partial}{\partial\theta} + \frac{1}{\operatorname{sen}^2\theta} \frac{\partial^2}{\partial\phi^2} \right) \left(S(\theta) \frac{1}{\sqrt{2\pi}} e^{im\phi} \right) = cS(\theta) \frac{1}{\sqrt{2\pi}} e^{im\phi}$$

$$-\hbar^2\left(\frac{\partial^2}{\partial\theta^2}+\cot\theta\frac{\partial}{\partial\theta}+\frac{1}{\operatorname{sen}^2\theta}\frac{\partial^2}{\partial\phi^2}\right)\left(S(\theta)\frac{1}{\sqrt{2\pi}}e^{im\phi}\right)=cS(\theta)\frac{1}{\sqrt{2\pi}}e^{im\phi}$$

$$\frac{d^2S}{d\theta^2}+\cot\theta\frac{dS}{d\theta}-\frac{m^2}{\operatorname{sen}^2\theta}S=-\frac{c}{\hbar^2}S$$

$$w=\cos\theta$$

$$S(\theta)=G(w)$$

$$(1-w^2)\frac{d^2G}{dw^2}-2w\frac{dG}{dw}+\left[\frac{c}{\hbar^2}-\frac{m^2}{1-w^2}\right]G(w)=0$$

$$G(w)=(1-w^2)^{|m|/2}H(w)$$

$$(1-w^2)H''-2(|m|+1)wH'+[c\hbar^{-2}-|m|(|m|+1)]H=0$$

$$H(w)=\sum_{j=0}^{\infty}a_jw^j$$

Relación de recurrencia:

$$a_{j+2}=\frac{[(j+|m|)(j+|m|+1)-c/\hbar^2]}{(j+1)(j+2)}a_j$$

$$c = \hbar^2 (k + |m|)(k + |m| + 1), \qquad k = 0,\ 1,\ 2, \ldots$$

Definimos:

$$l \equiv k + |m|$$

Como $|m| \leq l$ Entonces:

$$m = -l,\ -l+1,\ -l+2, ..., -1,\ 0,\ 1, ..., l-2,\ l-1,\ l$$

Los auto-valores de L^2 son:

$$c = l(l+1)\hbar^2, \qquad l = 0,\ 1,\ 2, \ldots$$

$$|\mathbf{L}| = [l(l+1)]^{1/2}\hbar$$

$$S_{l,m}(\theta) = \operatorname{sen}^{|m|}\theta \sum_{\substack{j=1,3,\ldots \\ \text{ó } j=0,2,\ldots}}^{l-|m|} a_j \cos^j\theta$$

$$P_l^{|m|}(w) \equiv \frac{l}{2^l l!}(1-w^2)^{|m|/2}\frac{d^{l+|m|}}{dw^{l+|m|}}(w^2-1)^l, \qquad l = 0, 1, 2, \ldots$$

$$P_0^0(w) = 1$$

$$P_1^0(w) = w$$

$$P_1^1(w) = (1-w^2)^{1/2}$$

$$P_2^0(w) = \frac{1}{2}(3w^2-1)$$

$$P_2^1(w) = 3w(1-w^2)^{1/2}$$

$$P_2^2(w) = 3 - 3w^2$$

$$S_{l,m}(\theta) = \left[\frac{2l+1}{2}\frac{(l-|m|)!}{(l+|m|)!}\right]^{1/2} P_l^{|m|}(\cos\theta)$$

$$Y_l^m(\theta,\phi) = S_{l,m}(\theta)T(\phi) = \frac{1}{\sqrt{2\pi}}S_{l,m}(\theta)e^{im\phi}$$

$$Y_l^m(\theta,\phi) = \left[\frac{2l+1}{4\pi}\frac{(l-|m|)!}{(l+|m|)!}\right]^{1/2} P_l^{|m|}(\cos\theta)e^{im\phi}$$

$$\hat{L}^2 Y_l^m(\theta,\phi) = l(l+1)\hbar^2 Y_l^m(\theta,\phi), \qquad l = 0, 1, 2, \ldots$$

$$\hat{L}_z Y_l^m(\theta,\phi) = m\hbar Y_l^m(\theta,\phi), \qquad m = -l, -l+1, \ldots, l-1, l$$

