Eq. Schrödinger em 3D
(potencial central)

Métodos de separação de variáveis em sistemas com simetria esférica

Mecânica quântica em três dimensões...

$$\mathcal{H}(p,q) = \frac{p^2}{2m} + V(r)$$

Equação de Schrödinger em 3D

A generalização para três dimensões é simples: $i\hbar\frac{\partial\Psi}{\partial t} = H\Psi;$

pela receita-padrão: $p_x \to \frac{\hbar}{i}\frac{\partial}{\partial x},\quad p_y \to \frac{\hbar}{i}\frac{\partial}{\partial y},\quad p_z \to \frac{\hbar}{i}\frac{\partial}{\partial z},$

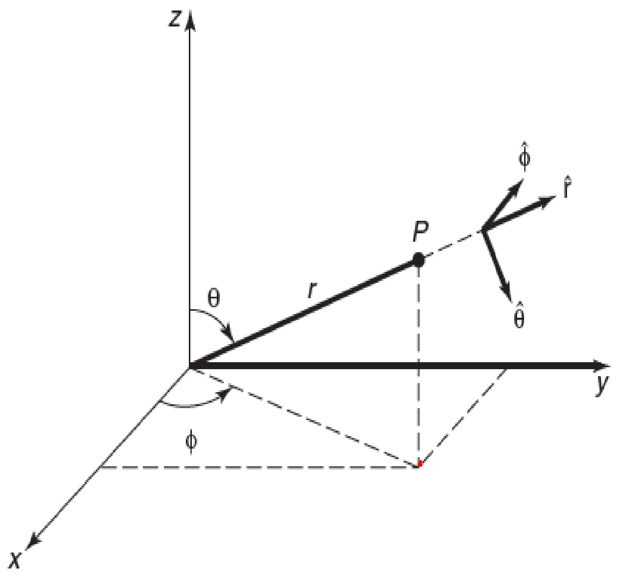
ou $\mathbf{p} \to \frac{\hbar}{i}\nabla,$. Assim $i\hbar\frac{\partial\Psi}{\partial t} = -\frac{\hbar^2}{2m}\nabla^2\Psi + V\Psi,$

em que

$$\boxed{\nabla^2 \equiv \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}}$$

é o **Laplaciano**, em coordenadas cartesianas.

Equação de Schrödinger em coordenadas esféricas



Nas **coordenadas esféricas**, o Laplaciano toma a forma de

Laplaciano, em coordenadas esféricas...

$$\nabla^2 = \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right) + \frac{1}{r^2 \operatorname{sen}\theta}\frac{\partial}{\partial \theta}\left(\operatorname{sen}\theta\frac{\partial}{\partial \theta}\right) + \frac{1}{r^2 \operatorname{sen}^2\theta}\left(\frac{\partial^2}{\partial \phi^2}\right).$$

Eq. de Schrödinger:

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

Separação de variáveis

$$\boxed{\psi(r,\theta,\phi) = R(r)Y(\theta,\phi).}$$

- **A equação angular**

$$\frac{1}{Y}\left\{\frac{1}{\text{sen}\theta}\frac{\partial}{\partial\theta}\left(\text{sen}\theta\frac{\partial Y}{\partial\theta}\right)+\frac{1}{\text{sen}^2\theta}\frac{\partial^2 Y}{\partial\phi^2}\right\}=-l(l+1)$$

- **A equação radial**

$$-\frac{\hbar^2}{2m}\frac{d^2u}{dr^2}+\left[V+\frac{\hbar^2}{2m}\frac{l(l+1)}{r^2}\right]u=Eu.$$

$$\boxed{\psi_{nlm}(r,\theta,\phi)=R_{nl}(r)Y_l^m(\theta,\phi),}$$

É conveniente que *R* e *Y* sejam normalizados separadamente:

$$\int_0^\infty |R|^2 r^2\,dr=1 \quad e \quad \int_0^{2\pi}\int_0^\pi |Y|^2\,\text{sen}\theta\,d\theta\,d\phi=1.$$

$$\boxed{Y(\theta,\phi)=\Theta(\theta)\Phi(\phi).}$$

$$\left\{\frac{1}{\Theta}\left[\text{sen}\theta\frac{d}{d\theta}\left(\text{sen}\theta\frac{d\Theta}{d\theta}\right)\right]+l(l+1)\text{sen}^2\theta\right\}+\frac{1}{\Phi}\frac{d^2\Phi}{d\phi^2}=0.$$

Harmônicos esféricos

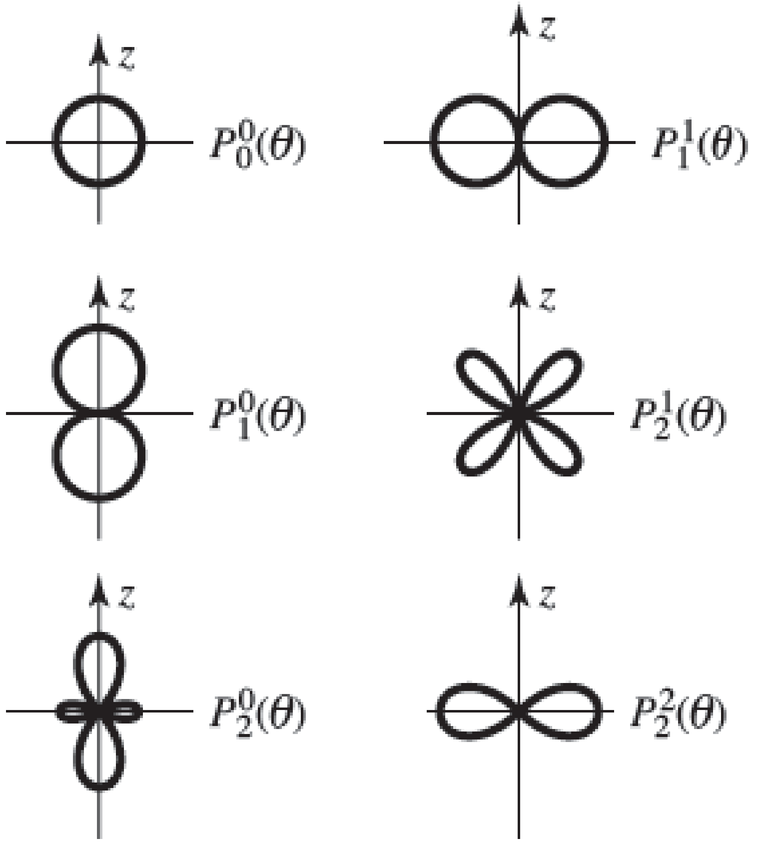
$Y_0^0=\left(\frac{1}{4\pi}\right)^{1/2}$	$Y_2^{\pm2}=\left(\frac{15}{32\pi}\right)^{1/2}\text{sen}^2\,\theta e^{\pm 2i\phi}$
$Y_1^0=\left(\frac{3}{4p}\right)^{1/2}\cos\theta$	$Y_3^0=\left(\frac{7}{16\pi}\right)^{1/2}(5\cos^3\theta-3\cos\theta)$
$Y_1^{\pm1}=\mp\left(\frac{3}{8\pi}\right)^{1/2}\text{sen}\,\theta e^{\pm i\phi}$	$Y_3^{\pm1}=\mp\left(\frac{21}{64\pi}\right)^{1/2}\text{sen}\,\theta\,(5\cos^2\theta-1)e^{\pm i\phi}$
$Y_2^0=\left(\frac{5}{16\pi}\right)^{1/2}(3\cos^2\theta-1)$	$Y_3^{\pm2}=\left(\frac{105}{32\pi}\right)^{1/2}\text{sen}^2\,\theta\cos\theta e^{\pm 2i\phi}$
$Y_2^{\pm1}=\mp\left(\frac{15}{8\pi}\right)^{1/2}\text{sen}\,\theta\cos\theta e^{\pm i\phi}$	$Y_3^{\pm3}=\mp\left(\frac{35}{64\pi}\right)^{1/2}\text{sen}^3\,\theta e^{\pm 3i\phi}$

$$Y_l^m(\theta,\phi)=\epsilon\sqrt{\frac{(2l+1)}{4\pi}\frac{(l-|m|)!}{(l+|m|)!}}e^{im\phi}P_l^m(\cos\theta),$$

$$\int_0^{2\pi}\int_0^\pi [Y_l^m(\theta,\phi)]^*[Y_{l'}^{m'}(\theta,\phi)]\,\text{sen}\theta\,d\theta\,d\phi=\delta_{ll'}\delta_{mm'}.$$

TABELA 4.2 Algumas funções associadas de Legendre, $P_l^m(\cos\theta)$: (a) forma funcional, (b) gráficos de $r = P_l^m(\cos\theta)$ (nesses gráficos, r diz qual a magnitude da função na direção θ; as figuras deveriam ser rotacionadas sobre o eixo z).

$P_0^0 = 1$	$P_2^0 = \frac{1}{2}(3\cos^2\theta - 1)$
$P_1^1 = \operatorname{sen}\theta$	$P_3^3 = 15\operatorname{sen}\theta(1-\cos^2\theta)$
$P_1^0 = \cos\theta$	$P_3^2 = 15\operatorname{sen}^2\theta\cos\theta$
$P_2^2 = 3\operatorname{sen}^2\theta$	$P_3^1 = \frac{3}{2}\operatorname{sen}\theta(5\cos^2\theta - 1)$
$P_2^1 = 3\operatorname{sen}\theta\cos\theta$	$P_3^0 = \frac{1}{2}(5\cos^3\theta - 3\cos\theta)$



$$Y_l^m(\theta,\phi) = \epsilon\sqrt{\frac{(2l+1)}{4\pi}\frac{(l-|m|)!}{(l+|m|)!}}e^{im\phi}P_l^m(\cos\theta),$$

Griffiths

Momento Angular

Propriedades da Álgebra, composição de momentos angulares
Importância das simetrias, estados moleculares....

