

# 5930300 – Química Quântica

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# Átomo de hidrogênio/hidrogenoide

$$\hat{H} = -\frac{\hbar^2}{2\mu} \nabla^2 - \frac{Ze^2}{4\pi\epsilon_0 r}$$

$$\hat{H}\psi_{nlm}(r, \theta, \phi) = E_n\psi_{nlm}(r, \theta, \phi)$$

$$E_n = -\frac{\mu Z^2 e^4}{8\epsilon_0^2 h^2} \frac{1}{n^2}$$

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

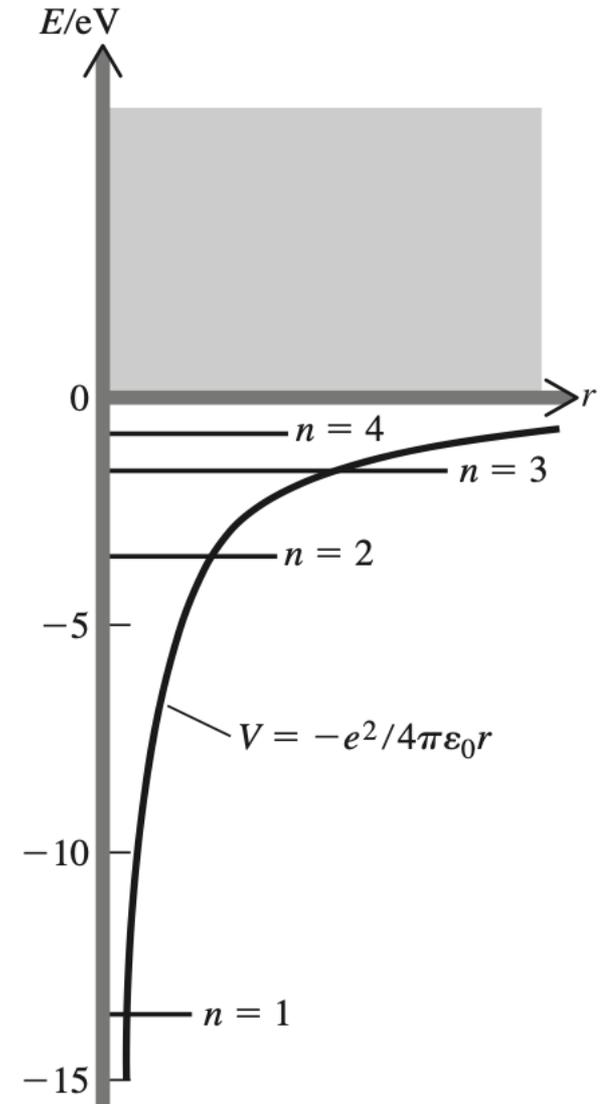
$$\hat{L}^2 \psi_{nlm}(r, \theta, \phi) = l(l+1)\hbar^2 \psi_{nlm}(r, \theta, \phi)$$

$$\hat{L}_z \psi_{nlm}(r, \theta, \phi) = m\hbar \psi_{nlm}(r, \theta, \phi)$$

$$n = 1, 2, 3, \dots$$

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

$$m = -l, -l+1, \dots, l-1, l$$



# Átomo de hidrogênio/hidrogenoide

## Funções de onda

$$\sigma = Zr/a_0$$

$$n = 1, \quad l = 0, \quad m = 0 \quad \psi_{100} = \frac{1}{\sqrt{\pi}} \left( \frac{Z}{a_0} \right)^{3/2} e^{-\sigma}$$

$$n = 2, \quad l = 0, \quad m = 0 \quad \psi_{200} = \frac{1}{\sqrt{32\pi}} \left( \frac{Z}{a_0} \right)^{3/2} (2 - \sigma) e^{-\sigma/2}$$

$$l = 1, \quad m = 0 \quad \psi_{210} = \frac{1}{\sqrt{32\pi}} \left( \frac{Z}{a_0} \right)^{3/2} \sigma e^{-\sigma/2} \cos \theta$$

$$l = 1, \quad m = \pm 1 \quad \psi_{21\pm 1} = \frac{1}{\sqrt{64\pi}} \left( \frac{Z}{a_0} \right)^{3/2} \sigma e^{-\sigma/2} \sin \theta e^{\pm i\phi}$$

# Átomo de hidrogênio/hidrogenoide

## Funções de onda

$$\sigma = Zr/a_0$$

$$\begin{aligned}n = 3, l = 0, m = 0 \quad \psi_{300} &= \frac{1}{81\sqrt{3\pi}} \left(\frac{Z}{a_0}\right)^{3/2} (27 - 18\sigma + 2\sigma^2)e^{-\sigma/3} \\l = 1, m = 0 \quad \psi_{310} &= \frac{1}{81} \left(\frac{2}{\pi}\right)^{1/2} \left(\frac{Z}{a_0}\right)^{3/2} (6\sigma - \sigma^2)e^{-\sigma/3} \cos \theta \\l = 1, m = \pm 1 \quad \psi_{31\pm 1} &= \frac{1}{81\sqrt{\pi}} \left(\frac{Z}{a_0}\right)^{3/2} (6\sigma - \sigma^2)e^{-\sigma/3} \sin \theta e^{\pm i\phi} \\l = 2, m = 0 \quad \psi_{320} &= \frac{1}{81\sqrt{6\pi}} \left(\frac{Z}{a_0}\right)^{3/2} \sigma^2 e^{-\sigma/3} (3 \cos^2 \theta - 1) \\l = 2, m = \pm 1 \quad \psi_{32\pm 1} &= \frac{1}{81\sqrt{\pi}} \left(\frac{Z}{a_0}\right)^{3/2} \sigma^2 e^{-\sigma/3} \sin \theta \cos \theta e^{\pm i\phi} \\l = 2, m = \pm 2 \quad \psi_{32\pm 2} &= \frac{1}{162\sqrt{\pi}} \left(\frac{Z}{a_0}\right)^{3/2} \sigma^2 e^{-\sigma/3} \sin^2 \theta e^{\pm 2i\phi}\end{aligned}$$

# Átomo de hidrogênio/hidrogenoide

## Funções de onda

$$\psi_{nlm}(r, \theta, \phi) = R_{nl}(r)\Theta_{lm}(\theta)\Phi_m(\phi)$$

Notação:  $(n, l, m) \rightarrow nl_m$

$l$	0	1	2	3	4	5
	$s$	$p$	$d$	$f$	$g$	$h$

- $(n = 1, l = 0, m = 0) \rightarrow 1s_0 \rightarrow 1s$
- $(n = 2, l = 0, m = 0) \rightarrow 2s_0 \rightarrow 2s$
- $(n = 2, l = 1, m = -1) \rightarrow 2p_{-1}$
- $(n = 2, l = 1, m = 0) \rightarrow 2p_0$
- $(n = 2, l = 1, m = 1) \rightarrow 2p_1$
- $(n = 3, l = 0, m = 0) \rightarrow 3s_0 \rightarrow 3s$
- $(n = 3, l = 1, m = -1) \rightarrow 3p_{-1}$
- $(n = 3, l = 1, m = 0) \rightarrow 3p_0$
- $(n = 3, l = 1, m = 1) \rightarrow 3p_1$
- $(n = 3, l = 2, m = -2) \rightarrow 3d_{-2}$
- ...