TABLA 5.1	$S_{l,m}(\theta)$
$l = 0:$	$S_{0,0} = \frac{1}{2}\sqrt{2}$
$l = 1:$	$S_{1,0} = \frac{1}{2}\sqrt{6}\cos\theta$
	$S_{1,\pm1} = \frac{1}{2}\sqrt{3}\,\mathrm{sen}\,\theta$
$l = 2:$	$S_{2,0} = \frac{1}{4}\sqrt{10}(3\cos^2\theta - 1)$
	$S_{2,\pm1} = \frac{1}{2}\sqrt{15}\,\mathrm{sen}\,\theta\cos\theta$
	$S_{2,\pm2} = \frac{1}{4}\sqrt{15}\,\mathrm{sen}^2\theta$
$l = 3:$	$S_{3,0} = \frac{3}{4}\sqrt{14}(\frac{5}{3}\cos^3\theta - \cos\theta)$
	$S_{3,\pm1} = \frac{1}{8}\sqrt{42}\,\mathrm{sen}\,\theta(5\cos^2\theta - 1)$
	$S_{3,\pm2} = \frac{1}{4}\sqrt{105}\,\mathrm{sen}^2\theta\cos\theta$
	$S_{3,\pm3} = \frac{1}{8}\sqrt{70}\,\mathrm{sen}^3\theta$

Armónicos esféricos

Table 8.3 The Spherical Harmonics $Y_\ell^{m_\ell}(\theta, \phi)$

$$Y_0^0 = \frac{1}{2\sqrt{\pi}}$$

$$Y_1^0 = \tfrac{1}{2}\sqrt{\frac{3}{\pi}} \cdot \cos\theta$$

$$Y_1^{\pm 1} = \mp\tfrac{1}{2}\sqrt{\frac{3}{2\pi}} \cdot \sin\theta \cdot e^{\pm i\phi}$$

$$Y_2^0 = \tfrac{1}{4}\sqrt{\frac{5}{\pi}} \cdot (3\cos^2\theta - 1)$$

$$Y_2^{\pm 1} = \mp\tfrac{1}{2}\sqrt{\frac{15}{2\pi}} \cdot \sin\theta \cdot \cos\theta \cdot e^{\pm i\phi}$$

$$Y_2^{\pm 2} = \tfrac{1}{4}\sqrt{\frac{15}{2\pi}} \cdot \sin^2\theta \cdot e^{\pm 2i\phi}$$

$$Y_3^0 = \tfrac{1}{4}\sqrt{\frac{7}{\pi}} \cdot (5\cos^3\theta - 3\cos\theta)$$

$$Y_3^{\pm 1} = \mp\tfrac{1}{8}\sqrt{\frac{21}{\pi}} \cdot \sin\theta \cdot (5\cos^2\theta - 1) \cdot e^{\pm i\phi}$$

$$Y_3^{\pm 2} = \tfrac{1}{4}\sqrt{\frac{105}{2\pi}} \cdot \sin^2\theta \cdot \cos\theta \cdot e^{\pm 2i\phi}$$

$$Y_3^{\pm 3} = \mp\tfrac{1}{8}\sqrt{\frac{35}{\pi}} \cdot \sin^3\theta \cdot e^{\pm 3i\phi}$$

Átomo de Hidrogeno

$$\hat{H} = \hat{T} + \hat{V} = -(\hbar^2/2m)\nabla^2 + V(r)$$

Laplaciano en esfèricas:

$$\nabla^2 = \frac{\partial^2}{\partial r^2} + \frac{2}{r}\frac{\partial}{\partial r} + \frac{1}{r^2}\frac{\partial^2}{\partial \theta^2} + \frac{1}{r^2}\operatorname{cotg}\theta\frac{\partial}{\partial \theta} + \frac{1}{r^2 \operatorname{sen}^2\theta}\frac{\partial^2}{\partial \phi^2}$$

OP. Momento Angular L^2 en esfèricas:

$$\hat{L}^2 = -\hbar^2\left(\frac{\partial^2}{\partial \theta^2} + \cot\theta\frac{\partial}{\partial \theta} + \frac{1}{\operatorname{sen}^2\theta}\frac{\partial^2}{\partial \phi^2}\right)$$

HAMILTONIANO EN ESFERICAS (átomo de Hidrógeno):

$$\hat{H} = -\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial r^2} + \frac{2}{r}\frac{\partial}{\partial r}\right) + \frac{1}{2mr^2}\hat{L}^2 + V(r)$$

$$\hat{H} = -\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial r^2} + \frac{2}{r}\frac{\partial}{\partial r}\right) + \frac{1}{2mr^2}\hat{L}^2 + V(r)$$

Se puede demostrar:

$$[\hat{H}, \hat{L}^2] = 0 \qquad \text{si } \; V = V(r)$$

$$[\hat{H}, \hat{L}_z] = 0 \qquad \text{si } \; V = V(r)$$

Entonces:

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

$$\hat{L}^2\psi = l(l+1)\hbar^2\psi\;, \qquad l = 0, 1, 2, \ldots$$

$$\hat{L}_z\psi = m\hbar\psi\;, \qquad m = -l, -l+1, \ldots, l$$

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

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

Proponemos:

$$\psi=R(r)Y_l^m(\theta,\phi)$$

$$-\frac{\hbar^2}{2m}\left(R''+\frac{2}{r}R'\right)+\frac{l(l+1)\hbar^2}{2mr^2}R+V(r)R=ER(r)$$

Ecuación Radial

Para el caso del átomo de hidrógeno $V(r) = \dfrac{e^2}{4\pi\varepsilon_0 r}$

$$-\frac{\hbar^2}{2m}\left(R'' + \frac{2}{r}R'\right) + \frac{l(l+1)\hbar^2}{2mr^2}R + V(r)R = ER(r)$$

Ecuación Radial para el átomo de hidrógeno

$$\frac{1}{r^2}\frac{d}{dr}\left(r^2\frac{dR}{dr}\right) + \frac{2m}{\hbar^2}\left[\left(\frac{e^2}{4\pi\varepsilon_0 r} + E\right) - \frac{l(l+1)}{r^2}\right]R = 0$$

$$\frac{1}{r^2}\frac{d}{dr}\left(r^2\frac{dR}{dr}\right)+\frac{2m}{\hbar^2}\left[\left(\frac{e^2}{4\pi\varepsilon_0 r}+E\right)-\frac{l(l+1)}{r^2}\right]R=0$$

Las soluciones se llaman funciones asociadas de LAGUERRE y las correspondientes energías son

$$E_n=-\frac{m}{2}\left(\frac{e^2}{4\pi\varepsilon_0\hbar}\right)^2\frac{1}{n^2}=-\frac{E_0}{n^2} \qquad n=1,2,3\ldots$$

Misma forma que obtuvo Bohr para el H.
La energía negativa indica que el electrón está ligado al núcleo

$n \longrightarrow$ **número cuántico principal**

Y se debe verificar que l = 0, 1, 2,…, (n-1)

Funciones radiales para el átomo de H

Table 8.4 The Radial Wavefunctions $R_{n\ell}(r)$ of Hydrogen-like Atoms for n = 1, 2, and 3

n	ℓ	$R_{n\ell}(r)$
1	0	$\left(\frac{Z}{a_0}\right)^{3/2} 2e^{-Zr/a_0}$
2	0	$\left(\frac{Z}{2a_0}\right)^{3/2} \left(2 - \frac{Zr}{a_0}\right) e^{-Zr/2a_0}$
2	1	$\left(\frac{Z}{2a_0}\right)^{3/2} \frac{Zr}{\sqrt{3}\,a_0} e^{-Zr/2a_0}$
3	0	$\left(\frac{Z}{3a_0}\right)^{3/2} 2\left[1 - \frac{2Zr}{3a_0} + \frac{2}{27}\left(\frac{Zr}{a_0}\right)^2\right] e^{-Zr/3a_0}$
3	1	$\left(\frac{Z}{3a_0}\right)^{3/2} \frac{4\sqrt{2}}{3} \frac{Zr}{a_0}\left(1 - \frac{Zr}{6a_0}\right) e^{-Zr/3a_0}$
3	2	$\left(\frac{Z}{3a_0}\right)^{3/2} \frac{2\sqrt{2}}{27\sqrt{5}} \left(\frac{Zr}{a_0}\right)^2 e^{-Zr/3a_0}$

Números cuánticos:

- Los tres números cuánticos son:
  - n: número cuántico principal
  - l: número cuántico orbital
  - m_l : número cuántico magnético
- Sus valores permitido son:
  - $n = 1, 2, 3, 4, . . .$
  - $l = 0, 1, 2, 3, . . . , n - 1$
  - $m_l = -l, -l + 1, . . . , 0, 1, . . . , l - 1, l$

Ejemplo: Indicar la cantidad de estados orbitales que existen para el nivel n=*3* del átomo de hidrógeno.