Momento angular

$$\mathbf{L} = \mathbf{r} \times \mathbf{p},$$

$$L_x = yp_z - zp_y, \quad L_y = zp_x - xp_z, \quad L_z = xp_y - yp_x.$$

$$p_x \to -i\hbar\partial / \partial x, p_y \to -i\hbar\partial / \partial y, p_z \to -i\hbar\partial / \partial z.$$

Os operadores L_x e L_y não comutam

$$[L_x, L_y] = [yp_z - zp_y, zp_x - xp_z]$$

$$= [yp_z, zp_x] - [yp_z, xp_z] - [zp_y, zp_x] + [zp_y, xp_z].$$

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

$$\boxed{[L_x, L_y] = i\hbar L_z; \quad [L_y, L_z] = i\hbar L_x; \quad [L_z, L_x] = i\hbar L_y.}$$

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

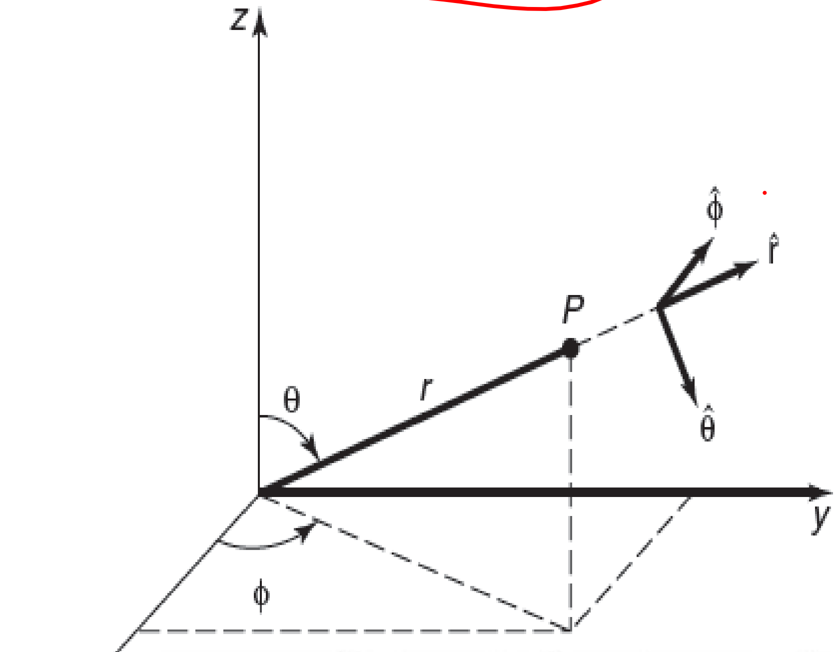
$$L_y = \frac{\hbar}{i}\left(+\cos\phi\frac{\partial}{\partial\theta} - \operatorname{sen}\phi\cot\theta\frac{\partial}{\partial\phi}\right),$$

$$L_z = \frac{\hbar}{i}\frac{\partial}{\partial\phi}.$$

$$-\frac{\hbar^2}{2m}\left[\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial\psi}{\partial r}\right) + \underbrace{\frac{1}{r^2\operatorname{sen}\theta}\frac{\partial}{\partial\theta}\left(\operatorname{sen}\theta\frac{\partial\psi}{\partial\theta}\right) + \frac{1}{r^2\operatorname{sen}^2\theta}\left(\frac{\partial^2\psi}{\partial\phi^2}\right)}_{\frac{1}{r^2}L^2}\right] + V\psi = E\psi.$$

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

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



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

$$\hat{\phi} = -(\sin\phi)\,\hat{\imath} + (\cos\phi)\,\hat{\jmath}.$$

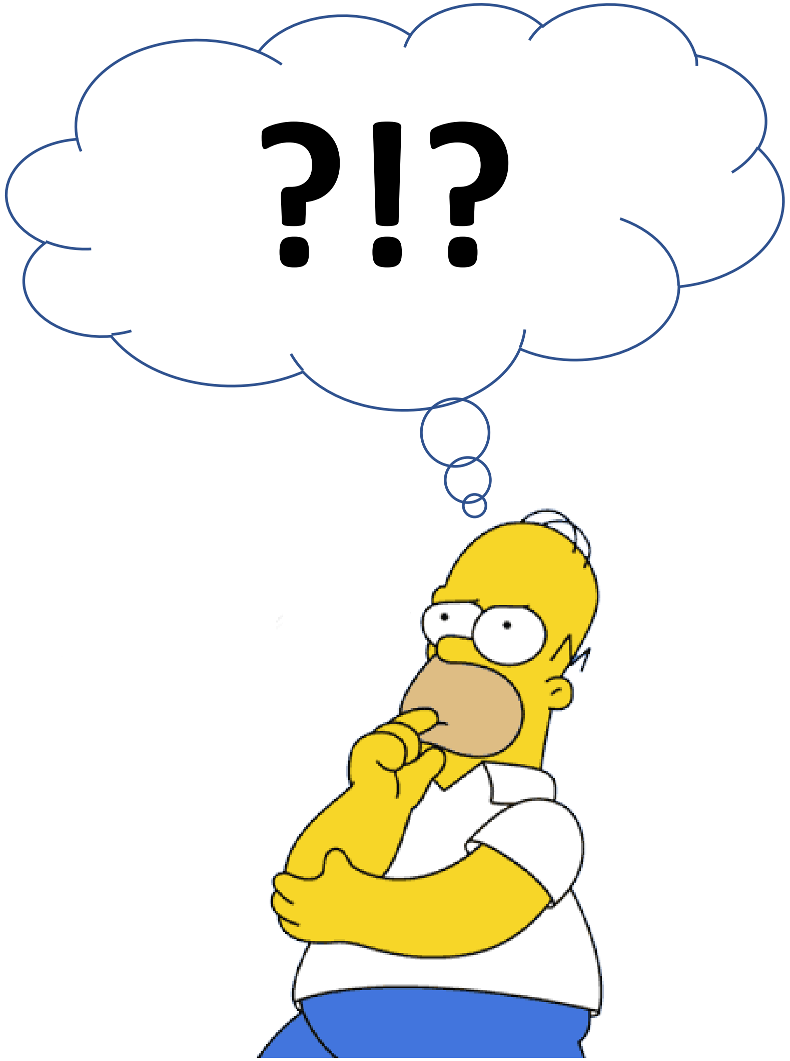
$$\mathbf{L} = -i\hbar\left[r(\hat{r}\times\hat{r})\frac{\partial}{\partial r} + (\hat{r}\times\hat{\theta})\frac{\partial}{\partial\theta} + (\hat{r}\times\hat{\phi})\frac{1}{\sin\theta}\frac{\partial}{\partial\phi}\right] \longrightarrow \mathbf{L} = -i\hbar\left(\hat{\phi}\frac{\partial}{\partial\theta}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

Momento angular

*Toda a **álgebra** do Momento Angular deriva disso(!!)*

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

$$[S_x, S_y] = i\hbar S_z, \quad [S_y, S_z] = i\hbar S_x, \quad [S_z, S_x] = i\hbar S_y.$$



Momento angular

*Toda a **álgebra** do Momento Angular deriva disso(!!)*

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

$$[S_x, S_y] = i\hbar S_z, \quad [S_y, S_z] = i\hbar S_x, \quad [S_z, S_x] = i\hbar S_y.$$

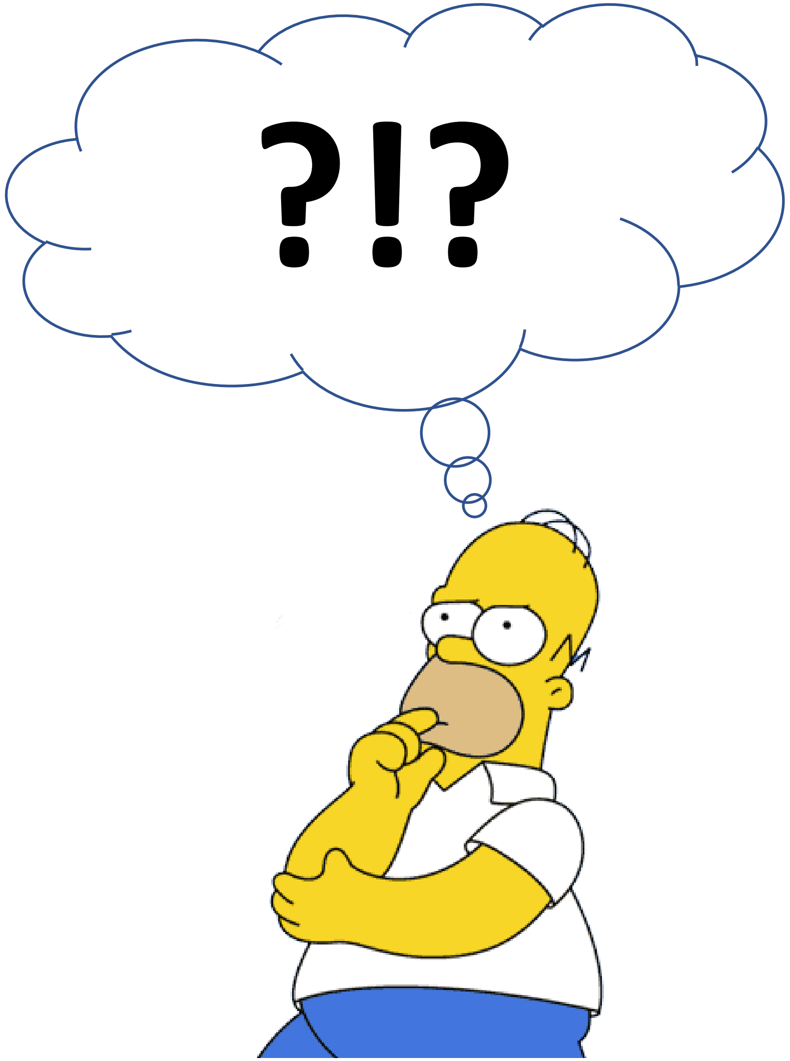
Usaremos a técnica do 'operador escada', muito similar à que aplicamos ao oscilador harmônico.

$$L_\pm \equiv L_x \pm i L_y.$$

Comutadores

$$[L^2, L_\pm] = 0.$$

$$[L_z, L_\pm] = \pm\hbar L_\pm.$$



Momento angular

*Toda a **álgebra** do Momento Angular deriva disso(!!)*

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

$$[S_x, S_y] = i\hbar S_z, \quad [S_y, S_z] = i\hbar S_x, \quad [S_z, S_x] = i\hbar S_y.$$