# Átomo de hidrogênio/hidrogenoide

## Soluções da equação de Schrödinger

Combinações lineares de estados degenerados são soluções da eq. de Schrödinger.

$$\begin{aligned}\hat{H}(c_1\psi_1 + c_2\psi_2) &= \hat{H}(c_1\psi_1) + \hat{H}(c_2\psi_2) \\ &= c_1\hat{H}\psi_1 + c_2\hat{H}\psi_2 \\ &= c_1E_1\psi_1 + c_2E_1\psi_2 \\ \hat{H}(c_1\psi_1 + c_2\psi_2) &= E_1(c_1\psi_1 + c_2\psi_2)\end{aligned}$$

# Átomo de hidrogênio/hidrogenoide

## Orbitais reais

$$2p_1 = N e^{-Zr/2a_0} r \sin \theta e^{i\phi}$$

$$2p_{-1} = N e^{-Zr/2a_0} r \sin \theta e^{-i\phi}$$

$$2p_0 = N' e^{-Zr/2a_0} \underbrace{r \cos \theta}_z = 2p_z$$

$$\begin{cases} x = r \sin \theta \cos \phi \\ y = r \sin \theta \sin \phi \\ z = r \cos \theta \end{cases}$$

$2p_x$  e  $2p_y$ ?

$$e^{\pm i\phi} = \cos \phi \pm i \sin \phi$$

$$2p_x \equiv \frac{2p_1 + 2p_{-1}}{\sqrt{2}} \propto x e^{-Zr/2a_0}$$

$$2p_y \equiv \frac{2p_1 - 2p_{-1}}{i\sqrt{2}} \propto y e^{-Zr/2a_0}$$

# Átomo de hidrogênio/hidrogenoide

## Orbitais reais

$$\psi_{1s} = \frac{1}{\sqrt{\pi}} \left( \frac{Z}{a_0} \right)^{3/2} e^{-\sigma}$$

$$\sigma = Zr/a_0$$

$$\psi_{2s} = \frac{1}{4\sqrt{2\pi}} \left( \frac{Z}{a_0} \right)^{3/2} (2 - \sigma)e^{-\sigma/2}$$

$$\psi_{2p_z} = \frac{1}{4\sqrt{2\pi}} \left( \frac{Z}{a_0} \right)^{3/2} \sigma e^{-\sigma/2} \cos \theta$$

$$\psi_{2p_x} = \frac{1}{4\sqrt{2\pi}} \left( \frac{Z}{a_0} \right)^{3/2} \sigma e^{-\sigma/2} \text{sen } \theta \cos \phi$$

$$\psi_{2p_y} = \frac{1}{4\sqrt{2\pi}} \left( \frac{Z}{a_0} \right)^{3/2} \sigma e^{-\sigma/2} \text{sen } \theta \text{sen } \phi$$

# Átomo de hidrogênio/hidrogenoide

## Orbitais reais

$$\psi_{3s} = \frac{1}{81\sqrt{3\pi}} \left( \frac{Z}{a_0} \right)^{3/2} (27 - 18\sigma + 2\sigma^2) e^{-\sigma/3} \quad \sigma = Zr/a_0$$

$$\psi_{3p_z} = \frac{\sqrt{2}}{81\sqrt{\pi}} \left( \frac{Z}{a_0} \right)^{3/2} \sigma(6 - \sigma) e^{-\sigma/3} \cos \theta$$

$$\psi_{3p_x} = \frac{\sqrt{2}}{81\sqrt{\pi}} \left( \frac{Z}{a_0} \right)^{3/2} \sigma(6 - \sigma) e^{-\sigma/3} \text{sen } \theta \cos \phi$$

$$\psi_{3p_y} = \frac{\sqrt{2}}{81\sqrt{\pi}} \left( \frac{Z}{a_0} \right)^{3/2} \sigma(6 - \sigma) e^{-\sigma/3} \text{sen } \theta \text{sen } \phi$$

# Átomo de hidrogênio/hidrogenoide

## Orbitais reais

$$\psi_{3d_{z^2}} = \frac{1}{81\sqrt{6\pi}} \left( \frac{Z}{a_0} \right)^{3/2} \sigma^2 e^{-\sigma/3} (3 \cos^2 \theta - 1) \quad \sigma = Zr/a_0$$

$$\psi_{3d_{xz}} = \frac{\sqrt{2}}{81\sqrt{\pi}} \left( \frac{Z}{a_0} \right)^{3/2} \sigma^2 e^{-\sigma/3} \sin \theta \cos \theta \cos \phi$$

$$\psi_{3d_{yz}} = \frac{\sqrt{2}}{81\sqrt{\pi}} \left( \frac{Z}{a_0} \right)^{3/2} \sigma^2 e^{-\sigma/3} \sin \theta \cos \theta \sin \phi$$

$$\psi_{3d_{x^2-y^2}} = \frac{1}{81\sqrt{2\pi}} \left( \frac{Z}{a_0} \right)^{3/2} \sigma^2 e^{-\sigma/3} \sin^2 \theta \cos 2\phi$$

$$\psi_{3d_{xy}} = \frac{1}{81\sqrt{2\pi}} \left( \frac{Z}{a_0} \right)^{3/2} \sigma^2 e^{-\sigma/3} \sin^2 \theta \sin 2\phi$$

# Átomo de hidrogênio/hidrogenoide

## Visualizando orbitais reais

$$\begin{aligned}\psi_{2p_z} &= \frac{1}{4\sqrt{2\pi}} \left( \frac{Z}{a_0} \right)^{3/2} \sigma e^{-\sigma/2} \cos \theta & \sigma &= Zr/a_0 \\ &= \frac{1}{4\sqrt{2\pi}} \left( \frac{Z}{a_0} \right)^{3/2} \frac{Zr}{a_0} e^{-Zr/2a_0} \cos \theta & Z &= 1 \\ &= \frac{1}{4\sqrt{2\pi}} \left( \frac{1}{a_0} \right)^{3/2} \frac{r \cos \theta}{a_0} e^{-r/2a_0} & r &= (x^2 + y^2 + z^2)^{1/2} \\ & & z &= r \cos \theta \\ &= \frac{1}{4\sqrt{2\pi}} \left( \frac{1}{a_0} \right)^{3/2} \frac{z}{a_0} e^{-(x^2+y^2+z^2)^{1/2}/2a_0} & \text{No plano } yz, x &= 0\end{aligned}$$
$$\psi_{2p_z}(x = 0, y, z) = \frac{1}{4\sqrt{2\pi}} \left( \frac{1}{a_0} \right)^{3/2} \frac{z}{a_0} e^{-(y^2+z^2)^{1/2}/2a_0}$$

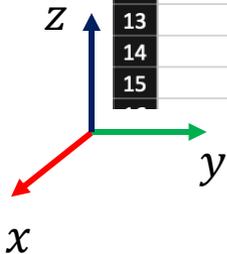
# Átomo de hidrogênio/hidrogenoide

## Visualizando orbitais reais

$$\psi_{2p_z}(x = 0, y, z) = \frac{1}{4\sqrt{2\pi}} \left( \frac{1}{a_0} \right)^{3/2} \frac{z}{a_0} e^{-(y^2+z^2)^{1/2}/2a_0}$$

$$=(1/(4*RAIZ(2*PI())))*\$A2*EXP(-RAIZ(B\$1^2 + \$A2^2)/2)$$

	A	B	C	D	E	F
1	z/y	-5,0	-4,9	...		
2	5,0					
3	4,9					
4	...					
5						
6						
7						
8						
9						
10						
11						
12						
13						
14						
15						



- Valores de z na coluna A (\$A2)
- Valores de y na linha 1 (B\$1)
- Cada célula com o valor da função/orbital

# Átomo de hidrogênio/hidrogenoide

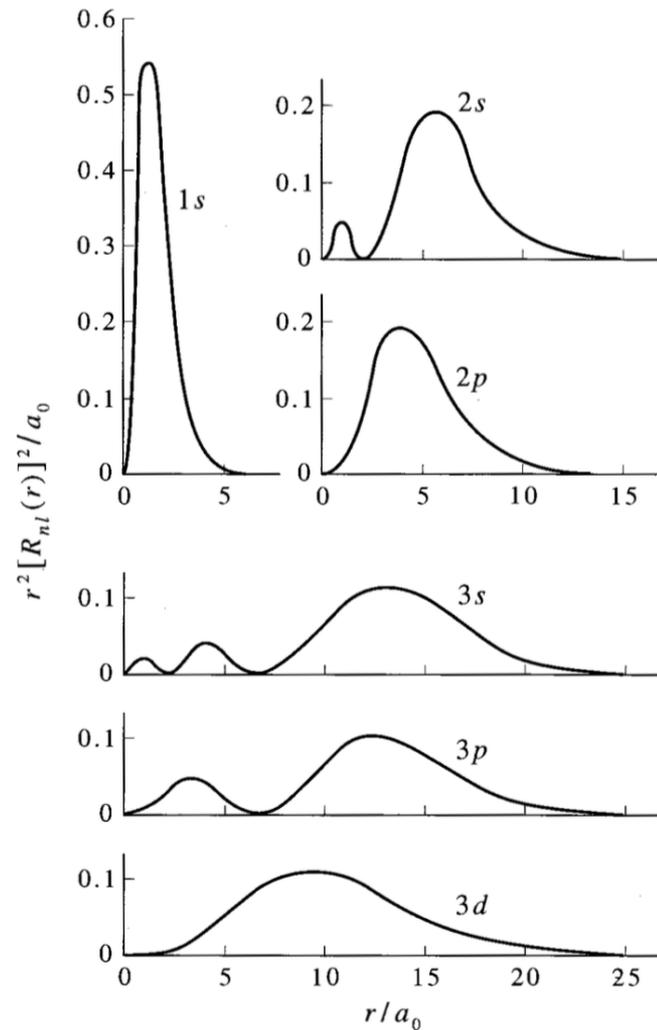
## Densidades de probabilidade radial

$$\begin{aligned}\text{Pr}(r \rightarrow r + dr) &= \int_0^{2\pi} \int_0^\pi |\psi|^2 r^2 dr \text{sen } \theta d\theta d\phi \\ &= |R_{nl}(r)|^2 r^2 dr \int_0^{2\pi} \int_0^\pi |\Theta_{lm}(\theta)|^2 |\Phi_m(\phi)|^2 \text{sen } \theta d\theta d\phi \\ &= |R_{nl}(r)|^2 r^2 dr\end{aligned}$$

