

4300375 - Física moderna I

# **Aula 12 – Física atômica: O átomo de hidrogênio**

parte 2

# Nesta aula...

- Terminaremos de resolver a equação de Schrödinger para o átomo de hidrogênio:
  - A solução da parte radial
  - A quantização da energia
  - Níveis de energia e linhas de emissão
  - O átomo de Schrödinger

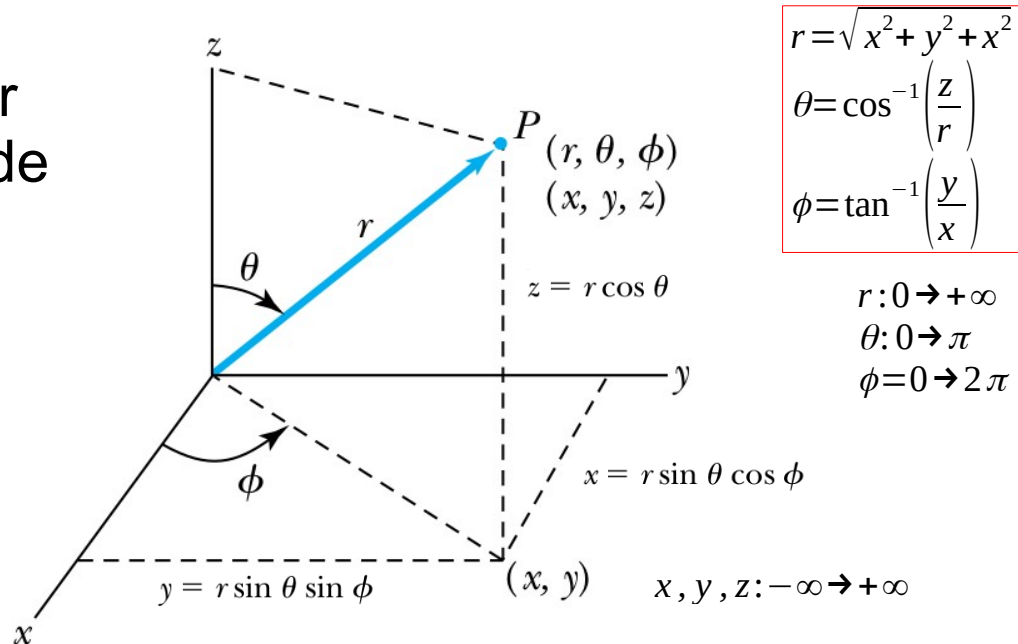
# As equações desacopladas

- Temos agora, de abordar as equações desacopladas para obter a solução completa para o átomo de hidrogênio!

$$\frac{1}{R(r)} \frac{d}{dr} \left( r^2 \frac{dR(r)}{dr} \right) + \frac{2mr^2}{\hbar^2} [E - V(r)] = C_1$$

$$-C_1 \cdot \sin^2 \theta - \frac{\sin \theta}{f(\theta)} \frac{d}{d\theta} \left( \sin \theta \frac{df(\theta)}{d\theta} \right) = C_2$$

$$\frac{1}{g(\phi)} \frac{d^2 g(\phi)}{d\phi^2} = C_2$$



$$V(r, \theta, \phi) = -\frac{K}{r} \quad \text{Potencial Coulombiano}$$

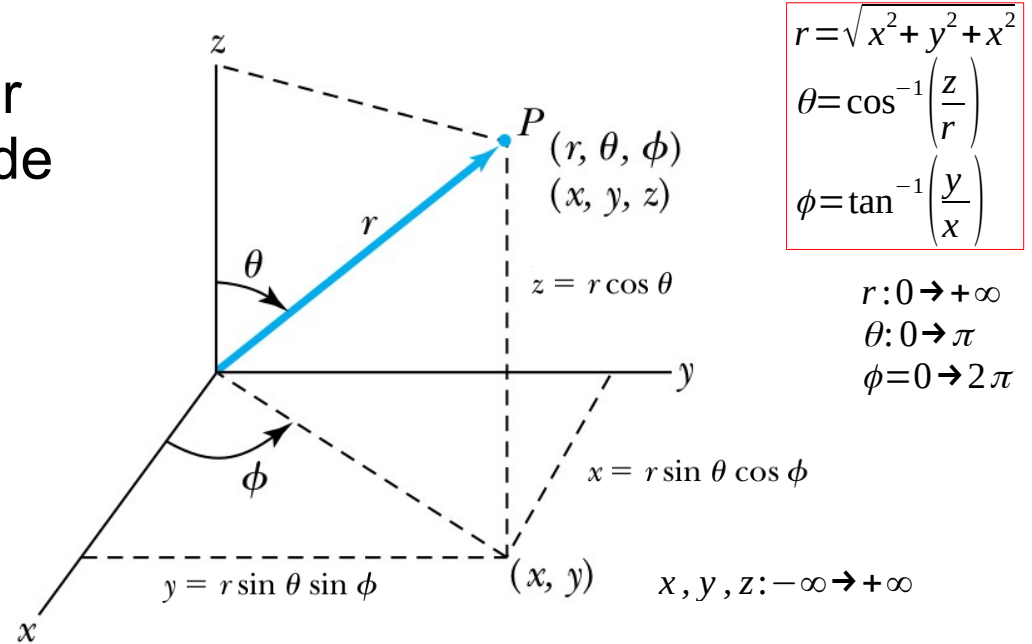
# As equações desacopladas

- Temos agora, de abordar as equações desacopladas para obter a solução completa para o átomo de hidrogênio!

$$\frac{1}{R(r)} \frac{d}{dr} \left( r^2 \frac{dR(r)}{dr} \right) + \frac{2mr^2}{\hbar^2} [E - V(r)] = C_1$$

$$f_{lm}(\theta) = \frac{(\sin \theta)^{|m|}}{2^l l!} \left[ \frac{d}{d(\cos \theta)} \right]^{l+|m|} (\cos^2 \theta - 1)^l$$

$$g(\phi) = e^{-im\phi}$$



$$V(r, \theta, \phi) = -\frac{K}{r} \quad \text{Potencial Coulombiano}$$

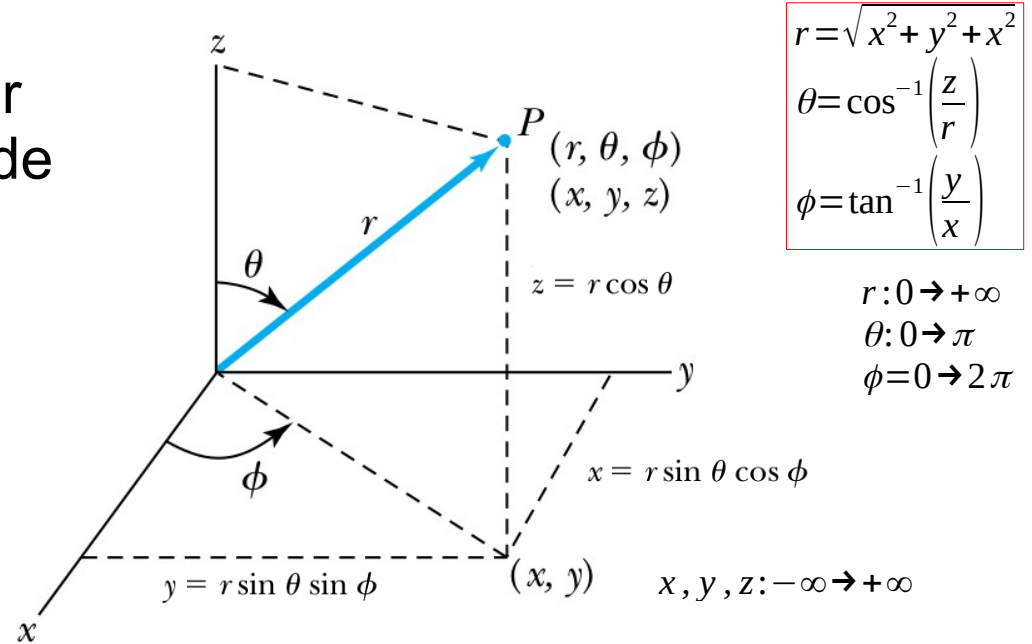
# As equações desacopladas

- Temos agora, de abordar as equações desacopladas para obter a solução completa para o átomo de hidrogênio!