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$$[L^2, L_\pm] = 0.$$

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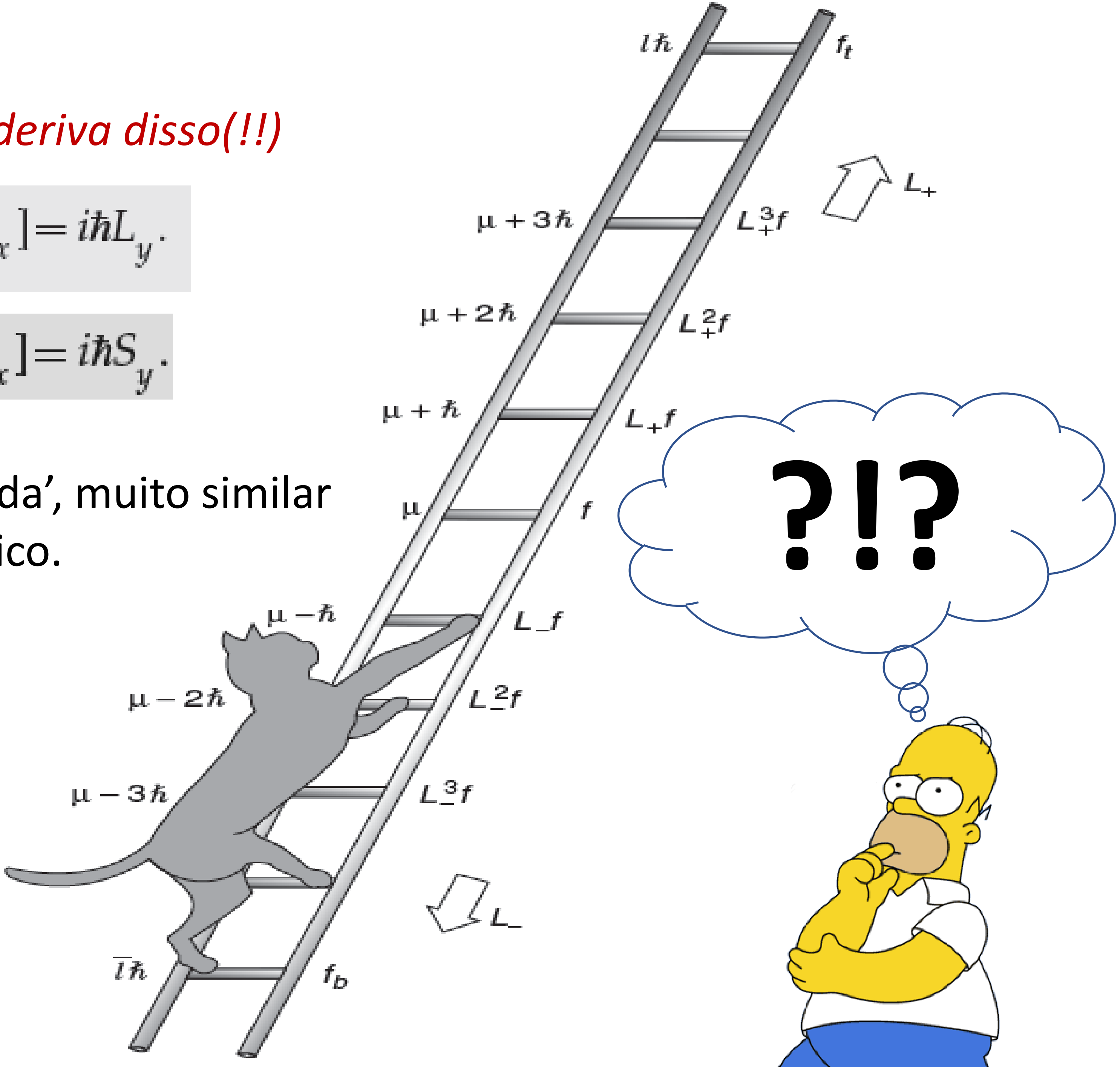
Espectro tipo "escada" !!

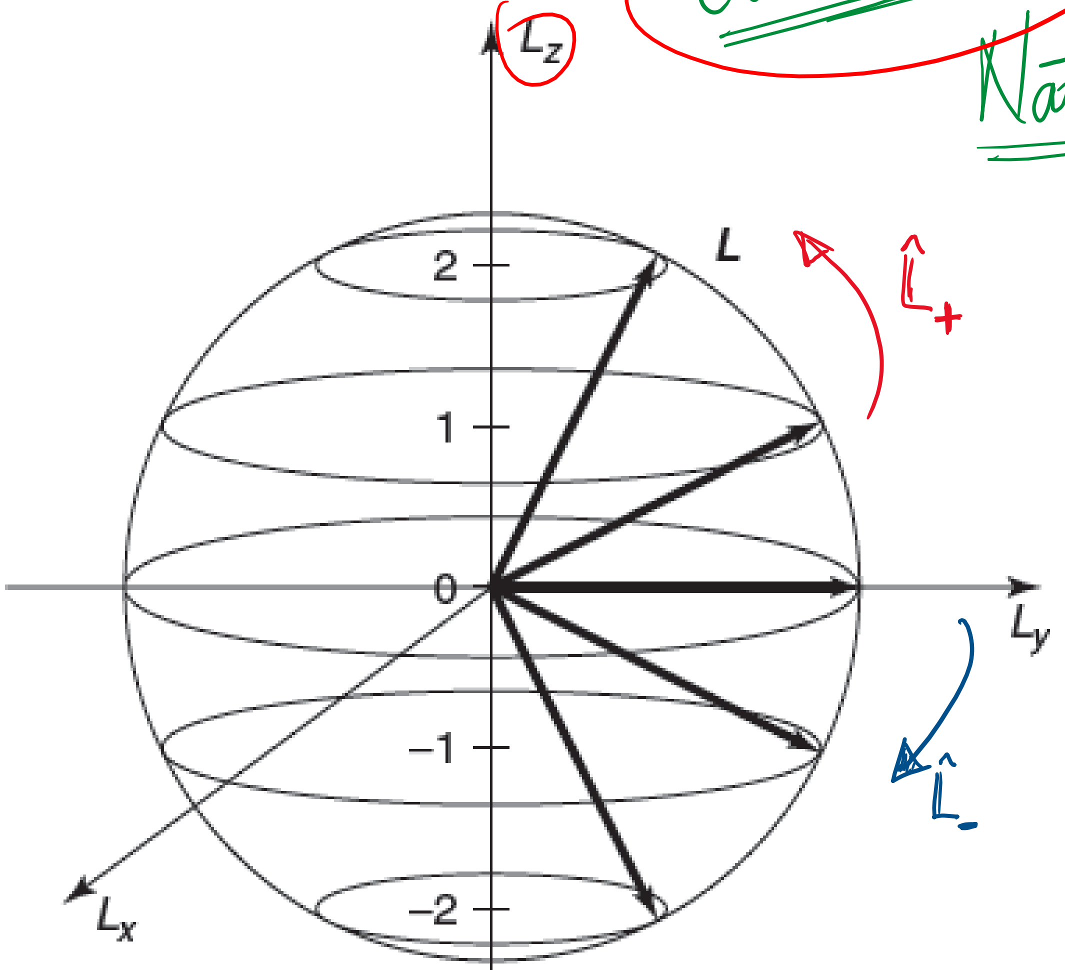
"raising" & "lowering" operator



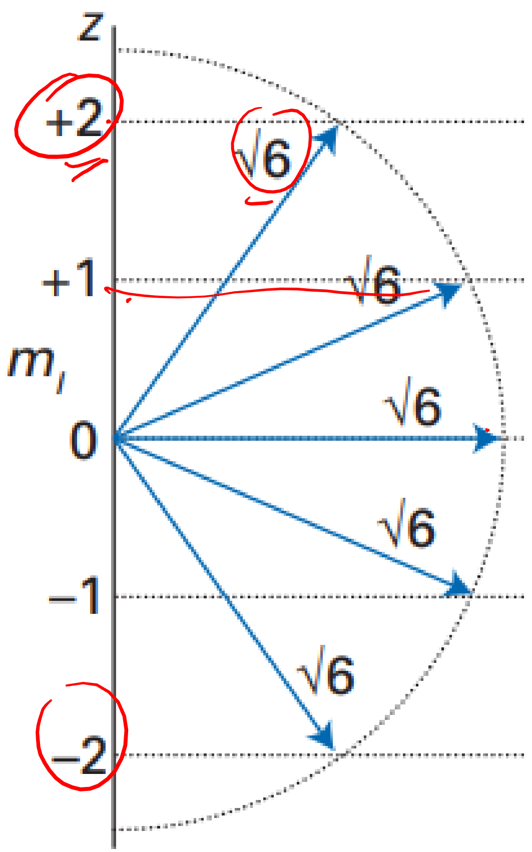
Autovalores de Lz

Cuidado!!

Não leve esta imagem a sério demais!



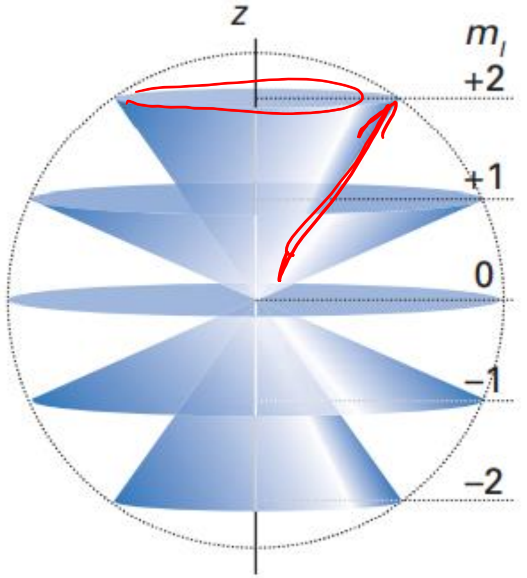
Estados do momento angular (para $l = 2$).