# Átomo de hidrogênio/hidrogenoide

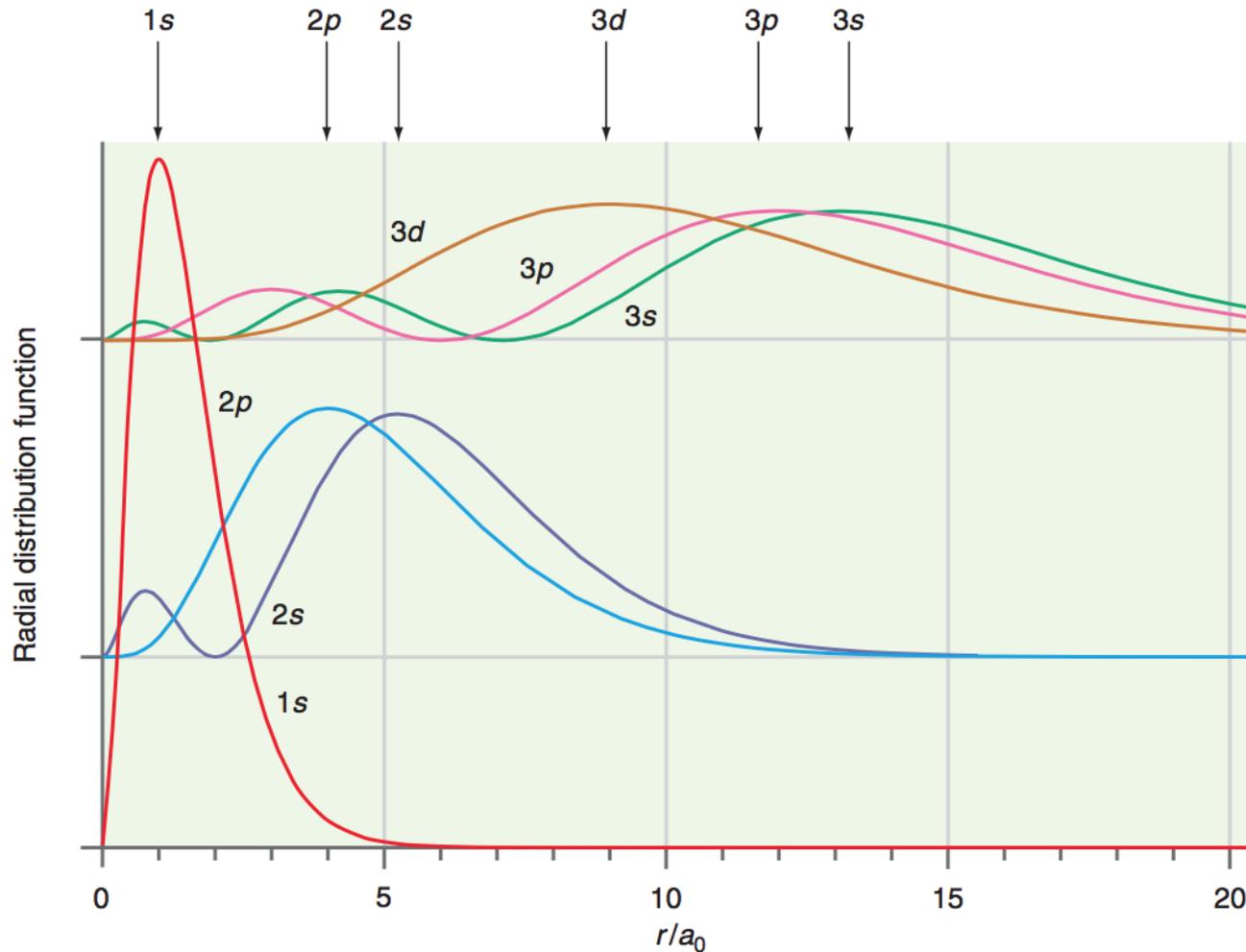
## Densidades de probabilidade radial

$$\text{Pr}(r \rightarrow r + dr) = |R_{nl}(r)|^2 r^2 dr$$



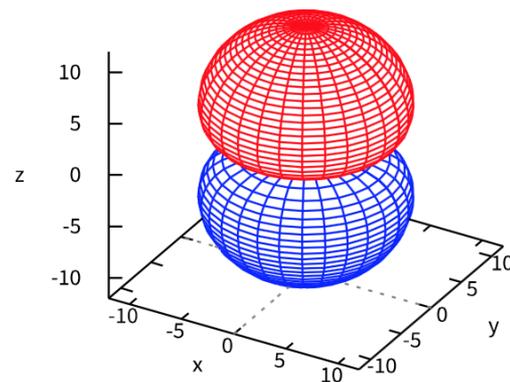
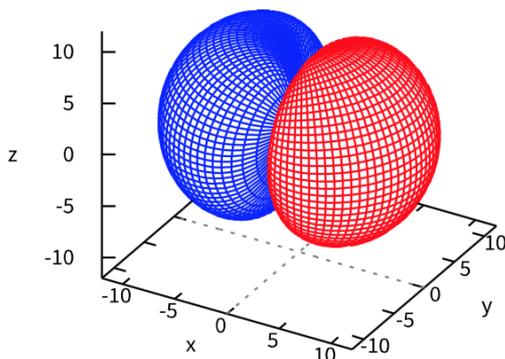
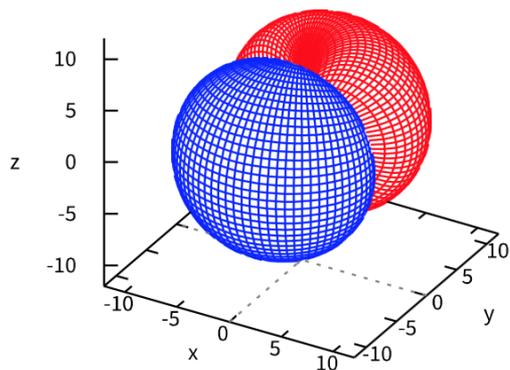
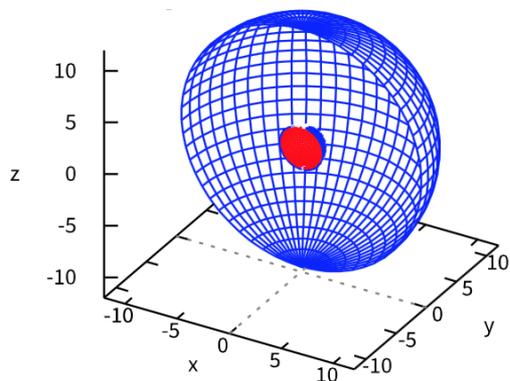
# Átomo de hidrogênio/hidrogenoide