$$\frac{1}{R(r)} \frac{d}{dr} \left( r^2 \frac{dR(r)}{dr} \right) + \frac{2mr^2}{\hbar^2} [E - V(r)] = C_1$$

$$f_{lm}(\theta) = \frac{(\sin \theta)^{|m|}}{2^{|l|} |l|!} \left[ \frac{d}{d(\cos \theta)} \right]^{|l+|m||} (\cos^2 \theta - 1)^l$$

$$g(\phi) = e^{-im\phi}$$



$$V(r, \theta, \phi) = -\frac{K}{r} \quad \text{Potencial Coulombiano}$$

# A parte radial do átomo de hidrogênio

- Solução da parte radial da equação de Schrödinger
- **Potencial Coulombiano**

$$\frac{1}{R(r)} \frac{d}{dr} \left( r^2 \frac{dR(r)}{dr} \right) + \frac{2mr^2}{\hbar^2} [E - V(r)] = C_1 \quad C_1 = l(l+1)$$

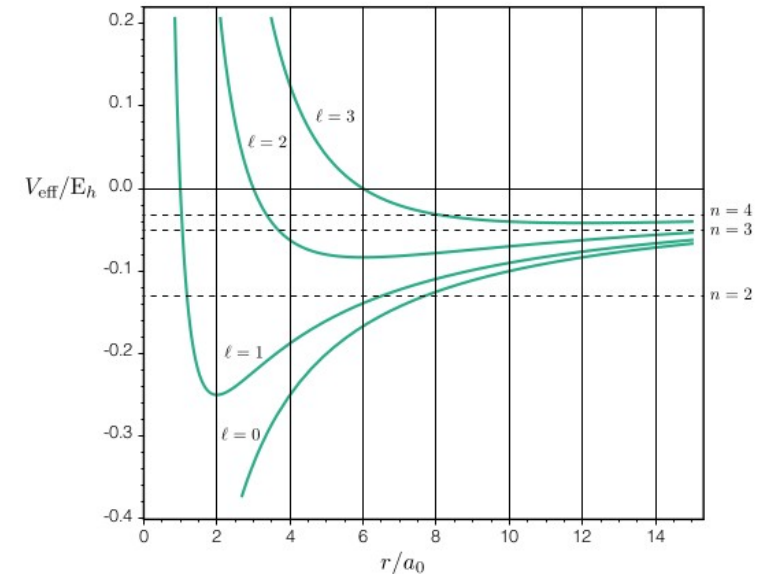
$$\frac{d}{dr} \left( r^2 \frac{dR(r)}{dr} \right) + \frac{2mr^2}{\hbar^2} \left[ E - \left( -\frac{K}{r} + \frac{\hbar^2 l(l+1)}{2mr^2} \right) \right] R(r) = 0$$

# A parte radial do átomo de hidrogênio

- Solução da parte radial da equação de Schrödinger
- **Potencial Coulombiano**

$$\frac{1}{R(r)} \frac{d}{dr} \left( r^2 \frac{dR(r)}{dr} \right) + \frac{2mr^2}{\hbar^2} [E - V(r)] = C_1 \quad C_1 = l(l+1)$$

$$\frac{d}{dr} \left( r^2 \frac{dR(r)}{dr} \right) + \frac{2mr^2}{\hbar^2} \left[ E - \underbrace{\left( -\frac{K}{r} + \frac{\hbar^2 l(l+1)}{2mr^2} \right)}_{V_{\text{efetivo}}(r)} \right] R(r) = 0$$



# Resolvendo a parte radial da eq. dif.

$$\frac{d}{dr} \left( r^2 \frac{dR(r)}{dr} \right) + \frac{2mr^2}{\hbar^2} \left[ E - \left( -\frac{K}{r} + \frac{\hbar^2 l(l+1)}{2mr^2} \right) \right] R(r) = 0$$



# Resolvendo a parte radial da eq. dif.

$$\frac{d}{dr} \left( r^2 \frac{dR(r)}{dr} \right) + \frac{2mr^2}{\hbar^2} \left[ E - \left( -\frac{K}{r} + \frac{\hbar^2 l(l+1)}{2mr^2} \right) \right] R(r) = 0$$

$$u(r) = r R(r)$$

$$\begin{aligned} \frac{d}{dr} \left( r^2 \frac{dR(r)}{dr} \right) &= \frac{d}{dr} \left( r^2 \frac{d}{dr} r^{-1} u(r) \right) \\ &= \frac{d}{dr} r^2 \left[ -r^{-2} u(r) + r^{-1} \frac{du(r)}{dr} \right] \\ &= \frac{d}{dr} \left[ -u(r) + r \frac{du(r)}{dr} \right] \\ &= -\frac{du(r)}{dr} + \frac{du(r)}{dr} + r \frac{d^2 u(r)}{dr^2} \\ &= r \frac{d^2 u(r)}{dr^2} \end{aligned}$$

# Resolvendo a parte radial da eq. dif.

$$\frac{d}{dr} \left( r^2 \frac{dR(r)}{dr} \right) + \frac{2mr^2}{\hbar^2} \left[ E - \left( -\frac{K}{r} + \frac{\hbar^2 l(l+1)}{2mr^2} \right) \right] R(r) = 0$$

$$u(r) = r R(r)$$

$$r \frac{d^2 u(r)}{dr^2} + \frac{2mr^2}{\hbar^2} \left[ E - \left( -\frac{K}{r} + \frac{\hbar^2 l(l+1)}{2mr^2} \right) \right] \frac{u(r)}{r} = 0$$

$$\begin{aligned} \frac{d}{dr} \left( r^2 \frac{dR(r)}{dr} \right) &= \frac{d}{dr} \left( r^2 \frac{d}{dr} r^{-1} u(r) \right) \\ &= \frac{d}{dr} r^2 \left[ -r^{-2} u(r) + r^{-1} \frac{du(r)}{dr} \right] \\ &= \frac{d}{dr} \left[ -u(r) + r \frac{du(r)}{dr} \right] \\ &= -\frac{du(r)}{dr} + \frac{du(r)}{dr} + r \frac{d^2 u(r)}{dr^2} \\ &= r \frac{d^2 u(r)}{dr^2} \end{aligned}$$