$l = 2$

$l(l+1)$

$2(2+1) = 6$



Spin

A teoria *algébrica* de spin é inspirada na teoria do momento angular orbital, a começar pelas relações de comutação fundamental:

$$[S_x, S_y] = i\hbar S_z, \quad [S_y, S_z] = i\hbar S_x, \quad [S_z, S_x] = i\hbar S_y.$$

Segue-se que (como antes) os autovetores de S^2 e S_z satisfazem

$$S^2 |sm\rangle = \hbar^2 s(s+1) |sm\rangle; \quad S_z |sm\rangle = \hbar m |sm\rangle;$$

e

$$S_\pm |sm\rangle = \hbar\sqrt{s(s+1) - m(m\pm 1)}\, |s(m\pm 1)\rangle,$$

$$s = 0, \frac{1}{2}, 1, \frac{3}{2}, \ldots; \quad m = -s, -s+1, \ldots, s-1, s.$$

Momento angular generalizado (total)

$$\vec{\mathbf{J}} = \vec{\mathbf{L}} + \vec{\mathbf{S}}$$

CUIDADO!!
espaços vetoriais distintos!!
(envolve produto tensorial)

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

$$[S_x, S_y] = i\hbar S_z, \quad [S_y, S_z] = i\hbar S_x, \quad [S_z, S_x] = i\hbar S_y.$$

$$[J_x, J_y] = i\hbar J_z, \quad [J_y, J_z] = i\hbar J_x, \quad [J_z, J_x] = i\hbar J_y$$

$$J_+ = J_x + iJ_y$$
$$J_- = J_x - iJ_y$$

$$\frac{1}{2}(J_+ + J_-) = \frac{1}{2}(J_x + iJ_y + J_x - iJ_y) = J_x$$

$$\frac{1}{2i}(J_+ - J_-) = \frac{1}{2i}(J_x + iJ_y - J_x + iJ_y) = J_y$$

$$[J^2, J_+] = [J^2, J_x + iJ_y] = [J^2, J_x] + i[J^2, J_y] = 0$$

$$[J_z, J_\pm] = [J_z, J_x \pm iJ_y] = [J_z, J_x] \pm i[J_z, J_y] = i\hbar J_y \pm i(-i\hbar J_x)$$
$$= \hbar(J_x \pm iJ_y) = \pm\hbar J_\pm$$

Atenção p/ os sinais

$$J^2 = J_- J_+ + J_z^2 + \hbar J_z$$
$$J^2 = J_z^2 + \tfrac{1}{2}(J_+ J_- + J_- J_+)$$

resulta em um espectro do tipo "escada" como osc. harmônico

Porém, a escada é limitada!!

$$J^2|j,m\rangle = h^2 j(j+1)|j,m\rangle$$
$$J_z|j,m\rangle = m\hbar|j,m\rangle$$

$$J_+|j,m\rangle = \hbar\sqrt{j(j+1) - m(m+1)}|j,m+1\rangle$$
$$J_-|j,m\rangle = \hbar\sqrt{j(j+1) - m(m-1)}|j,m-1\rangle$$

$$J_+|j,m=j\rangle = 0$$
$$J_-|j,m=-j\rangle = 0$$

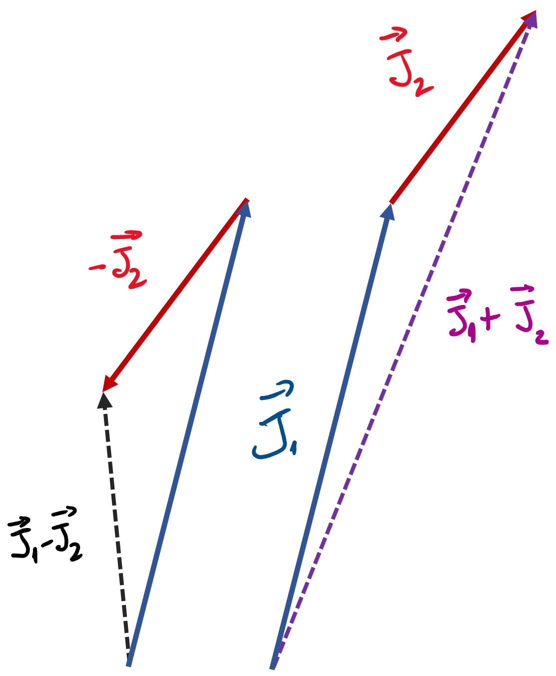
Soma (composição) de Momentos angulares

$$\boxed{\vec{\mathbf{J}} = \vec{\mathbf{L}} + \vec{\mathbf{S}}} \Rightarrow \vec{J} = \vec{L} \otimes \mathbb{1} + \mathbb{1} \otimes \vec{S} \Rightarrow \left\{ \begin{array}{l} J^2 |j\,m\rangle = j(j+1)\hbar^2 |j\,m\rangle \\ J_z |j,m\rangle = m\hbar |j\,m\rangle \\ j = \{(\ell+s), \dots |\ell - s|\} \\ m = \{-j, \dots, j\} \end{array} \right.$$

$$\vec{J} = \vec{J}_1 + \vec{J}_2$$

$$|j_1\, m_1\rangle |j_2\, m_2\rangle \leftrightarrow |j\, m\rangle$$

$$\left\{ \begin{array}{l} j = (j_1 + j_2),\ (j_1 + j_2 - 1), \dots |j_1 - j_2| \\ m = j,\ j-1, \dots, -j \end{array} \right.$$



Exemplo: $j_1 = 1$, $j_2 = 1/2$

Vetores: $\begin{pmatrix} \cdot \\ \cdot \\ \cdot \end{pmatrix} \otimes \begin{pmatrix} \cdot \\ \cdot \end{pmatrix} = \begin{pmatrix} \cdot \\ \cdot \\ \cdot \\ \cdot \\ \cdot \\ \cdot \end{pmatrix}$

ops.: $(3\times3) \otimes (2\times2) = (6\times6)$

Soma de momentos angulares

$$|sm\rangle = \sum_{m_1+m_2=m} \underbrace{C^{s_1 s_2 s}_{m_1 m_2 m}\,|s_1 m_1\rangle |s_2 m_2\rangle}_{\text{Combinação linear da base dos estados Zeeman.}}$$

O estado combinado $|j\ m\rangle$ com spin total s e componente-z igual a m será uma combinação linear dos estados compostos $|j_1\ m_1\rangle|j_2\ m_2\rangle$:

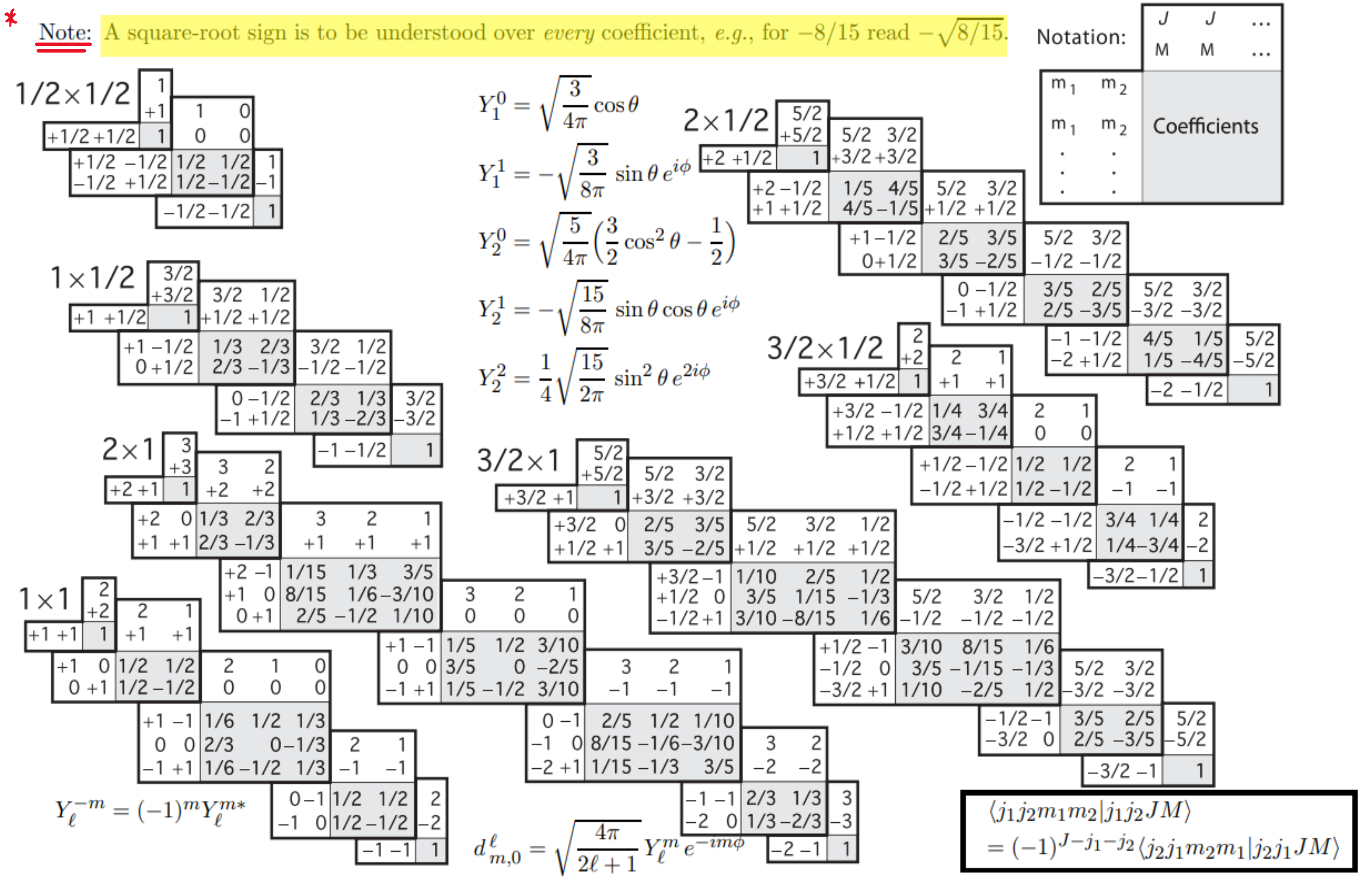
$$|j_1 m_1\rangle|j_2 m_2\rangle \rightarrow |j_1 j_2; m_1 m_2\rangle \equiv |m_1 m_2\rangle$$

$$|j\,m\rangle = \sum_{m_1}\sum_{m_2} \underbrace{\langle m_1 m_2 | j\, m\rangle}_{\text{Coef. de Clebsch-Gordan}} |m_1 m_2\rangle$$

↳ Elementos da matriz de transf. da base $|m_1 m_2\rangle \rightarrow |j, m\rangle$

$m_1 = \{-j_1, \ldots, j_1\}$
$m_2 = \{-j_2, \ldots, j_2\}$
$j = \{(j_1+j_2), (j_1+j_2-1), \ldots |j_1-j_2|\}$

Coeficientes de Clebsch-Gordan


* Note: A square-root sign is to be understood over *every* coefficient, *e.g.*, for −8/15 read $-\sqrt{8/15}$.