## Densidades de probabilidade radial



# Átomo de hidrogênio/hidrogenoide

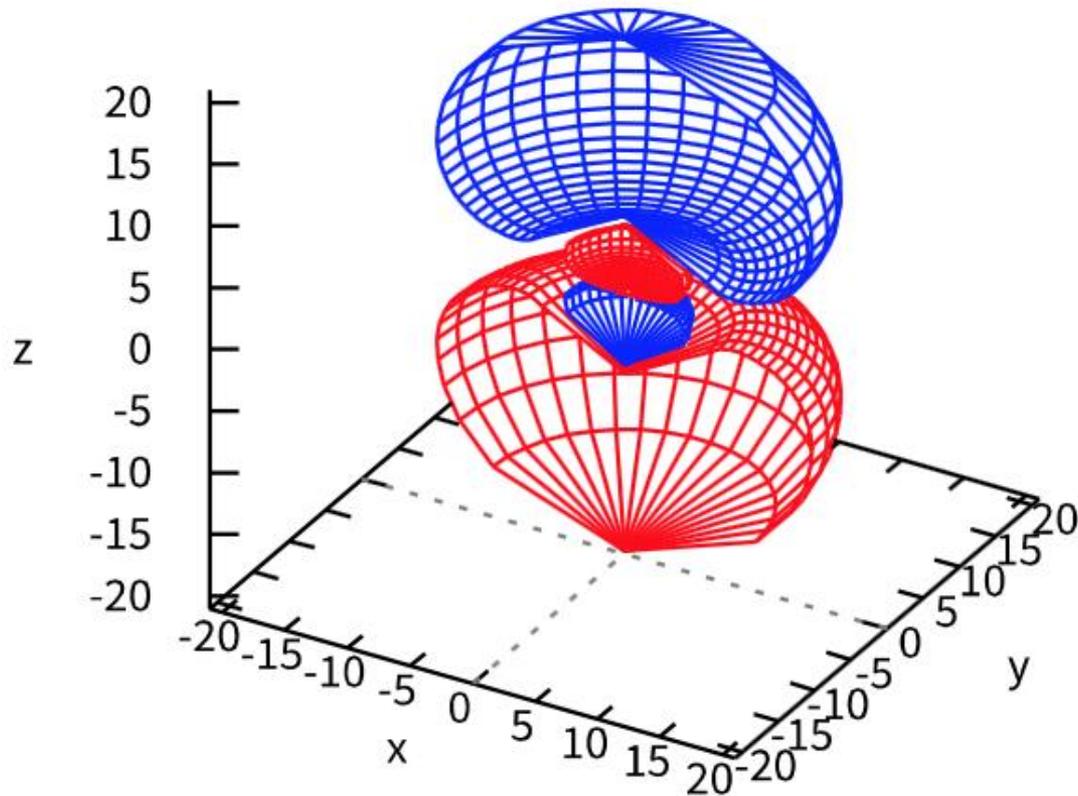
## Isosuperfícies – $n = 2$



*J. Chem. Educ.* 2014, 91, 10, 1739–1741 (<https://doi.org/10.1021/ed500470q>)

# Átomo de hidrogênio/hidrogenoide

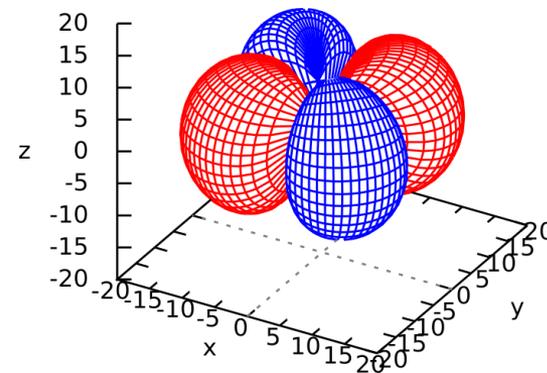
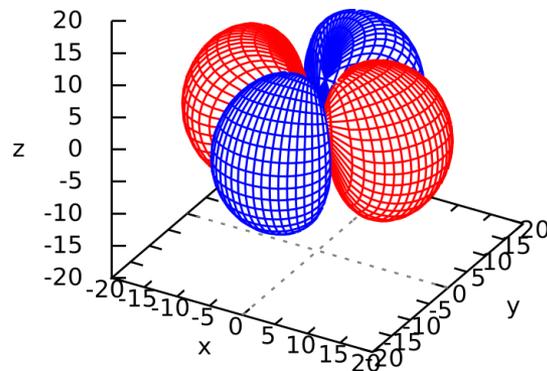
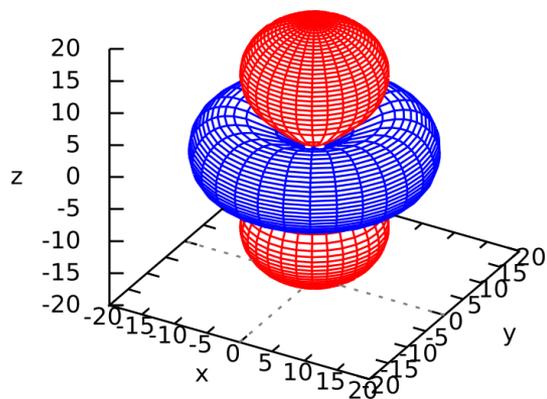
## Isosuperfícies – $3p_z$



*J. Chem. Educ.* 2014, 91, 10, 1739–1741 (<https://doi.org/10.1021/ed500470q>)

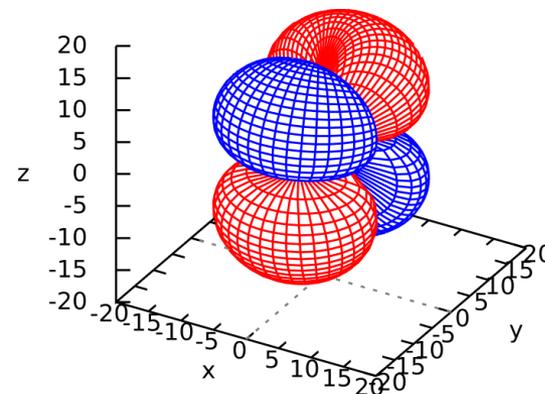
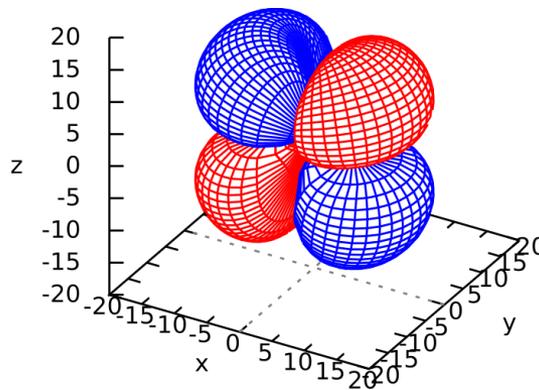
# Átomo de hidrogênio/hidrogenoide

## Isosuperfícies – 3d



$3d_{z^2}, 3d_{x^2-y^2}, 3d_{xy}$

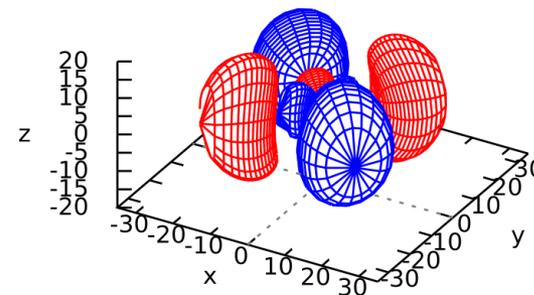
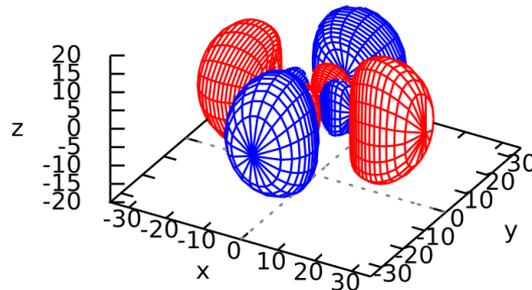
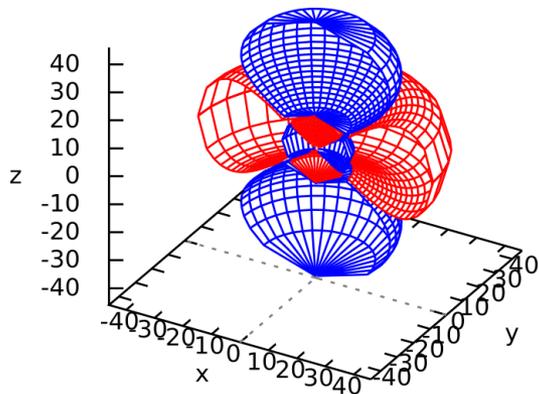
$3d_{yz}, 3d_{xz}$



*J. Chem. Educ.* 2014, 91, 10, 1739–1741 (<https://doi.org/10.1021/ed500470q>)