# Resolvendo a parte radial da eq. dif.

$$\frac{d}{dr} \left( r^2 \frac{dR(r)}{dr} \right) + \frac{2mr^2}{\hbar^2} \left[ E - \left( -\frac{K}{r} + \frac{\hbar^2 l(l+1)}{2mr^2} \right) \right] R(r) = 0$$

$$u(r) = r R(r)$$

$$r \frac{d^2 u(r)}{dr^2} + \frac{2mr^2}{\hbar^2} \left[ E - \left( -\frac{K}{r} + \frac{\hbar^2 l(l+1)}{2mr^2} \right) \right] \frac{u(r)}{r} = 0$$

$$\frac{d^2 u(r)}{dr^2} + \frac{2m}{\hbar^2} \left[ E - \left( -\frac{K}{r} + \frac{\hbar^2 l(l+1)}{2mr^2} \right) \right] u(r) = 0$$

$$\frac{d^2 u(r)}{dr^2} + \left[ \frac{2mE}{\hbar^2} + \frac{2mK}{\hbar^2 r} - \frac{l(l+1)}{r^2} \right] u(r) = 0$$

$$\begin{aligned} \frac{d}{dr} \left( r^2 \frac{dR(r)}{dr} \right) &= \frac{d}{dr} \left( r^2 \frac{d}{dr} r^{-1} u(r) \right) \\ &= \frac{d}{dr} r^2 \left[ -r^{-2} u(r) + r^{-1} \frac{du(r)}{dr} \right] \\ &= \frac{d}{dr} \left[ -u(r) + r \frac{du(r)}{dr} \right] \\ &= -\frac{du(r)}{dr} + \frac{du(r)}{dr} + r \frac{d^2 u(r)}{dr^2} \\ &= r \frac{d^2 u(r)}{dr^2} \end{aligned}$$

# Resolvendo a parte radial da eq. dif.

$$\frac{d^2 u(r)}{dr^2} + \left[ \frac{2mE}{\hbar^2} + \frac{2mK}{\hbar^2 r} - \frac{l(l+1)}{r^2} \right] u(r) = 0 \quad \left( \frac{\epsilon}{2} \right)^2 = - \frac{2mE}{\hbar^2} \quad x = r \epsilon$$

# Resolvendo a parte radial da eq. dif.

$$\frac{d^2 u(r)}{dr^2} + \left[ \frac{2mE}{\hbar^2} + \frac{2mK}{\hbar^2 r} - \frac{l(l+1)}{r^2} \right] u(r) = 0 \quad \left( \frac{\epsilon}{2} \right)^2 = - \frac{2mE}{\hbar^2} \quad x = r \epsilon$$

$$\frac{d^2 u(x)}{dx^2} + \left[ -\frac{1}{4} + \frac{2mK}{\hbar^2 \epsilon x} - \frac{l(l+1)}{x^2} \right] u(x) = 0$$

# Resolvendo a parte radial da eq. dif.

$$\frac{d^2 u(r)}{dr^2} + \left[ \frac{2mE}{\hbar^2} + \frac{2mK}{\hbar^2 r} - \frac{l(l+1)}{r^2} \right] u(r) = 0 \quad \left( \frac{\epsilon}{2} \right)^2 = - \frac{2mE}{\hbar^2} \quad x = r \epsilon$$

$$\frac{d^2 u(x)}{dx^2} + \left[ -\frac{1}{4} + \frac{2mK}{\hbar^2 \epsilon x} - \frac{l(l+1)}{x^2} \right] u(x) = 0$$

$$\frac{d^2 u_j^k(x)}{dx^2} + \left[ -\frac{1}{4} + \frac{2j+k+1}{2x} - \frac{k^2-1}{4x^2} \right] u(x) = 0$$

$$u_j^k(x) = e^{-x/2} x^{(k+1)/2} L_j^k(x)$$

# Resolvendo a parte radial da eq. dif.

$$\frac{d^2 u(r)}{dr^2} + \left[ \frac{2mE}{\hbar^2} + \frac{2mK}{\hbar^2 r} - \frac{l(l+1)}{r^2} \right] u(r) = 0$$

$$\left( \frac{\epsilon}{2} \right)^2 = - \frac{2mE}{\hbar^2} \quad x = r \epsilon$$

$$\frac{d^2 u(x)}{dx^2} + \left[ -\frac{1}{4} + \frac{2mK}{\hbar^2 \epsilon x} - \frac{l(l+1)}{x^2} \right] u(x) = 0$$

$$\frac{d^2 u_j^k(x)}{dx^2} + \left[ -\frac{1}{4} + \frac{2j+k+1}{2x} - \frac{k^2-1}{4x^2} \right] u(x) = 0$$

$$u_j^k(x) = e^{-x/2} x^{(k+1)/2} L_j^k(x) \quad k \text{ e } j \text{ índices inteiros!}$$

Zoológico  
das equações diferenciais



# Resolvendo a parte radial da eq. dif.

$$\frac{d^2 u(x)}{dx^2} + \left[ -\frac{1}{4} + \frac{2mK}{\hbar^2 \epsilon x} - \frac{l(l+1)}{x^2} \right] u(x) = 0$$

$$\frac{d^2 u_j^k(x)}{dx^2} + \left[ -\frac{1}{4} + \frac{2j+k+1}{2x} - \frac{k^2-1}{4x^2} \right] u(x) = 0$$

$$u_j^k(x) = e^{-x/2} x^{(k+1)/2} L_j^k(x)$$

$k$  e  $j$  índices  
inteiros!



# Resolvendo a parte radial da eq. dif.

$$\frac{d^2 u(x)}{dx^2} + \left[ -\frac{1}{4} + \frac{2mK}{\hbar^2 \epsilon x} - \frac{l(l+1)}{x^2} \right] u(x) = 0$$

$$\frac{d^2 u_j^k(x)}{dx^2} + \left[ -\frac{1}{4} + \frac{2j+k+1}{2x} - \frac{k^2-1}{4x^2} \right] u(x) = 0$$

$$u_j^k(x) = e^{-x/2} x^{(k+1)/2} L_j^k(x)$$

$k$  e  $j$  índices  
inteiros!

$$l(l+1) = \frac{k^2-1}{4}$$

$$\begin{aligned} k^2 &= 4l^2 + 4l + 1 \\ &= (2l+1)^2 \Rightarrow k = 2l+1 \end{aligned}$$

$$\frac{k+1}{2} = \frac{2l+2}{2} = l+1$$

# Resolvendo a parte radial da eq. dif.

$$\frac{d^2 u(x)}{dx^2} + \left[ -\frac{1}{4} + \frac{2mK}{\hbar^2 \epsilon x} - \frac{l(l+1)}{x^2} \right] u(x) = 0$$

$$\frac{d^2 u_j^k(x)}{dx^2} + \left[ -\frac{1}{4} + \frac{2j+k+1}{2x} - \frac{k^2-1}{4x^2} \right] u(x) = 0$$

$$u_j^k(x) = e^{-x/2} x^{(k+1)/2} L_j^k(x)$$

$k$  e  $j$  índices  
inteiros!

$$l(l+1) = \frac{k^2-1}{4}$$

$$k^2 = 4l^2 + 4l + 1 \\ = (2l+1)^2 \Rightarrow k = 2l+1$$

$$\frac{k+1}{2} = \frac{2l+2}{2} = l+1$$

$$\frac{2mK}{\hbar^2 \epsilon} = \frac{2j+k+1}{2} \quad \frac{2j+k+1}{2} = \frac{2j+(2l+1)+1}{2} = j+l+1 = n \quad j = n-l-1$$

# Resolvendo a parte radial da eq. dif.

$$\frac{2mK}{\hbar^2 \epsilon} = \frac{2j+k+1}{2} \quad \frac{2j+k+1}{2} = \frac{2j+(2l+1)+1}{2} = \underbrace{j+l+1}_{\substack{\text{número} \\ \text{inteiro!}}}$$