$l = 0, 1, 2, 3, \ldots, n - 1$

$m_l = -l, -l + 1, .., 0,. , l - 1, l$

Para n=*3* los valores permitidos para l *son 0, 1 y 2*

Si l =0 , $m_l = 0$

Si l =1 , hay 3 valores posibles para m_l = -1, 0,1

Si l =2 , hay 5 valores posibles para m_l = -2,-1, 0,1,2

l	m_l
0	0
1	-1 0 1
2	-2 -1 0 1 2

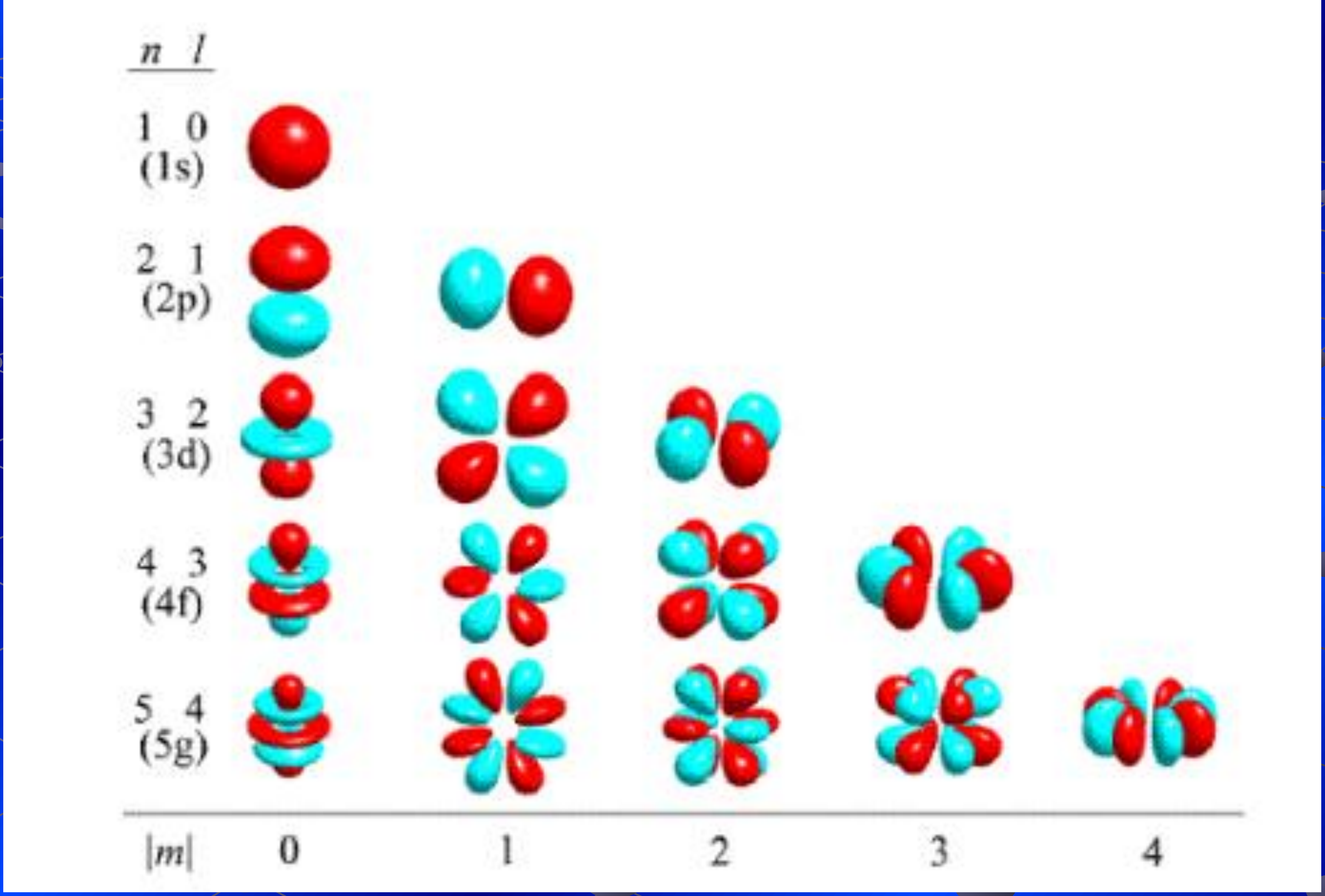
Hay 9 estados posibles

Se acostumbra especificar los estados del electrón con distinto momento angular con una letra

l =	0	1	2	3	4	5 . . .
Letra =	*s*	*p*	*d*	*f*	*g*	*h* . . .

Los estados atómicos usualmente se refieren por sus valores de n y l

Un estado con $n = 2$ y $l = 1$ se llama estado 2*p* .


n l
1 0
(1s)
2 1
(2p)
3 2
(3d)
4 3
(4f)
5 4
(5g)
|m|
0
1
2
3
4