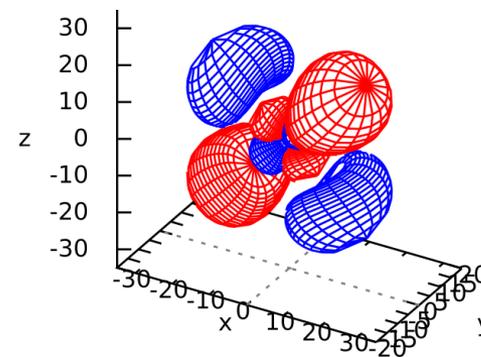
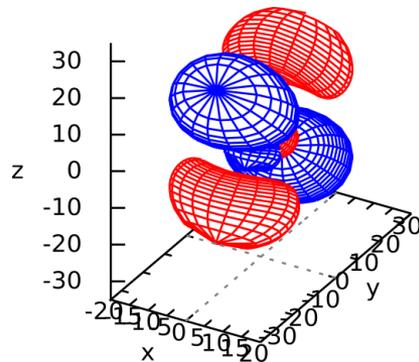
# Átomo de hidrogênio/hidrogenoide

## Isosuperfícies – $4d$



$$4d_{z^2}, 4d_{x^2-y^2}, 4d_{xy}$$

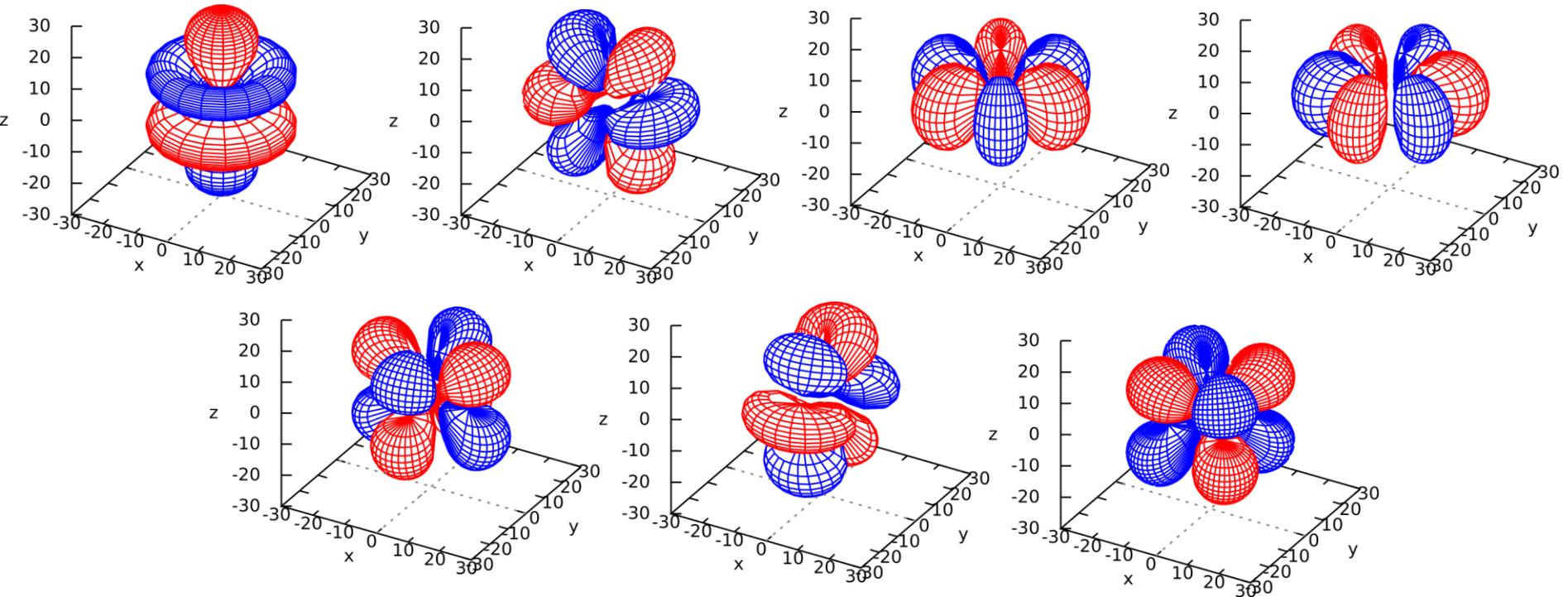
$$4d_{yz}, 4d_{xz}$$



*J. Chem. Educ.* 2014, 91, 10, 1739–1741 (<https://doi.org/10.1021/ed500470q>)

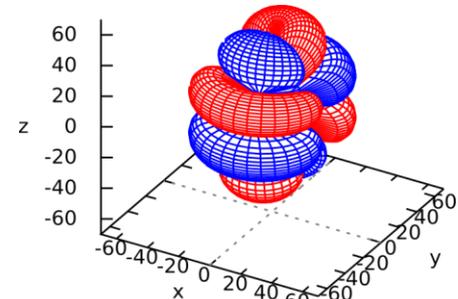
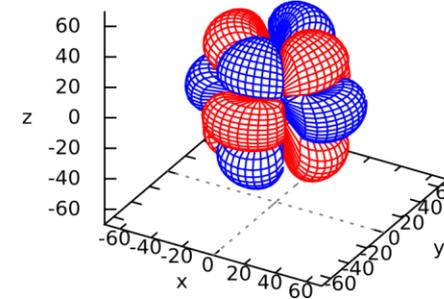
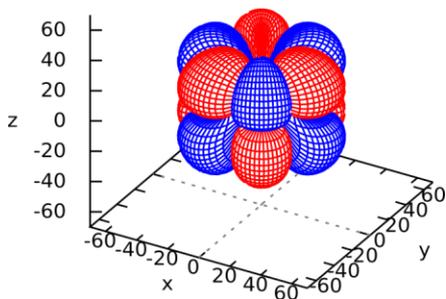
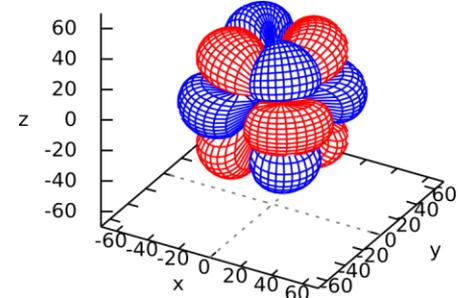
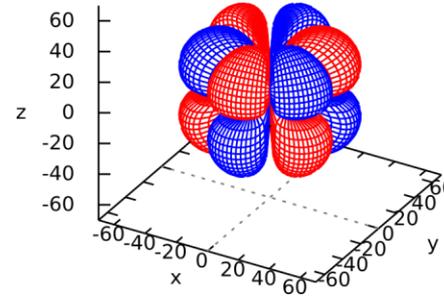
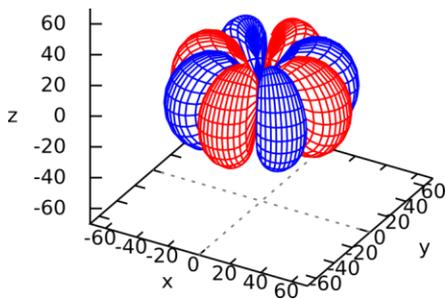
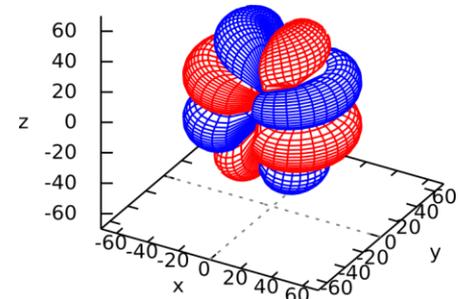
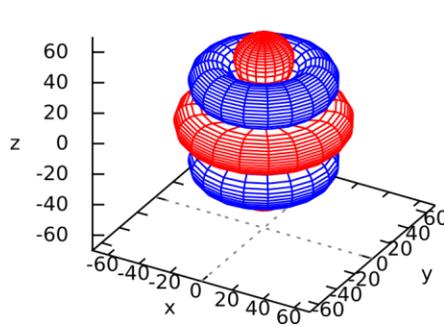
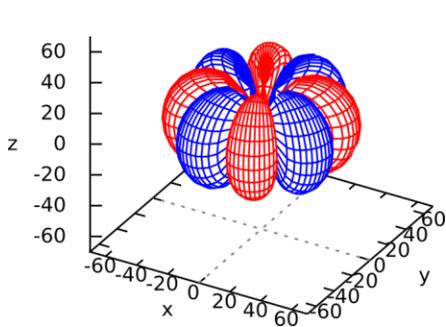
# Átomo de hidrogênio/hidrogenoide