# Resolvendo a parte radial da eq. dif.

$$\frac{2mK}{\hbar^2 \epsilon} = \frac{2j+k+1}{2} \quad \frac{2j+k+1}{2} = \frac{2j+(2l+1)+1}{2} = \underbrace{j+l+1}_{\substack{\text{número} \\ \text{inteiro!}}}$$

$$\frac{2mK}{\hbar^2 \epsilon} = j+l+1 = n \quad \longrightarrow \quad \frac{m^2 K^2}{\hbar^4} \left( -\frac{\hbar^2}{2mE} \right) = n^2$$

$\frac{\epsilon^2}{4} = -\frac{2mE}{\hbar^2}$

# Resolvendo a parte radial da eq. dif.

$$\frac{2mK}{\hbar^2 \epsilon} = \frac{2j+k+1}{2} \quad \frac{2j+k+1}{2} = \frac{2j+(2l+1)+1}{2} = \underbrace{j+l+1}$$

número  
inteiro!

$$\frac{2mK}{\hbar^2 \epsilon} = j+l+1 = n \quad \xrightarrow{\quad} \quad \frac{m^2 K^2}{\hbar^4} \left( -\frac{\hbar^2}{2mE} \right) = n^2 \quad \xrightarrow{\quad} \quad E_n = -\frac{mZ^2 e^4}{8h^2 \epsilon_0 n^2}$$

$\frac{\epsilon^2}{4} = -\frac{2mE}{\hbar^2}$        $K = \frac{Ze^2}{4\pi\epsilon_0}$

# Resolvendo a parte radial da eq. dif.

$$\frac{2mK}{\hbar^2 \epsilon} = \frac{2j+k+1}{2} \quad \frac{2j+k+1}{2} = \frac{2j+(2l+1)+1}{2} = \underbrace{j+l+1}$$

número  
inteiro!

$$\frac{2mK}{\hbar^2 \epsilon} = j+l+1 = n \quad \longrightarrow \quad \frac{m^2 K^2}{\hbar^4} \left( -\frac{\hbar^2}{2mE} \right) = n^2 \quad \longrightarrow \quad E_n = -\frac{mZ^2 e^4}{8h^2 \epsilon_0 n^2}$$

$\frac{\epsilon^2}{4} = -\frac{2mE}{\hbar^2}$        $K = \frac{Ze^2}{4\pi\epsilon_0}$

$$\Delta E = \frac{mZ^2 e^4}{8h^2 \epsilon_0} \left( \frac{1}{n_i^2} - \frac{1}{n_f^2} \right)$$

Fórmula de  
Rydberg!

# Resolvendo a parte radial da eq. dif.

$$\frac{2mK}{\hbar^2 \epsilon} = \frac{2j+k+1}{2} \quad \frac{2j+k+1}{2} = \frac{2j+(2l+1)+1}{2} = j+l+1$$

número inteiro!

$$\frac{2mK}{\hbar^2 \epsilon} = j+l+1 = n \quad \xrightarrow{\frac{\epsilon^2}{4} = -\frac{2mE}{\hbar^2}} \quad \frac{m^2 K^2}{\hbar^4} \left( -\frac{\hbar^2}{2mE} \right) = n^2 \quad \xrightarrow{K = \frac{Ze^2}{4\pi\epsilon_0}} \quad E_n = -\frac{mZ^2 e^4}{8h^2 \epsilon_0 n^2}$$

$$\Delta E = \frac{mZ^2 e^4}{8h^2 \epsilon_0} \left( \frac{1}{n_i^2} - \frac{1}{n_f^2} \right)$$

Fórmula de Rydberg!

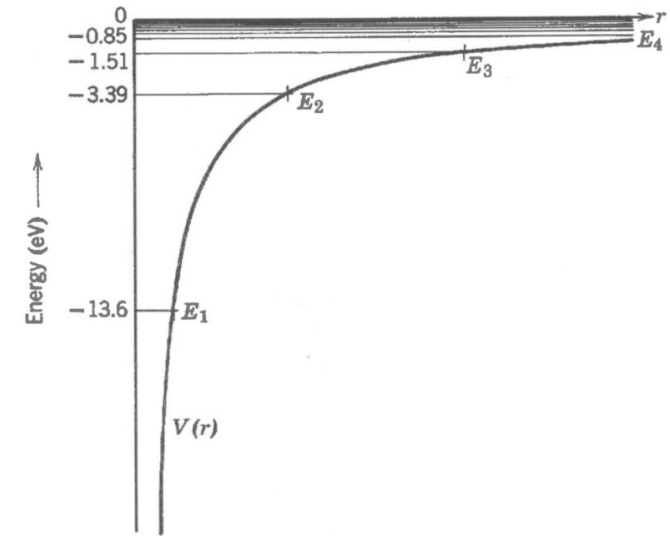
Energia dos estados só depende de n, não depende de nenhum número quântico de momento angular!!

# A energia dos estados e as transições

- Na solução da parte radial, analogamente ao que aconteceu com a solução do potencial harmônico, encontramos que a **energia dos estados é quantizada** para satisfazer a equação de Schrödinger e a condição de normalização

$$E_n = -\frac{\mu}{2} \left( \frac{e^2}{4\pi\epsilon_0\hbar} \right)^2 \frac{1}{n^2} = -\frac{13,6}{n^2}$$

- **Resultado igual ao de Bohr!**



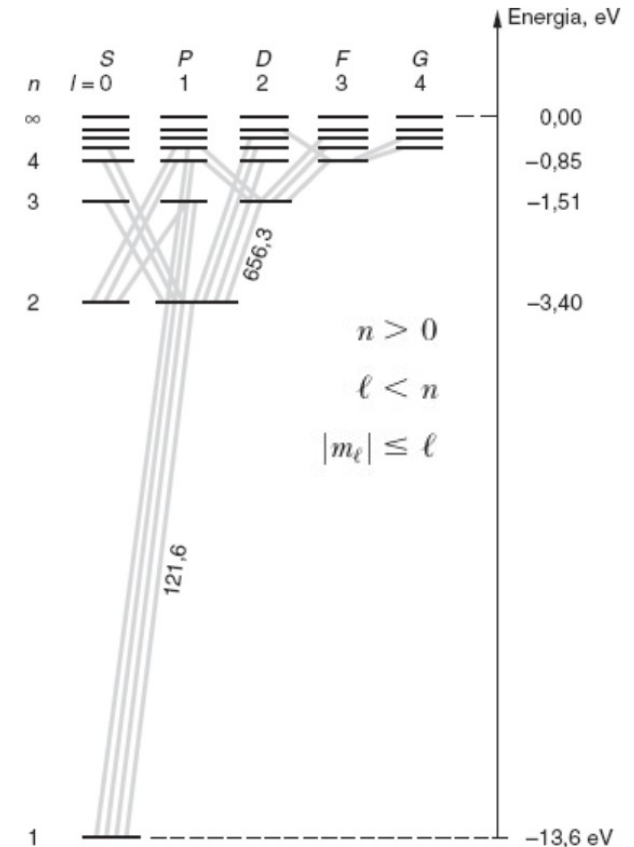


# A energia dos estados e as transições

- Na solução da parte radial, analogamente ao que aconteceu com a solução do potencial harmônico, encontramos que a **energia dos estados é quantizada** para satisfazer a equação de Schrödinger e a condição de normalização

$$E_n = -\frac{\mu}{2} \left( \frac{e^2}{4\pi\epsilon_0\hbar} \right)^2 \frac{1}{n^2} = -\frac{13,6}{n^2}$$