Notation: J J … / M M … ; m_1 m_2 / m_1 m_2 / ⋮ ⋮ : Coefficients

1/2×1/2
1 / +1 — +1/2 +1/2: 1
1 0 / 0 0 — +1/2 −1/2: 1/2 1/2 ; −1/2 +1/2: 1/2 −1/2
1 / −1 — −1/2 −1/2: 1

1×1/2
3/2 / +3/2 — +1 +1/2: 1
3/2 1/2 / +1/2 +1/2 — +1 −1/2: 1/3 2/3 ; 0 +1/2: 2/3 −1/3
3/2 1/2 / −1/2 −1/2 — 0 −1/2: 2/3 1/3 ; −1 +1/2: 1/3 −2/3
3/2 / −3/2 — −1 −1/2: 1

2×1/2
5/2 / +5/2 — +2 +1/2: 1
5/2 3/2 / +3/2 +3/2 — +2 −1/2: 1/5 4/5 ; +1 +1/2: 4/5 −1/5
5/2 3/2 / +1/2 +1/2 — +1 −1/2: 2/5 3/5 ; 0 +1/2: 3/5 −2/5
5/2 3/2 / −1/2 −1/2 — 0 −1/2: 3/5 2/5 ; −1 +1/2: 2/5 −3/5
5/2 3/2 / −3/2 −3/2 — −1 −1/2: 4/5 1/5 ; −2 +1/2: 1/5 −4/5
5/2 / −5/2 — −2 −1/2: 1

3/2×1/2
2 / +2 — +3/2 +1/2: 1
2 1 / +1 +1 — +3/2 −1/2: 1/4 3/4 ; +1/2 +1/2: 3/4 −1/4
2 1 / 0 0 — +1/2 −1/2: 1/2 1/2 ; −1/2 +1/2: 1/2 −1/2
2 1 / −1 −1 — −1/2 −1/2: 3/4 1/4 ; −3/2 +1/2: 1/4 −3/4
2 / −2 — −3/2 −1/2: 1

2×1
3 / +3 — +2 +1: 1
3 2 / +2 +2 — +2 0: 1/3 2/3 ; +1 +1: 2/3 −1/3
3 2 1 / +1 +1 +1 — +2 −1: 1/15 1/3 3/5 ; +1 0: 8/15 1/6 −3/10 ; 0 +1: 2/5 −1/2 1/10
3 2 1 / 0 0 0 — +1 −1: 1/5 1/2 3/10 ; 0 0: 3/5 0 −2/5 ; −1 +1: 1/5 −1/2 3/10
3 2 1 / −1 −1 −1 — 0 −1: 2/5 1/2 1/10 ; −1 0: 8/15 −1/6 −3/10 ; −2 +1: 1/15 −1/3 3/5
3 2 / −2 −2 — −1 −1: 2/3 1/3 ; −2 0: 1/3 −2/3
3 / −3 — −2 −1: 1

3/2×1
5/2 / +5/2 — +3/2 +1: 1
5/2 3/2 / +3/2 +3/2 — +3/2 0: 2/5 3/5 ; +1/2 +1: 3/5 −2/5
5/2 3/2 1/2 / +1/2 +1/2 +1/2 — +3/2 −1: 1/10 2/5 1/2 ; +1/2 0: 3/5 1/15 −1/3 ; −1/2 +1: 3/10 −8/15 1/6
5/2 3/2 1/2 / −1/2 −1/2 −1/2 — +1/2 −1: 3/10 8/15 1/6 ; −1/2 0: 3/5 −1/15 −1/3 ; −3/2 +1: 1/10 −2/5 1/2
5/2 3/2 / −3/2 −3/2 — −1/2 −1: 3/5 2/5 ; −3/2 0: 2/5 −3/5
5/2 / −5/2 — −3/2 −1: 1

1×1
2 / +2 — +1 +1: 1
2 1 / +1 +1 — +1 0: 1/2 1/2 ; 0 +1: 1/2 −1/2
2 1 0 / 0 0 0 — +1 −1: 1/6 1/2 1/3 ; 0 0: 2/3 0 −1/3 ; −1 +1: 1/6 −1/2 1/3
2 1 / −1 −1 — 0 −1: 1/2 1/2 ; −1 0: 1/2 −1/2
2 / −2 — −1 −1: 1

$$Y_1^0 = \sqrt{\frac{3}{4\pi}}\cos\theta$$
$$Y_1^1 = -\sqrt{\frac{3}{8\pi}}\sin\theta\, e^{i\phi}$$
$$Y_2^0 = \sqrt{\frac{5}{4\pi}}\left(\frac{3}{2}\cos^2\theta - \frac{1}{2}\right)$$
$$Y_2^1 = -\sqrt{\frac{15}{8\pi}}\sin\theta\cos\theta\, e^{i\phi}$$
$$Y_2^2 = \frac{1}{4}\sqrt{\frac{15}{2\pi}}\sin^2\theta\, e^{2i\phi}$$
$$Y_\ell^{-m} = (-1)^m Y_\ell^{m*}$$
$$d^\ell_{m,0} = \sqrt{\frac{4\pi}{2\ell+1}}\,Y_\ell^m\, e^{-im\phi}$$
$$\langle j_1 j_2 m_1 m_2 | j_1 j_2 J M\rangle = (-1)^{J-j_1-j_2}\langle j_2 j_1 m_2 m_1 | j_2 j_1 J M\rangle$$

Essa tabela* também funciona ao contrário:

$$|s_1 m_1\rangle|s_2 m_2\rangle = \sum_s C^{s_1 s_2 s}_{m_1 m_2 m}\,|sm\rangle.$$

Exemplo Griffiths*

http://pdg.lbl.gov/

Clebsch-Gordan Coefficients, Spherical Harmonics, and d Functions

Note: A square-root sign is to be understood over *every* coefficient, *e.g.*, for $-8/15$ read $-\sqrt{8/15}$.

Notation:

		J	J	...
		M	M	...
m_1	m_2	Coefficients		
m_1	m_2			
.	.			

$$Y_1^0 = \sqrt{\frac{3}{4\pi}}\cos\theta$$

$$Y_1^1 = -\sqrt{\frac{3}{8\pi}}\sin\theta\, e^{i\phi}$$

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

$$Y_2^1 = -\sqrt{\frac{15}{8\pi}}\sin\theta\cos\theta\, e^{i\phi}$$

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

$$Y_\ell^{-m} = (-1)^m Y_\ell^{m*}$$

$$d^{\ell}_{m,0} = \sqrt{\frac{4\pi}{2\ell+1}}\, Y_\ell^m\, e^{-im\phi}$$

$$\langle j_1 j_2 m_1 m_2 | j_1 j_2 J M\rangle = (-1)^{J-j_1-j_2}\langle j_2 j_1 m_2 m_1 | j_2 j_1 J M\rangle$$

$1/2\times 1/2$

m_1	m_2	$J=1$, $M=+1$
+1/2	+1/2	1

m_1	m_2	$J=1$, $M=0$	$J=0$, $M=0$
+1/2	−1/2	1/2	1/2
−1/2	+1/2	1/2	−1/2

m_1	m_2	$J=1$, $M=-1$
−1/2	−1/2	1

$1\times 1/2$

m_1	m_2	$J=3/2$, $M=+3/2$
+1	+1/2	1

m_1	m_2	$J=3/2$, $M=+1/2$	$J=1/2$, $M=+1/2$
+1	−1/2	1/3	2/3
0	+1/2	2/3	−1/3

m_1	m_2	$J=3/2$, $M=-1/2$	$J=1/2$, $M=-1/2$
0	−1/2	2/3	1/3
−1	+1/2	1/3	−2/3

m_1	m_2	$J=3/2$, $M=-3/2$
−1	−1/2	1

2×1

m_1	m_2	$J=3$, $M=+3$
+2	+1	1

m_1	m_2	$J=3$, $M=+2$	$J=2$, $M=+2$
+2	0	1/3	2/3
+1	+1	2/3	−1/3

m_1	m_2	$J=3$, $M=+1$	$J=2$, $M=+1$	$J=1$, $M=+1$
+2	−1	1/15	1/3	3/5
+1	0	8/15	1/6	−3/10
0	+1	2/5	−1/2	1/10

m_1	m_2	$J=3$, $M=0$	$J=2$, $M=0$	$J=1$, $M=0$
+1	−1	1/5	1/2	3/10
0	0	3/5	0	−2/5
−1	+1	1/5	−1/2	3/10

m_1	m_2	$J=3$, $M=-1$	$J=2$, $M=-1$	$J=1$, $M=-1$
0	−1	2/5	1/2	1/10
−1	0	8/15	−1/6	−3/10
−2	+1	1/15	−1/3	3/5

m_1	m_2	$J=3$, $M=-2$	$J=2$, $M=-2$
−1	−1	2/3	1/3
−2	0	1/3	−2/3

m_1	m_2	$J=3$, $M=-3$
−2	−1	1

1×1

m_1	m_2	$J=2$, $M=+2$
+1	+1	1

m_1	m_2	$J=2$, $M=+1$	$J=1$, $M=+1$
+1	0	1/2	1/2
0	+1	1/2	−1/2

m_1	m_2	$J=2$, $M=0$	$J=1$, $M=0$	$J=0$, $M=0$
+1	−1	1/6	1/2	1/3
0	0	2/3	0	−1/3
−1	+1	1/6	−1/2	1/3

m_1	m_2	$J=2$, $M=-1$	$J=1$, $M=-1$
0	−1	1/2	1/2
−1	0	1/2	−1/2

m_1	m_2	$J=2$, $M=-2$
−1	−1	1

$2\times 1/2$

m_1	m_2	$J=5/2$, $M=+5/2$
+2	+1/2	1

m_1	m_2	$J=5/2$, $M=+3/2$	$J=3/2$, $M=+3/2$
+2	−1/2	1/5	4/5
+1	+1/2	4/5	−1/5

m_1	m_2	$J=5/2$, $M=+1/2$	$J=3/2$, $M=+1/2$
+1	−1/2	2/5	3/5
0	+1/2	3/5	−2/5

m_1	m_2	$J=5/2$, $M=-1/2$	$J=3/2$, $M=-1/2$
0	−1/2	3/5	2/5
−1	+1/2	2/5	−3/5

m_1	m_2	$J=5/2$, $M=-3/2$	$J=3/2$, $M=-3/2$
−1	−1/2	4/5	1/5
−2	+1/2	1/5	−4/5

m_1	m_2	$J=5/2$, $M=-5/2$
−2	−1/2	1

$3/2\times 1/2$

m_1	m_2	$J=2$, $M=+2$
+3/2	+1/2	1

m_1	m_2	$J=2$, $M=+1$	$J=1$, $M=+1$
+3/2	−1/2	1/4	3/4
+1/2	+1/2	3/4	−1/4

m_1	m_2	$J=2$, $M=0$	$J=1$, $M=0$
+1/2	−1/2	1/2	1/2
−1/2	+1/2	1/2	−1/2

m_1	m_2	$J=2$, $M=-1$	$J=1$, $M=-1$
−1/2	−1/2	3/4	1/4
−3/2	+1/2	1/4	−3/4

m_1	m_2	$J=2$, $M=-2$
−3/2	−1/2	1

$3/2\times 1$

m_1	m_2	$J=5/2$, $M=+5/2$
+3/2	+1	1

m_1	m_2	$J=5/2$, $M=+3/2$	$J=3/2$, $M=+3/2$
+3/2	0	2/5	3/5
+1/2	+1	3/5	−2/5

m_1	m_2	$J=5/2$, $M=+1/2$	$J=3/2$, $M=+1/2$	$J=1/2$, $M=+1/2$
+3/2	−1	1/10	2/5	1/2
+1/2	0	3/5	1/15	−1/3
−1/2	+1	3/10	−8/15	1/6