## Isosuperfícies – $4f$



# Átomo de hidrogênio/hidrogenoide

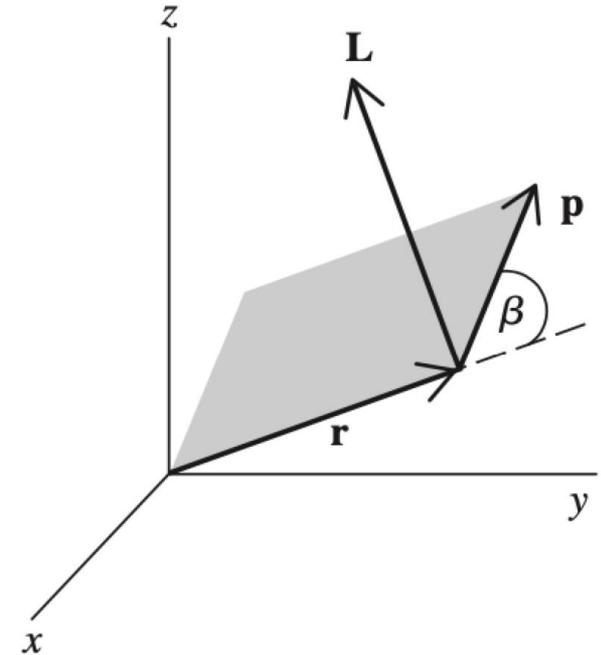
## Isosuperfícies – $5g$



# Momento angular ( $\vec{L}$ )

- Quantidade conservada no movimento orbital
- Quantizado em mecânica quântica (associado a número quântico)

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



# Momento angular

## Magnitude $|\vec{L}|$

$$\hat{L}^2 \psi_{nlm} = l(l+1)\hbar^2 \psi_{nlm} \quad l(l+1)\hbar^2 \text{ é o autovalor de } \hat{L}^2 \text{ para o estado } \psi_{nlm}.$$

Para o estado  $1s$  ( $\psi_{100}$ ):  $l = 0$

$$\hat{L}^2 \psi_{100} = 0(0+1)\hbar^2 \psi_{100}$$
$$|L|^2 = 0$$

$$|L| = 0$$

Para o estado  $2s$  ( $\psi_{200}$ ):  $l = 0$

$$|L| = 0$$

Para o estado  $2p_0$  ( $\psi_{210}$ ):  $l = 1$

$$\hat{L}^2 \psi_{210} = 1(1+1)\hbar^2 \psi_{210}$$
$$= 2\hbar^2 \psi_{210}$$

$$|L|^2 = 2\hbar^2$$

$$|L| = \sqrt{2}\hbar$$

# Momento angular

## Magnitude $|\vec{L}|$

$$\hat{L}^2 \psi_{nlm} = l(l+1)\hbar^2 \psi_{nlm}$$

$$|L| = \sqrt{l(l+1)}\hbar$$

- Para estados *s* ( $l = 0$ ):  $|L| = 0$ .
- Para estados *p* ( $l = 1$ ):  $|L| = \sqrt{2}\hbar$ .
- Para estados *d* ( $l = 2$ ):  $|L| = \sqrt{6}\hbar$ .
- Para estados *f* ( $l = 3$ ):  $|L| = \sqrt{12}\hbar$ .

# Momento angular

## Orientação $L_z$

$$\hat{L}_z \psi_{nlm} = m\hbar \psi_{nlm}$$

$m\hbar$  é o autovalor de  $\hat{L}_z$  para o estado  $\psi_{nlm}$ .

Para o estado  $2s$  ( $\psi_{200}$ ):  $m = 0$   $\hat{L}_z \psi_{200} = 0\hbar \psi_{200}$   
 $L_z = 0$

Para o estado  $2p_1$  ( $\psi_{211}$ ):  $m = 1$   $\hat{L}_z \psi_{211} = 1\hbar \psi_{211}$   
 $L_z = \hbar$

Para o estado  $2p_0$  ( $\psi_{210}$ ):  $m = 0$   $\hat{L}_z \psi_{210} = 0\hbar \psi_{210}$   
 $L_z = 0$

Para o estado  $2p_{-1}$  ( $\psi_{21-1}$ ):  $m = -1$   $\hat{L}_z \psi_{21-1} = -1\hbar \psi_{21-1}$   
 $L_z = -\hbar$

# Momento angular

Magnitude  $|\vec{L}|$  e orientação  $L_z$

$$\hat{L}^2 \psi_{nlm} = l(l+1)\hbar^2 \psi_{nlm}$$

$$|L| = \sqrt{l(l+1)}\hbar$$

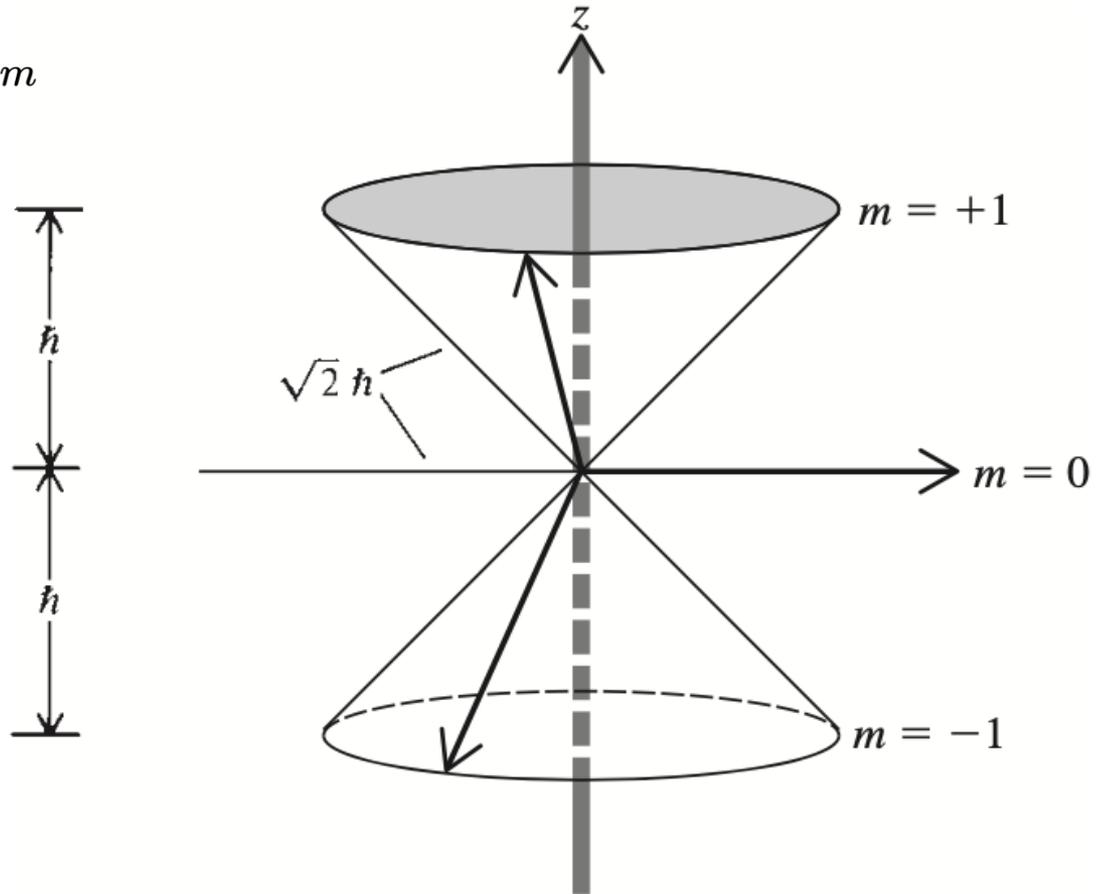
$$\hat{L}_z \psi_{nlm} = m\hbar \psi_{nlm}$$

$$L_z = m\hbar$$

Para estados  $2p$ :

$$|L| = \sqrt{2}\hbar$$

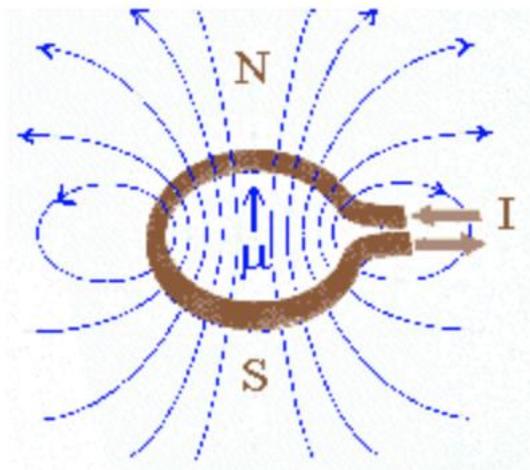
$$L_z = \begin{cases} \hbar \\ 0 \\ -\hbar \end{cases}$$