- Resultado igual ao de Bohr!**



# A energia dos estados e as transições

- As equações diferenciais impõem **restrições sobre os valores possíveis dos números quânticos:**

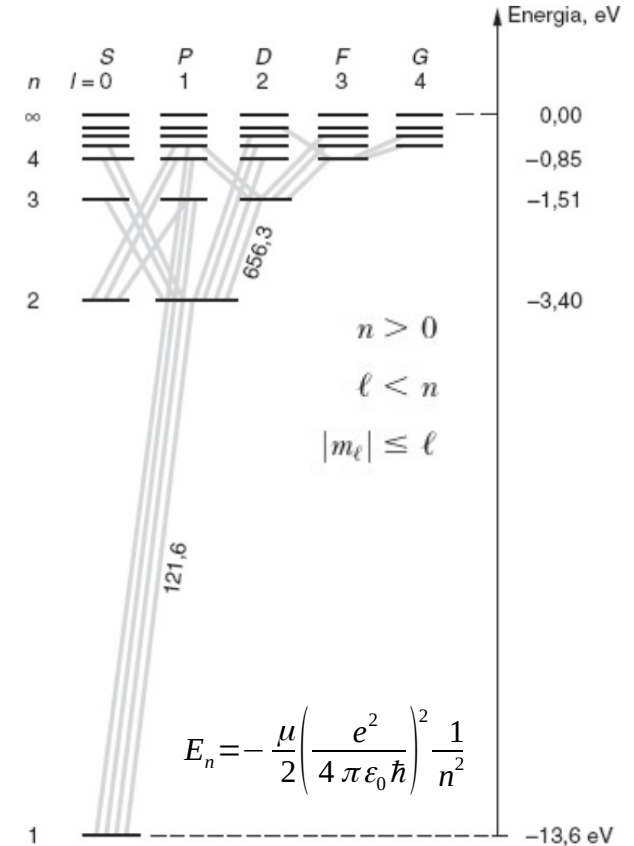
$$\frac{2j+k+1}{2} = \frac{2j+(2l+1)+1}{2} = j+l+1 = n \quad \text{Do slide 18!}$$

$$j = n - l - 1$$

- $j$  deve sempre ser maior ou igual a zero!
  - $l$  pode ser 0, logo o menor  $n$  será 1
  - $l$  não pode ser maior nem igual a  $n$

- Vínculo entre os números quânticos:

$n = 1, 2, 3, 4, \dots$	: inteiro (camada)
$l = 0, 1, 2, 3, \dots, n-1$	: inteiro (subcamada)
$m = -l, -l+1, \dots, 0, 1, \dots, l-1, l$	: inteiro (orbital)



# A parte radial do átomo de hidrogênio

- Desfazendo todas as transformações que fizemos até agora:

$$R_{nl}(r) = A_{nl} e^{-r/a_0 n} \left( \frac{2r}{a_0 n} \right)^l L_n^l(2r/a_0 n)$$

$$a_0 = \frac{4 \pi \epsilon_0 \hbar^2}{m e^2}$$

Polinômio de Laguerre

$$L_n^l(x) = (-1)^{2l+1} \frac{d^{2l+1}}{dx^{2l+1}} \left[ e^x \frac{d^{n+l}}{dx^{n+l}} (e^{-x} x^{n+l}) \right]$$

# A parte radial do átomo de hidrogênio

- Polinômios de Laguerre também são tabelados!

$n$	$\ell$	$R_{n\ell}(r)$
1	0	$\frac{2}{(a_0)^{3/2}} e^{-r/a_0}$
2	0	$\left(2 - \frac{r}{a_0}\right) \frac{e^{-r/2a_0}}{(2a_0)^{3/2}}$
2	1	$\frac{r}{a_0} \frac{e^{-r/2a_0}}{\sqrt{3}(2a_0)^{3/2}}$
3	0	$\frac{1}{(a_0)^{3/2}} \frac{2}{81\sqrt{3}} \left(27 - 18\frac{r}{a_0} + 2\frac{r^2}{a_0^2}\right) e^{-r/3a_0}$
3	1	$\frac{1}{(a_0)^{3/2}} \frac{4}{81\sqrt{6}} \left(6 - \frac{r}{a_0}\right) \frac{r}{a_0} e^{-r/3a_0}$
3	2	$\frac{1}{(a_0)^{3/2}} \frac{4}{81\sqrt{30}} \frac{r^2}{a_0^2} e^{-r/3a_0}$

# A parte radial do átomo de hidrogênio

$$P(r) dr = r^2 R^*(r) R(r) dr \int_0^\pi |f(\theta)|^2 \sin \theta d\theta \int_0^{2\pi} |g(\phi)|^2 d\phi$$

$$P_{nl}(r) dr = r^2 |R_{nl}(r)|^2 dr \quad P_{nl}(r) = r^2 |R_{nl}(r)|^2$$

$$r_{nlm}^- = \int_{-\infty}^{\infty} (\psi^* \hat{r} \psi) r^2 \sin \theta dr d\theta d\phi$$

$$r_{nl}^- = \frac{n^2 a_0}{Z} \left\{ 1 + \frac{1}{2} \left[ 1 - \frac{l(l+1)}{n^2} \right] \right\}$$

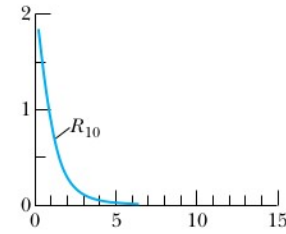
# A parte radial do átomo de hidrogênio

$$P(r) dr = r^2 R^*(r) R(r) dr \int_0^\pi |f(\theta)|^2 \sin \theta d\theta \int_0^{2\pi} |g(\phi)|^2 d\phi$$

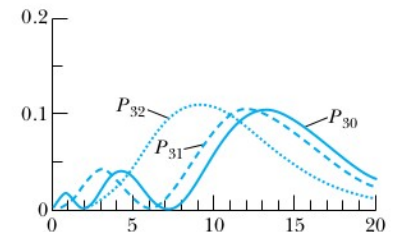
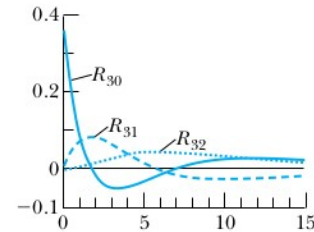
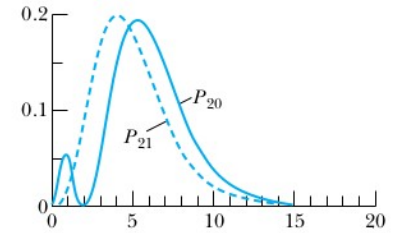
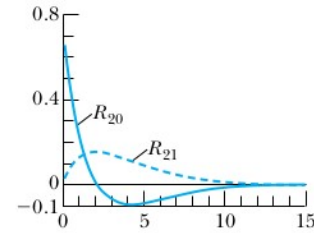
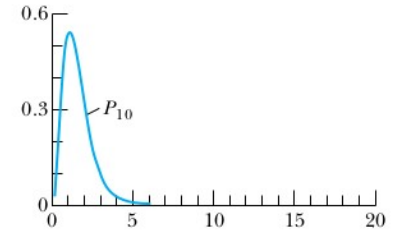
$$P_{n\ell}(r) dr = r^2 |R_{n\ell}(r)|^2 dr \quad P_{n\ell}(r) = r^2 |R_{n\ell}(r)|^2$$