m_1	m_2	$J=5/2$, $M=-1/2$	$J=3/2$, $M=-1/2$	$J=1/2$, $M=-1/2$
+1/2	−1	3/10	8/15	1/6
−1/2	0	3/5	−1/15	−1/3
−3/2	+1	1/10	−2/5	1/2

m_1	m_2	$J=5/2$, $M=-3/2$	$J=3/2$, $M=-3/2$
−1/2	−1	3/5	2/5
−3/2	0	2/5	−3/5

m_1	m_2	$J=5/2$, $M=-5/2$
−3/2	−1	1

http://pdg.lbl.gov/

$$\mathbf{S} \equiv \mathbf{S}^{(1)} + \mathbf{S}^{(2)}.$$

$$s = (s_1 + s_2),\quad (s_1 + s_2 - 1),\quad (s_1 + s_2 - 2), \ldots,\quad |s_1 - s_2|.$$

$$\vec{J} = \vec{S} = \hat{S}_1 \otimes \hat{1} + \hat{1} \otimes \hat{S}_2 \Rightarrow$$

$$\begin{pmatrix} 1 \\ 0 \end{pmatrix} \otimes \begin{pmatrix} \alpha \\ \beta \end{pmatrix}$$

m_{s1}	m_{s2}	$\|1,+1\rangle$	$\|1,0\rangle$	$\|0,0\rangle$	$\|1,-1\rangle$
$+\frac{1}{2}$	$+\frac{1}{2}$	1	0	0	0
$+\frac{1}{2}$	$-\frac{1}{2}$	0	$1/2^{1/2}$	$1/2^{1/2}$	0
$-\frac{1}{2}$	$+\frac{1}{2}$	0	$1/2^{1/2}$	$-1/2^{1/2}$	0
$-\frac{1}{2}$	$-\frac{1}{2}$	0	0	0	1

Coef. de Clebsch-Gordan

$$S = (S_1 + S_2)\ ;\ (S_1 + S_2 - 1) \ldots |S_1 - S_2|$$

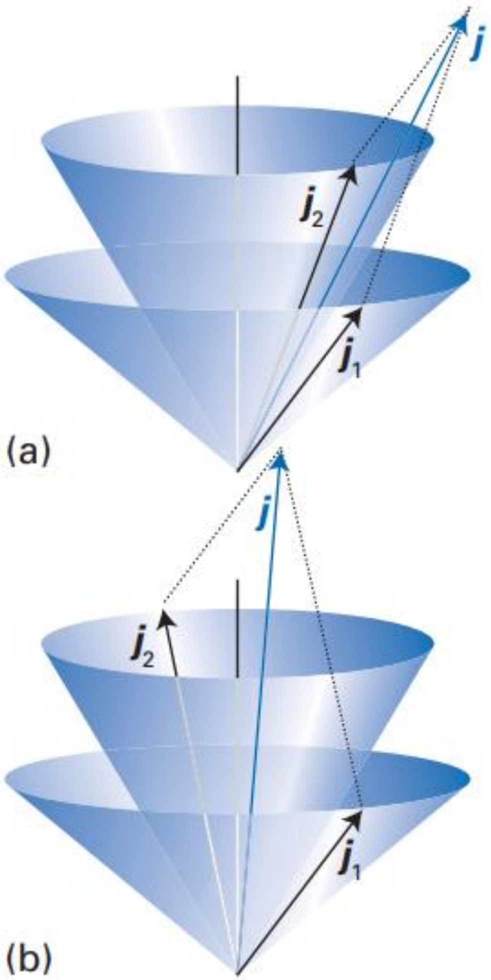
$$J = (J_1 + J_2)\ ;\ (J_2 + J_1 - 1), \ldots |J_1 - J_2|$$

módulo da diferença

$$\left\{\begin{array}{ll} |1\ 1\rangle & = \uparrow\uparrow \\ |1\ 0\rangle & = \frac{1}{\sqrt{2}}(\uparrow\downarrow + \downarrow\uparrow) \\ |1 -1\rangle & = \downarrow\downarrow \end{array}\right\} \quad s = 1 \text{ (tripleto)}.$$

$$\left\{|0\ 0\rangle = \frac{1}{\sqrt{2}}(\uparrow\downarrow - \downarrow\uparrow)\right\} \quad s = 0 \text{ (singleto)}.$$

Modelo vetorial da soma de momento angular & acoplamento



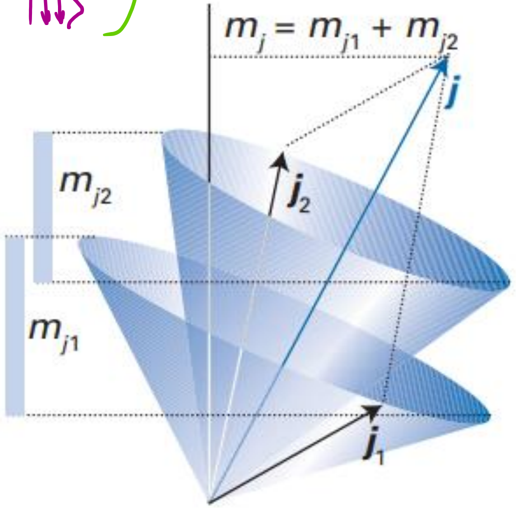
"desacoplado"

$|j\,m\rangle$

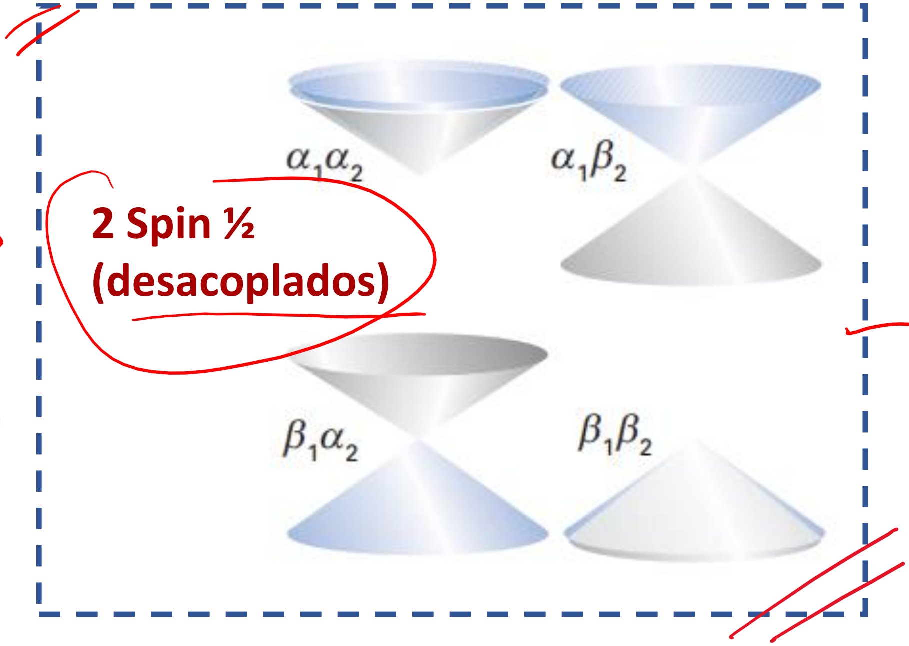
$|j_1 m_1\rangle|j_2 m_2\rangle$

$\uparrow\downarrow$

$|\uparrow\uparrow\rangle$
$|\uparrow\downarrow\rangle$
$|\downarrow\uparrow\rangle$
$|\downarrow\downarrow\rangle$

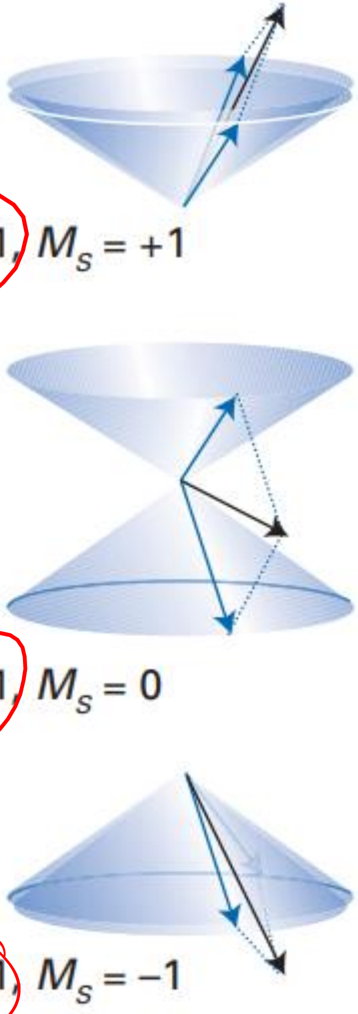


"acoplado"

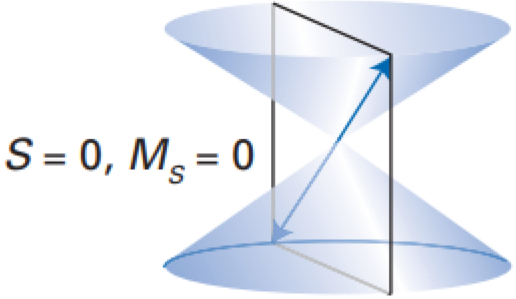


$|s, m_s\rangle$

$|j\, m_j\rangle$



2 Spins ½ (acoplados)



singleto

tripleto

Átomo de hidrogênio

$$-\frac{\hbar^2}{2m}\frac{d^2u}{dr^2}+\left[-\frac{e^2}{4\pi\epsilon_0}\frac{1}{r}+\frac{\hbar^2}{2m}\frac{l(l+1)}{r^2}\right]u=Eu. \quad \rightarrow \quad \frac{d^2u}{d\rho^2}=\left[1-\frac{\rho_0}{\rho}+\frac{l(l+1)}{\rho^2}\right]u.$$