# Momento angular

## Número quântico magnético ( $m$ )

- Partícula carregada eletricamente em movimento equivale a uma corrente elétrica.
- Corrente elétrica numa curva fechada gera campo magnético equivalente a um ímã (dipolo magnético,  $\mu$ )



# Momento angular

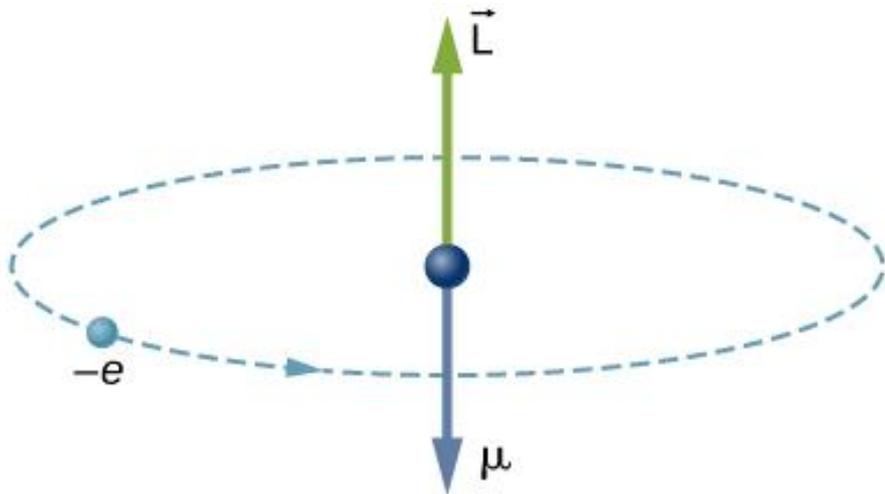
## Número quântico magnético ( $m$ )

Do eletromagnetismo:

$$\vec{\mu}_l = q \frac{\vec{v} \times \vec{r}}{2}$$

$$= q \frac{\vec{L}}{2m}$$

$$= -\frac{e\vec{L}}{2m_e}$$



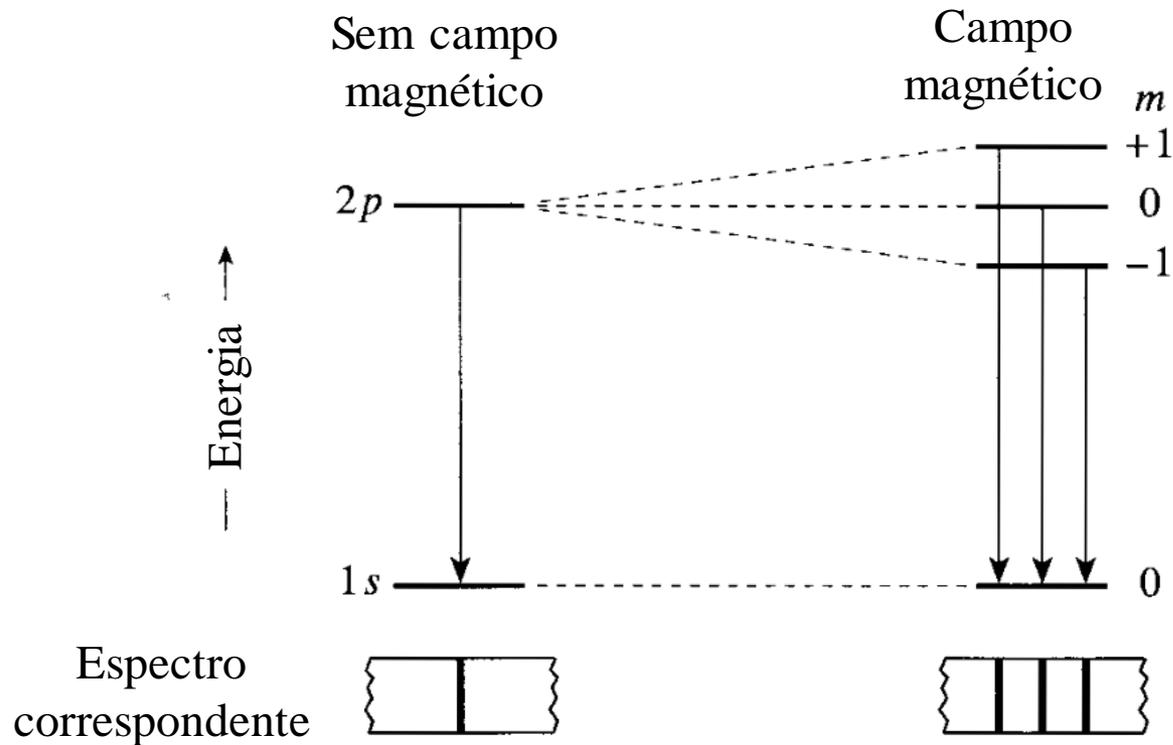
# Momento angular

## Número quântico magnético ( $m$ )

- O movimento orbital dos elétrons gera um campo magnético.
- Na presença de um campo magnético externo, o momento magnético orbital interage com o campo.
- A magnitude da interação depende do número quântico magnético,  $m$ .

# Momento angular

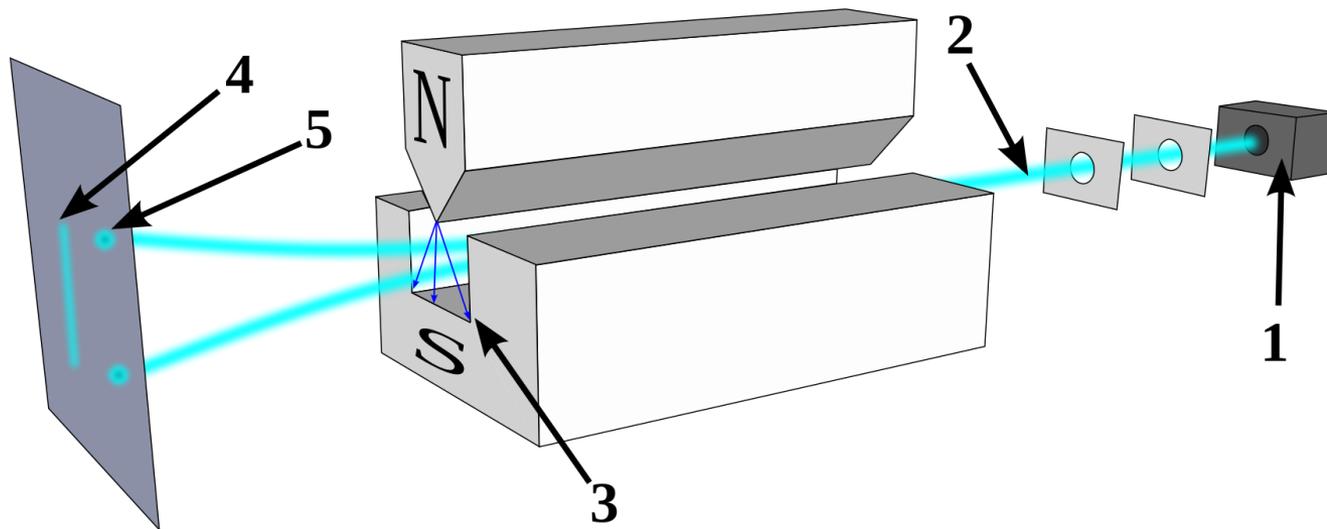
## Número quântico magnético ( $m$ )