$n$	$\ell$	$R_{n\ell}(r)$
1	0	$\frac{2}{(a_0)^{3/2}} e^{-r/a_0}$
2	0	$\left(2 - \frac{r}{a_0}\right) \frac{e^{-r/2a_0}}{(2a_0)^{3/2}}$
2	1	$\frac{r}{a_0} \frac{e^{-r/2a_0}}{\sqrt{3}(2a_0)^{3/2}}$
3	0	$\frac{1}{(a_0)^{3/2}} \frac{2}{81\sqrt{3}} \left(27 - 18\frac{r}{a_0} + 2\frac{r^2}{a_0^2}\right) e^{-r/3a_0}$
3	1	$\frac{1}{(a_0)^{3/2}} \frac{4}{81\sqrt{6}} \left(6 - \frac{r}{a_0}\right) \frac{r}{a_0} e^{-r/3a_0}$
3	2	$\frac{1}{(a_0)^{3/2}} \frac{4}{81\sqrt{30}} \frac{r^2}{a_0^2} e^{-r/3a_0}$

Radial wave functions ( $R_{n\ell}$ )



Radial probability distribution ( $P_{n\ell}$ )



Radius ( $a_0$ )

(a)

Radius ( $a_0$ )

(b)

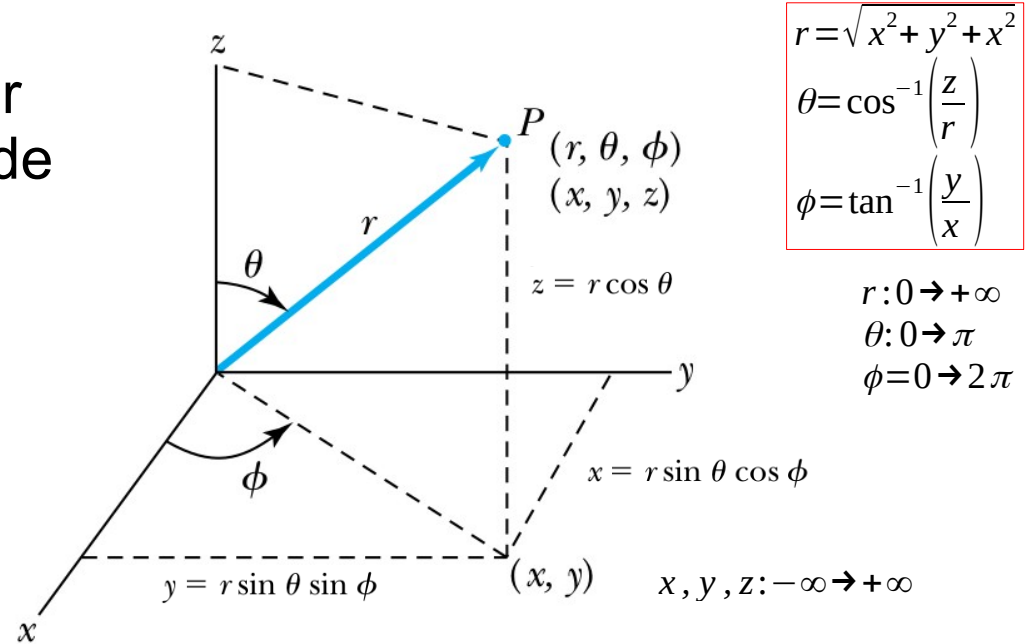
# As equações desacopladas

- Temos agora, de abordar as equações desacopladas para obter a solução completa para o átomo de hidrogênio!

$$\frac{1}{R(r)} \frac{d}{dr} \left( r^2 \frac{dR(r)}{dr} \right) + \frac{2mr^2}{\hbar^2} [E - V(r)] = C_1$$

$$f_{lm}(\theta) = \frac{(\sin \theta)^{|m|}}{2^{|l|} |l|!} \left[ \frac{d}{d(\cos \theta)} \right]^{|l+|m||} (\cos^2 \theta - 1)^l$$

$$g(\phi) = e^{-im\phi}$$



$$r = \sqrt{x^2 + y^2 + z^2}$$

$$\theta = \cos^{-1} \left( \frac{z}{r} \right)$$

$$\phi = \tan^{-1} \left( \frac{y}{x} \right)$$

$$r: 0 \rightarrow +\infty$$

$$\theta: 0 \rightarrow \pi$$

$$\phi: 0 \rightarrow 2\pi$$

$$V(r, \theta, \phi) = -\frac{K}{r} \quad \text{Potencial Coulombiano}$$

# As equações desacopladas

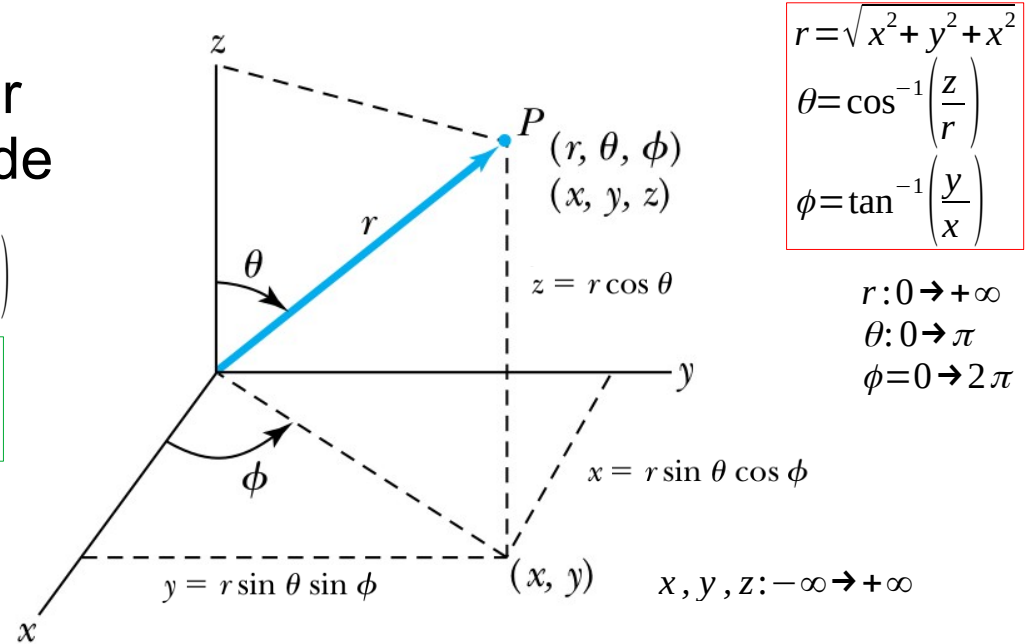
- Temos agora, de abordar as equações desacopladas para obter a solução completa para o átomo de hidrogênio!