A função de onda radial

As funções de onda espaciais para o hidrogênio são classificadas por três números quânticos: n, l, m:

$$\psi_{nlm}(r,\theta,\phi)=R_{nl}(r)Y_l^m(\theta,\phi),$$

$$\int \psi^*_{nlm}\psi_{n'l'm'}r^2\operatorname{sen}\theta\, dr\, d\theta\, d\phi=\delta_{nn'}\delta_{ll'}\delta_{mm'}.$$

$$R_{nl}(r)=\frac{1}{r}\rho^{l+1}e^{-\rho}v(\rho),$$

$$v(\rho)=L^{2l+1}_{n-l-1}(2\rho),$$

$$L^p_{q-p}(x)\equiv(-1)^p\left(\frac{d}{dx}\right)^p L_q(x)$$ (Polinômios associados de Laguerre)

$$L_q(x)\equiv e^x\left(\frac{d}{dx}\right)^q(e^{-x}x^q)$$ (Polinômios de Laguerre)

Energia: fórmula de Bohr

$$E_n=-\left[\frac{m}{2\hbar^2}\left(\frac{e^2}{4\pi\epsilon_0}\right)^2\right]\frac{1}{n^2}=\frac{E_1}{n^2},\quad n=1,2,3,\ldots$$

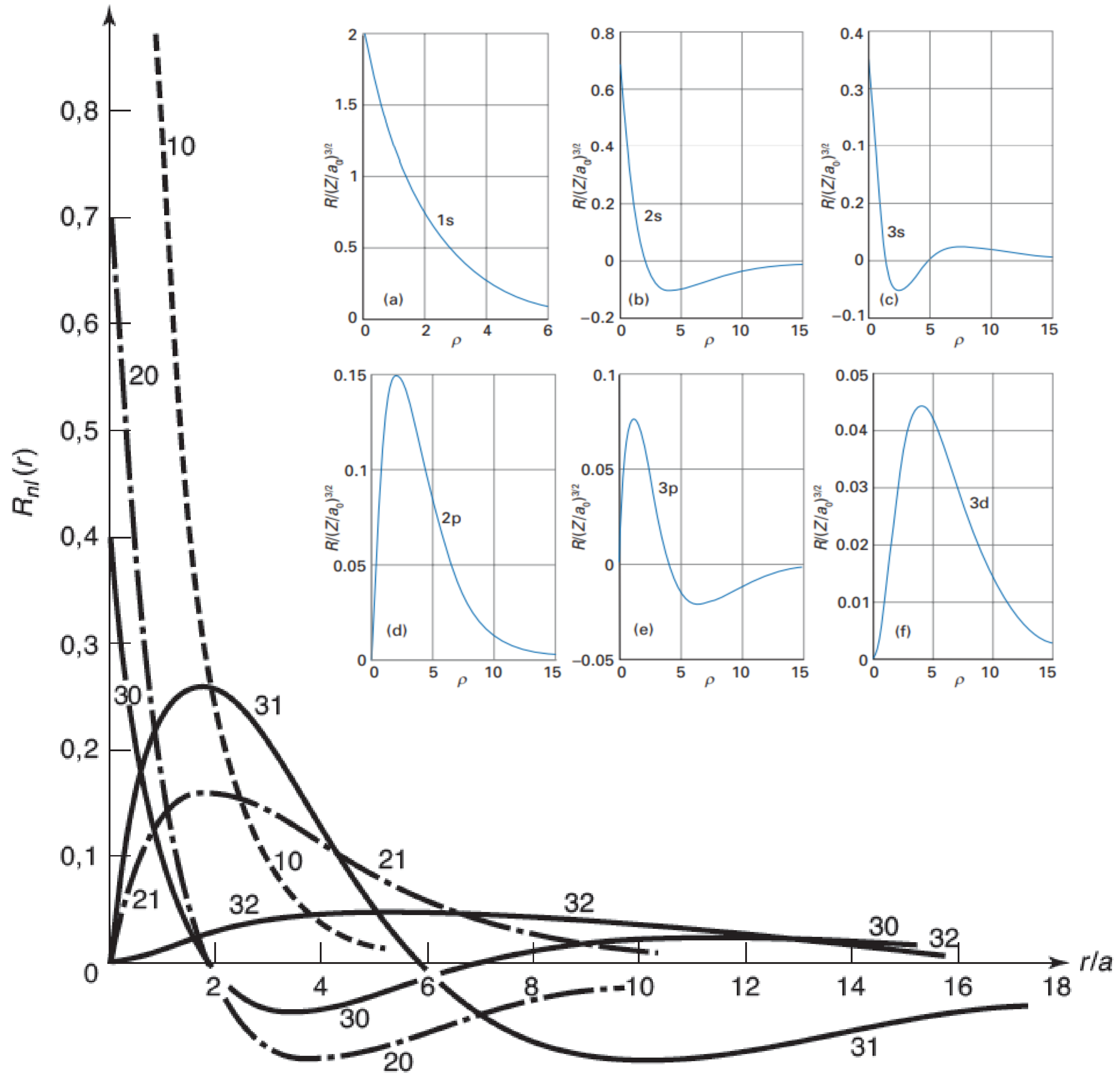
$$d(n)=\sum_{l=0}^{n-1}(2l+1)=n^2.$$

Raio de Bohr

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

$$a\equiv\frac{4\pi\epsilon_0\hbar^2}{me^2}=0{,}529\times10^{-10}\,\mathrm{m}$$

Primeiras funções de onda radiais do H



$$R_{10} = 2a^{-3/2}\exp(-r/a) \rightsquigarrow |\psi_{100}|^2 = \frac{1}{\pi}\left(\frac{1}{a_0}\right)^3 e^{-(2r/a_0)}$$

$$R_{20} = \frac{1}{\sqrt{2}}a^{-3/2}\left(1-\frac{1}{2}\frac{r}{a}\right)\exp(-r/2a)$$

$$R_{21} = \frac{1}{\sqrt{24}}a^{-3/2}\frac{r}{a}\exp(-r/2a)$$

$$R_{30} = \frac{2}{\sqrt{27}}a^{-3/2}\left(1-\frac{2}{3}\frac{r}{a}+\frac{2}{27}\left(\frac{r}{a}\right)^2\right)\exp(-r/3a)$$

$$R_{31} = \frac{8}{27\sqrt{6}}a^{-3/2}\left(1-\frac{1}{6}\frac{r}{a}\right)\left(\frac{r}{a}\right)\exp(-r/3a)$$

$$R_{32} = \frac{4}{81\sqrt{30}}a^{-3/2}\left(\frac{r}{a}\right)^2\exp(-r/3a)$$

$$R_{40} = \frac{1}{4}a^{-3/2}\left(1-\frac{3}{4}\frac{r}{a}+\frac{1}{8}\left(\frac{r}{a}\right)^2-\frac{1}{192}\left(\frac{r}{a}\right)^3\right)\exp(-r/4a)$$

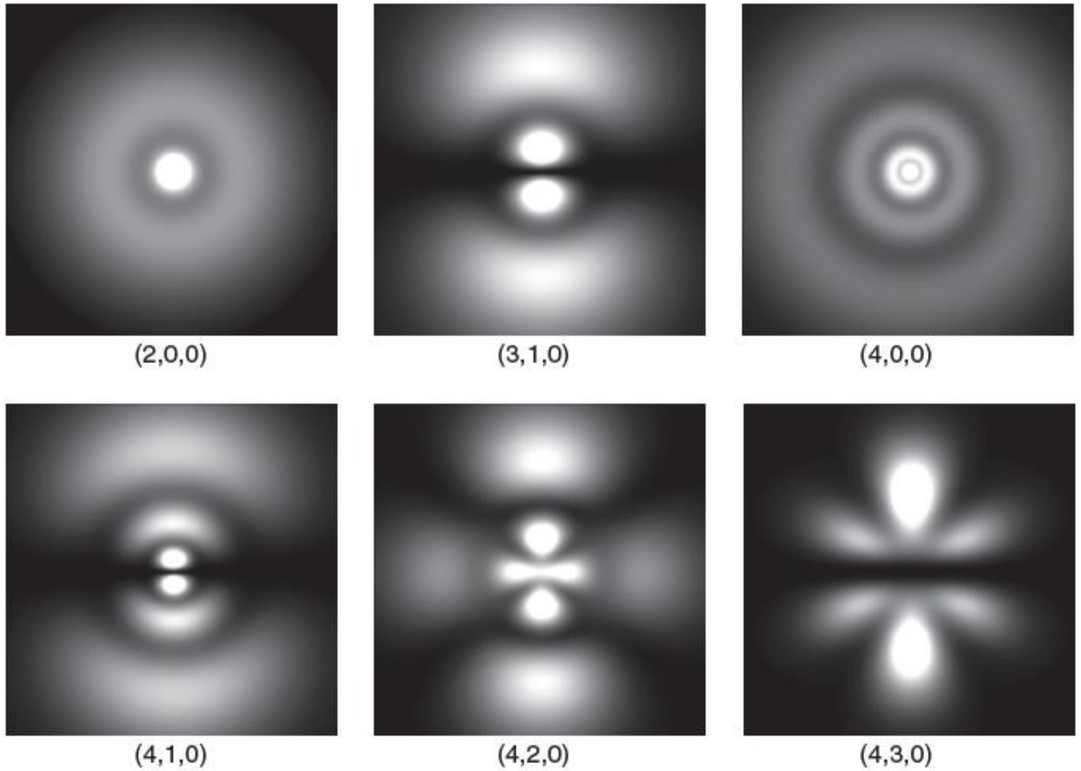
$$R_{41} = \frac{\sqrt{5}}{16\sqrt{3}}a^{-3/2}\left(1-\frac{1}{4}\frac{r}{a}+\frac{1}{80}\left(\frac{r}{a}\right)^2\right)\frac{r}{a}\exp(-r/4a)$$

$$R_{42} = \frac{1}{64\sqrt{5}}a^{-3/2}\left(1-\frac{1}{12}\frac{r}{a}\right)\left(\frac{r}{a}\right)^2\exp(-r/4a)$$