$$\text{Efeito Zeeman: } \Delta E \propto m$$

# Spin eletrônico

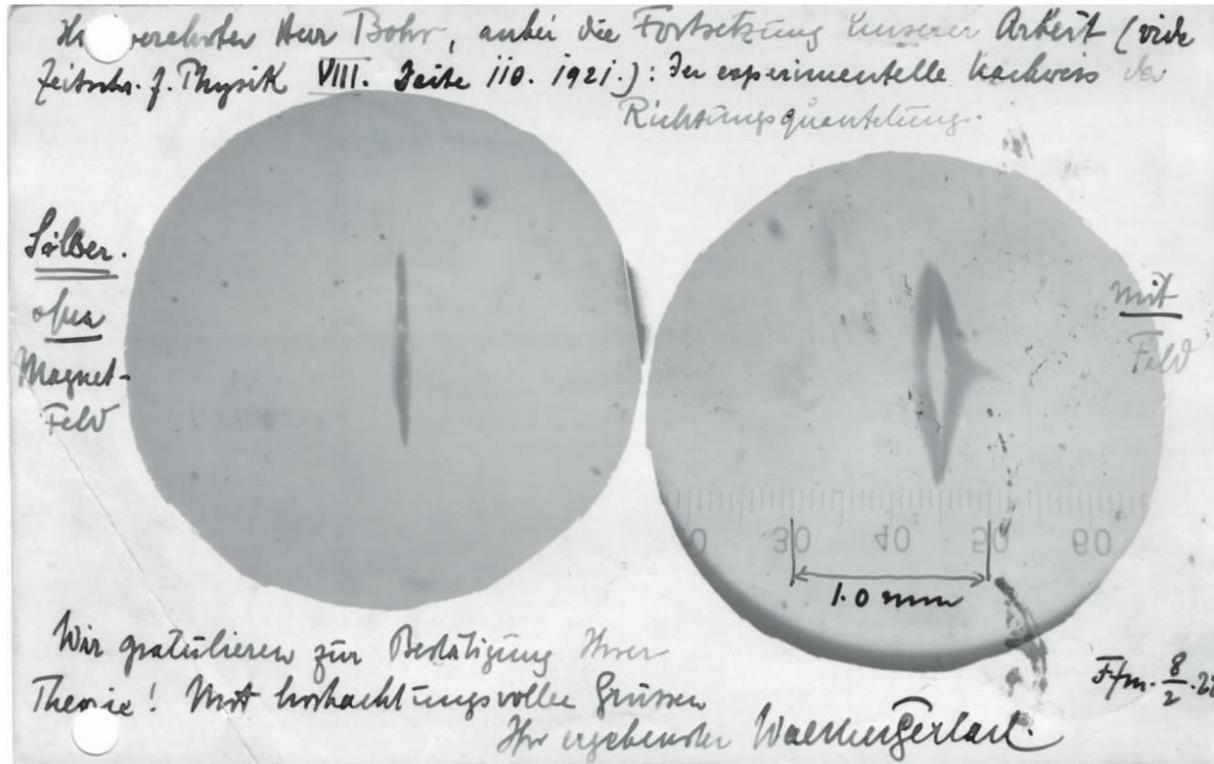
## Experimento de Stern–Gerlach



1. Forno
2. Feixe de átomos de prata
3. Campo magnético não homogêneo
4. Resultado esperado classicamente (distribuição contínua)
5. Resultado observado

# Spin eletrônico

## Experimento de Stern–Gerlach



- Dois componentes.
- Discretização.
- Comportamento quântico.

# Spin eletrônico

## Experimento de Stern–Gerlach

Poderia ser o momento angular orbital o responsável pelo desdobramento?

- Se  $l = 0$ ,  $m = 0$ , sem desdobramento.
- Se  $l = 1$ ,  $m = 1, 0, -1$ , três componentes.
- Se  $l = 1$ ,  $m = 2, 1, 0, -1, -2$ , cinco componentes.
- Para momento angular orbital  $l$ , há  $2l + 1$  componentes.

Configuração eletrônica Ag:  $[\text{Kr}]4d^{10}5s^1$ .

# Spin eletrônico

## Experimento de Stern–Gerlach

Poderia ser a “rotação do elétron” a responsável pelo desdobramento?

$$\vec{\mu} = q \frac{\vec{L}}{2m} = \frac{-e}{2m_e} \vec{r}_e \times \vec{p} = -\frac{e}{2m_e} \vec{r}_e \times m_e \vec{v} = -\frac{e \vec{r}_e \times \vec{v}}{2}$$

$$|\mu_s| = \frac{e r_e v}{2}$$

$$|\mu_s| = 9,284\,764\,7043(28) \times 10^{-24} \text{ J T}^{-1} \quad (\text{Medido experimentalmente})$$

Qual deve ser a velocidade de rotação do elétron para produzir esse momento magnético?

$$v = \frac{2|\mu_s|}{e r_e}$$

# Spin eletrônico

## Experimento de Stern–Gerlach

Qual deve ser a velocidade de rotação do elétron para produzir esse momento magnético?

$$v = \frac{2|\mu_s|}{e r_e}$$

Qual é o raio do elétron?

$$r_e < 10^{-22} \text{ m}$$

$$v > \frac{2 \times (9 \times 10^{-24} \text{ J T}^{-1})}{(2 \times 10^{-19} \text{ C}) \times (10^{-22} \text{ m})}$$

$$v > 9 \times 10^{17} \text{ m s}^{-1} \gg c \approx 3 \times 10^8 \text{ m s}^{-1}$$

H. Dehmelt, Experiments on the Structure of an Individual Elementary Particle. *Science* **247**, 539–545 (1990).

# Spin eletrônico

- Momento angular intrínseco sem análogo clássico.
- Definitivamente não é rotação.
- Introduzido na mecânica quântica (não-relativística) como postulado.

# Spin eletrônico

Os números quânticos de spin ( $s$  e  $m_s$ ) são análogos aos números quânticos de momento angular orbital ( $l$  e  $m_l$ ).

$l \rightarrow 2l + 1$  componentes

$s \rightarrow 2s + 1$  componentes

$$2s + 1 = 2$$

Experimento de Stern–Gerlach

$$s = \frac{1}{2} \quad m_s = \begin{cases} +\frac{1}{2} \\ -\frac{1}{2} \end{cases} \quad \text{para o elétron.}$$

# Spin eletrônico

$$|S| = [s(s + 1)]^{1/2} \hbar$$

$$S_z = m_s \hbar \quad m_s = -s, -s + 1, \dots, s - 1, s$$

$$s = \frac{1}{2} \quad m_s = \begin{cases} +\frac{1}{2} \\ -\frac{1}{2} \end{cases} \quad \text{para o elétron.}$$

# Spin eletrônico

Duas funções de spin:

$$\alpha = \alpha(\omega)$$

$$\beta = \beta(\omega)$$

$\omega$  é a variável de spin. Só o operador de spin opera sobre ela.

$$\begin{aligned}\hat{S}^2 \alpha(\omega) &= s(s+1)\hbar^2 \alpha(\omega) \\ &= \frac{3}{4}\hbar^2 \alpha(\omega)\end{aligned}$$

$$\begin{aligned}\hat{S}^2 \beta(\omega) &= s(s+1)\hbar^2 \beta(\omega) \\ &= \frac{3}{4}\hbar^2 \beta(\omega)\end{aligned}$$

$$\begin{aligned}\hat{S}_z \alpha(\omega) &= m_s \hbar \alpha(\omega) \\ &= +\frac{1}{2}\hbar \alpha(\omega)\end{aligned}$$

$$\begin{aligned}\hat{S}_z \beta(\omega) &= m_s \hbar \beta(\omega) \\ &= -\frac{1}{2}\hbar \beta(\omega)\end{aligned}$$

# Spin eletrônico

Para incluir o spin nas funções de onda, multiplicamos a função espacial  $(x, y, z)$  pela função de spin.

$$\Psi(x, y, z, \omega) = \begin{cases} \psi_{nlm_l}(x, y, z)\alpha(\omega) \\ \psi_{nlm_l}(x, y, z)\beta(\omega) \end{cases}$$

↓  
spin-orbital

↓                      ↓  
orbital                  função de spin

# Spin eletrônico

- Parte espacial: 3 variáveis → 3 números quântico
- Parte de spin: 1 variável → 1 número quântico

$$\Psi_{nlm_l m_s}(x, y, z, \omega)$$

São necessários 4 números quânticos para especificar completamente o estado de um elétron no átomo de hidrogênio.