$$x = \left( \frac{2r}{a_0 n} \right)$$

$$R_{nl}(r) = A_{nl} e^{-x/2} x^l (-1)^{2l+1} \frac{d^{2l+1}}{dx^{2l+1}} \left[ e^x \frac{d^{n+l}}{dx^{n+l}} (e^{-x} x^{n+1}) \right]$$

$$f_{lm}(\theta) = \frac{(\sin \theta)^{|m|}}{2^l l!} \left[ \frac{d}{d(\cos \theta)} \right]^{|l+m|} (\cos^2 \theta - 1)^l$$

$$g(\phi) = e^{-im\phi}$$



$$r = \sqrt{x^2 + y^2 + z^2}$$

$$\theta = \cos^{-1} \left( \frac{z}{r} \right)$$

$$\phi = \tan^{-1} \left( \frac{y}{x} \right)$$

$$r: 0 \rightarrow +\infty$$

$$\theta: 0 \rightarrow \pi$$

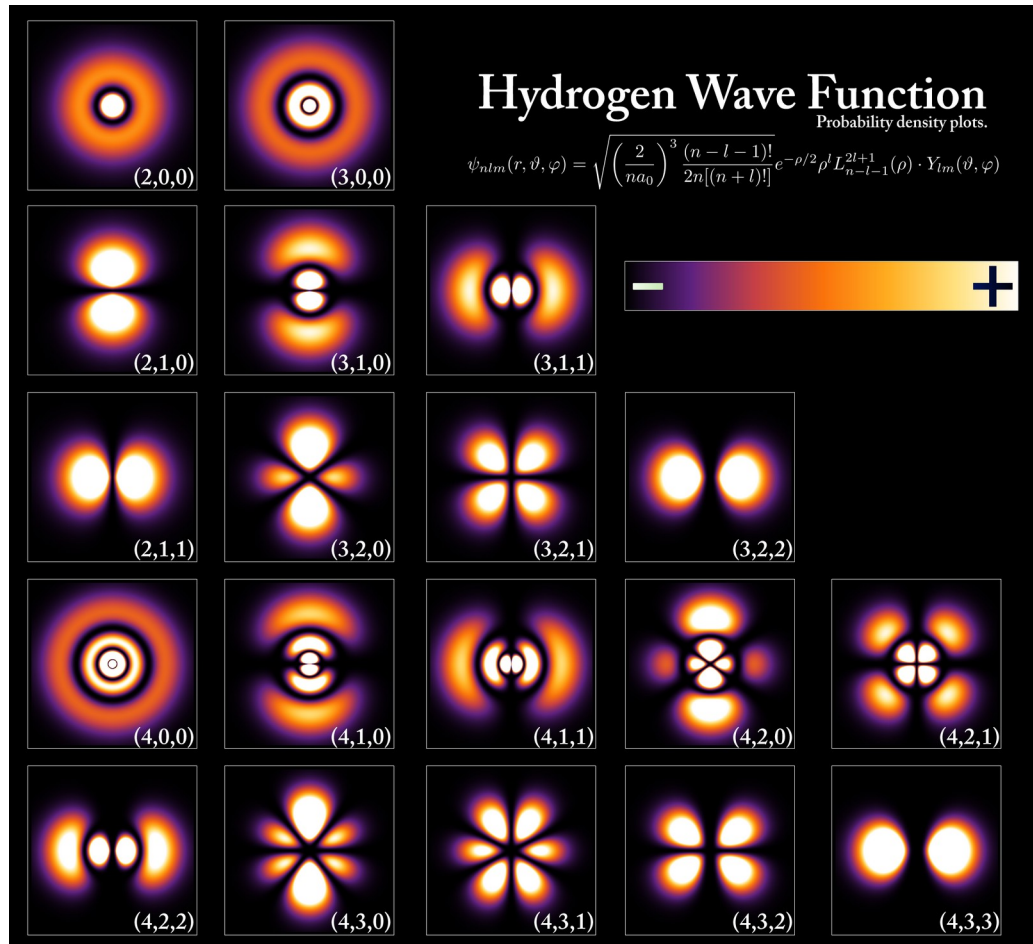
$$\phi: 0 \rightarrow 2\pi$$

$$V(r, \theta, \phi) = -\frac{K}{r}$$

Potencial  
Coulombiano



# Visualizando a solução



# Notação química!

- A notação química veio antes da era da mecânica quântica
- Veio da necessidade de se nomear as linhas de espectroscopia de emissão (espectros de emissão)

Camada:

$n = 1 \ 2 \ 3 \ 4 \ 5$        $\leftarrow$  valor numérico  
 $K \ L \ M \ N \ O$        $\leftarrow$  símbolo

Subcamada:

$l = 0 \ 1 \ 2 \ 3 \ 4$        $\leftarrow$  valor numérico  
 $s \ p \ d \ f \ g$        $\leftarrow$  símbolo

- Assim, funções de onda com número quântico:

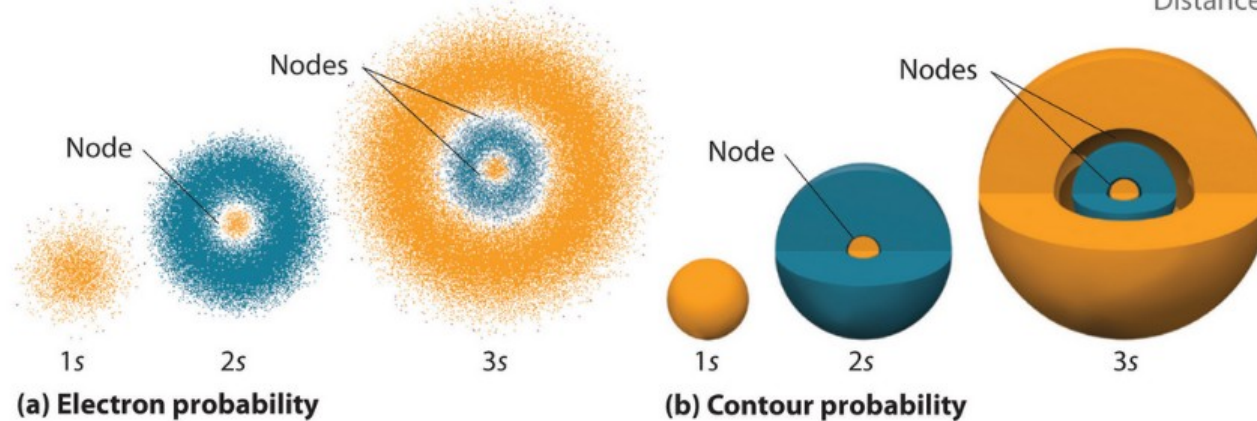
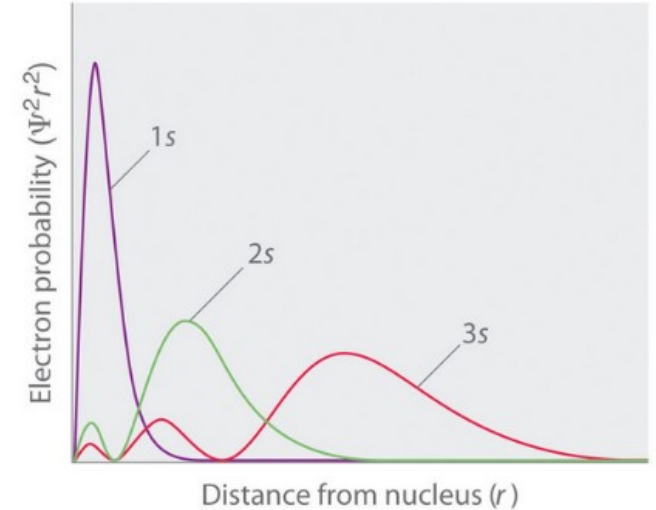
$n=1, l=0$  é nomeada como o estado 1s

$n=2, l=1$  é nomeada como o estado 2p



# Distribuição eletrônica na subcamada s

- Se estende por regiões maiores quando o número quântico principal aumenta
- Apresenta nós, e quanto maior o número quântico principal, mais nós são presentes