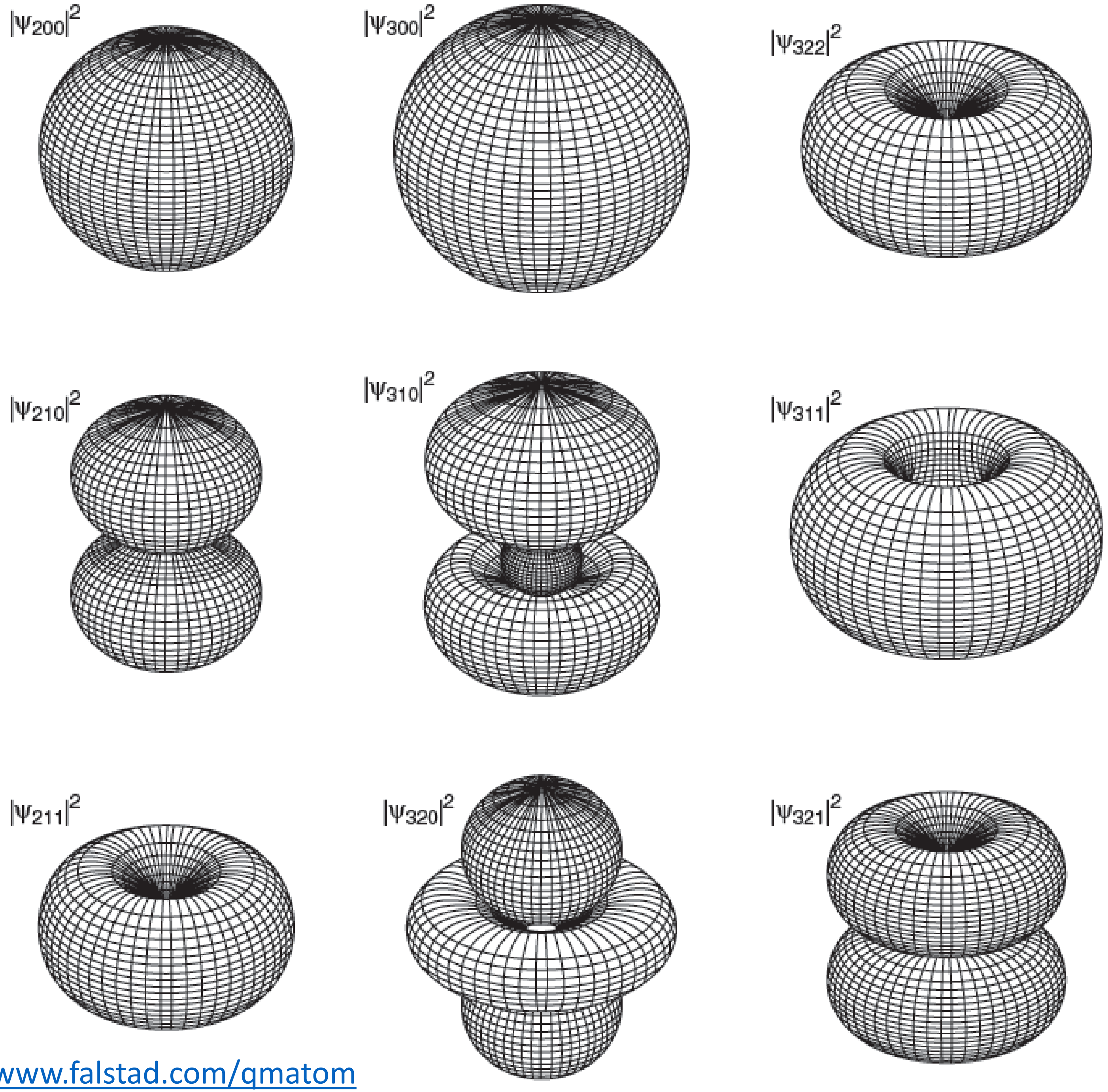
$$R_{43} = \frac{1}{768\sqrt{35}}a^{-3/2}\left(\frac{r}{a}\right)^3\exp(-r/4a)$$

Função de onda do átomo de hidrogênio

$$\psi_{nlm} = \sqrt{\left(\frac{2}{na}\right)^3 \frac{(n-l-1)!}{2n[(n+l)!]^3}}\, e^{-r/na}\left(\frac{2r}{na}\right)^l \left[L^{2l+1}_{n-l-1}(2r/na)\right] Y_l^m(\theta,\phi).$$



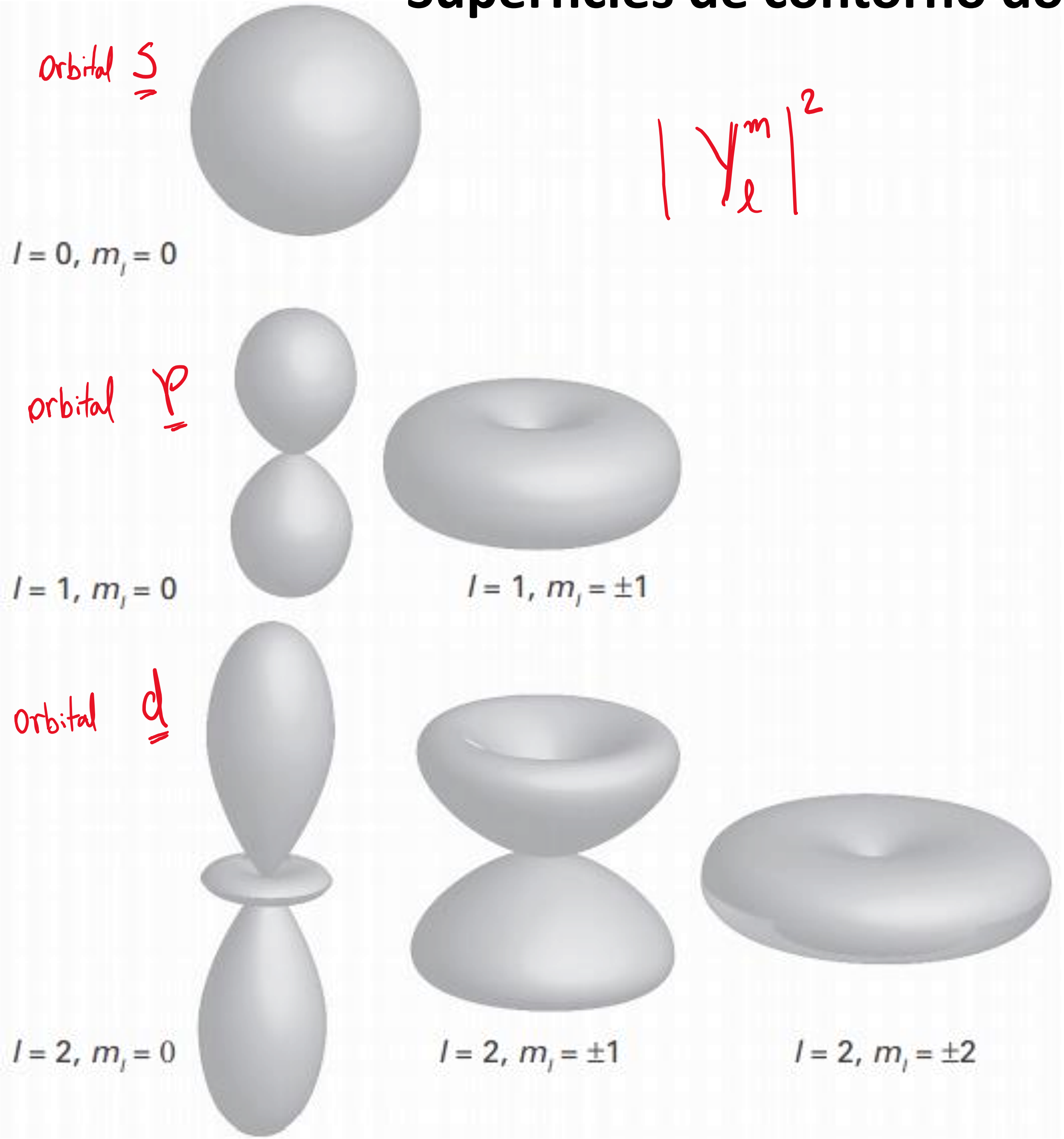
visualização da parte radial
(densidade de probabilidade)

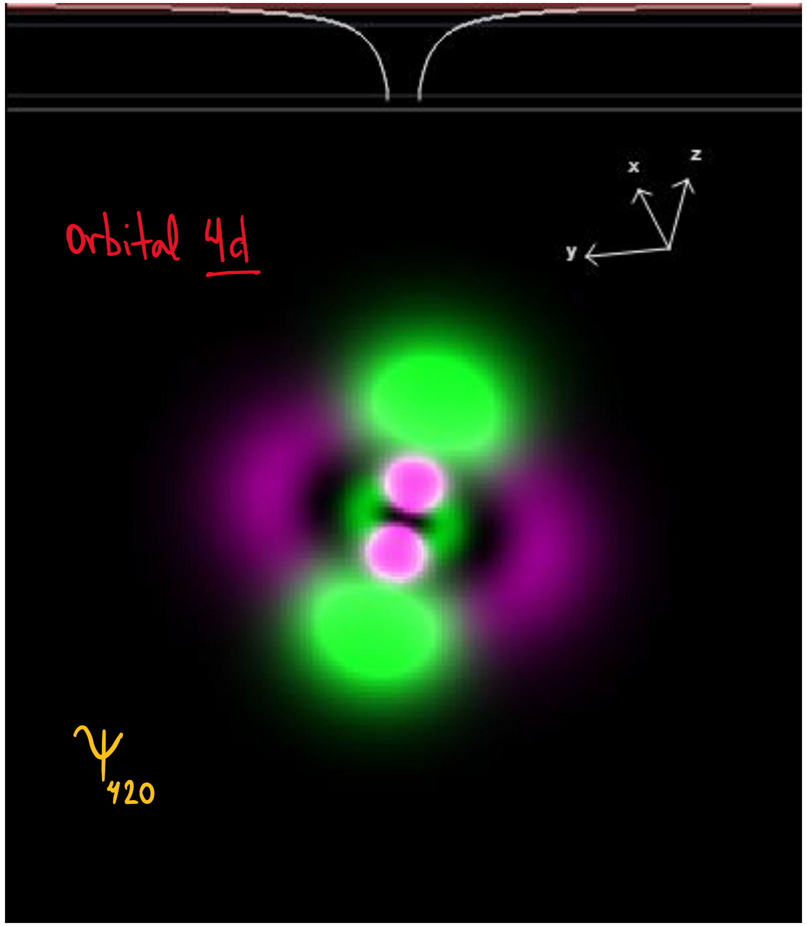


Sugestão: acesse o link para explorar de forma interativa http://www.falstad.com/qmatom

Superfícies de contorno dos orbitais atômicos (1e)

$$\left| Y_l^m \right|^2$$





Sugestão: explore outros orbitais de forma interativa @ http://www.falstad.com/qmatom