## Hydrogen Atoms under Magnification: Direct Observation of the Nodal Structure of Stark States

A. S. Stodolna,<sup>1,\*</sup> A. Rouzée,<sup>1,2</sup> F. Lépine,<sup>3</sup> S. Cohen,<sup>4</sup> F. Robicheaux,<sup>5</sup>  
A. Gijbtsen,<sup>1</sup> J. H. Jungmann,<sup>1</sup> C. Bordas,<sup>3</sup> and M. J. J. Vrakking<sup>1,2,\*</sup>

<sup>1</sup>FOM Institute AMOLF, Science Park 104, 1098 XG Amsterdam, Netherlands

<sup>2</sup>Max-Born-Institut, Max Born Straße 2A, D-12489 Berlin, Germany

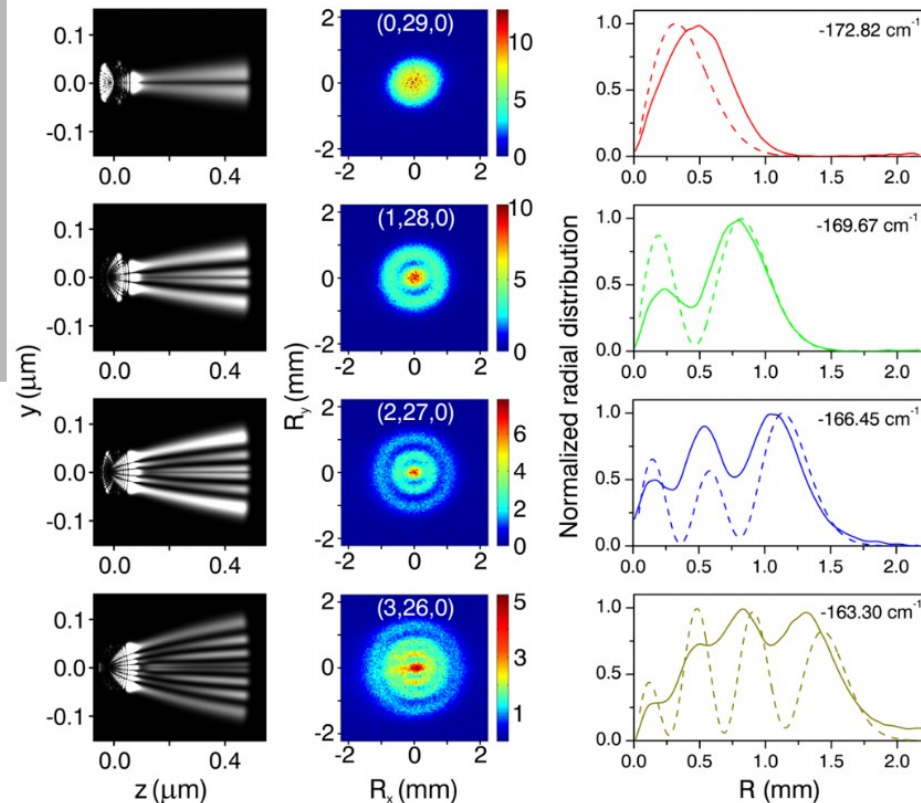
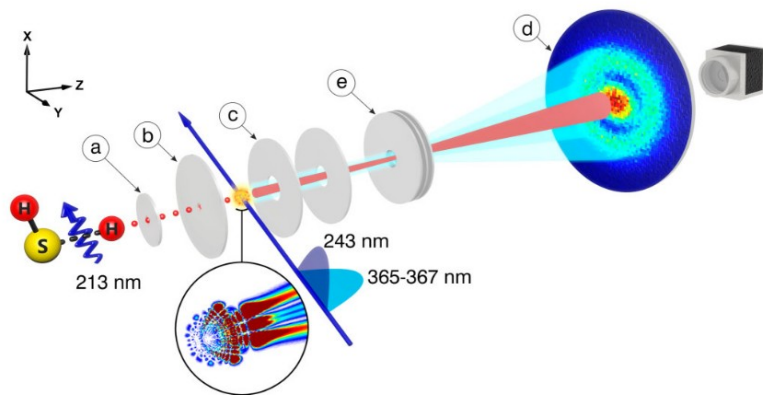
<sup>3</sup>Institut Lumière Matière, Université Lyon 1, CNRS, UMR 5306, 10 Rue Ada Byron, 69622 Villeurbanne Cedex, France

<sup>4</sup>Atomic and Molecular Physics Laboratory, Physics Department, University of Ioannina, 45110 Ioannina, Greece

<sup>5</sup>Department of Physics, Auburn University, Auburn, Alabama 36849, USA

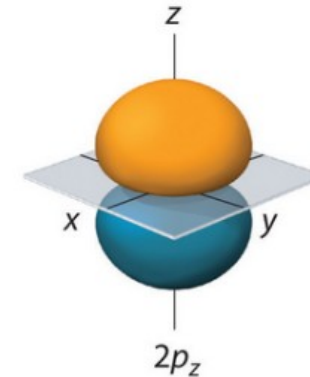
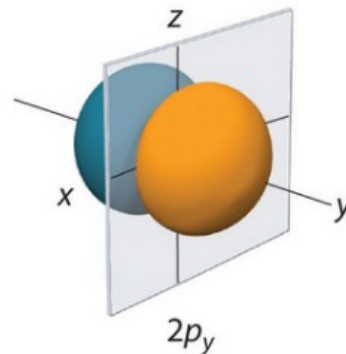
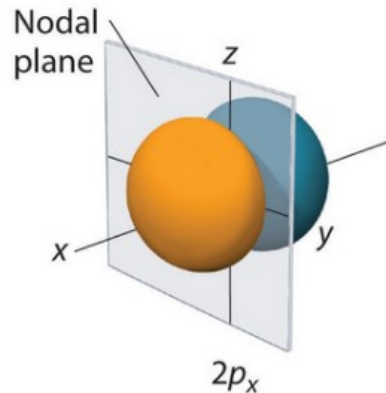
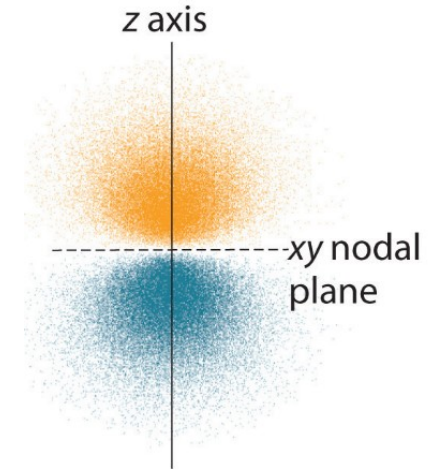
(Received 18 January 2013; revised manuscript received 13 March 2013; published 20 May 2013)

To describe the microscopic properties of matter, quantum mechanics uses wave functions, whose structure and time dependence is governed by the Schrödinger equation. In atoms the charge distributions described by the wave function are rarely observed. The hydrogen atom is unique, since it only has one electron and, in a dc electric field, the Stark Hamiltonian is exactly separable in terms of parabolic coordinates  $(\eta, \xi, \varphi)$ . As a result, the microscopic wave function along the  $\xi$  coordinate that exists in the vicinity of the atom, and the projection of the continuum wave function measured at a macroscopic distance, share the same nodal structure. In this Letter, we report photoionization microscopy experiments where this nodal structure is directly observed. The experiments provide a validation of theoretical predictions that have been made over the last three decades.



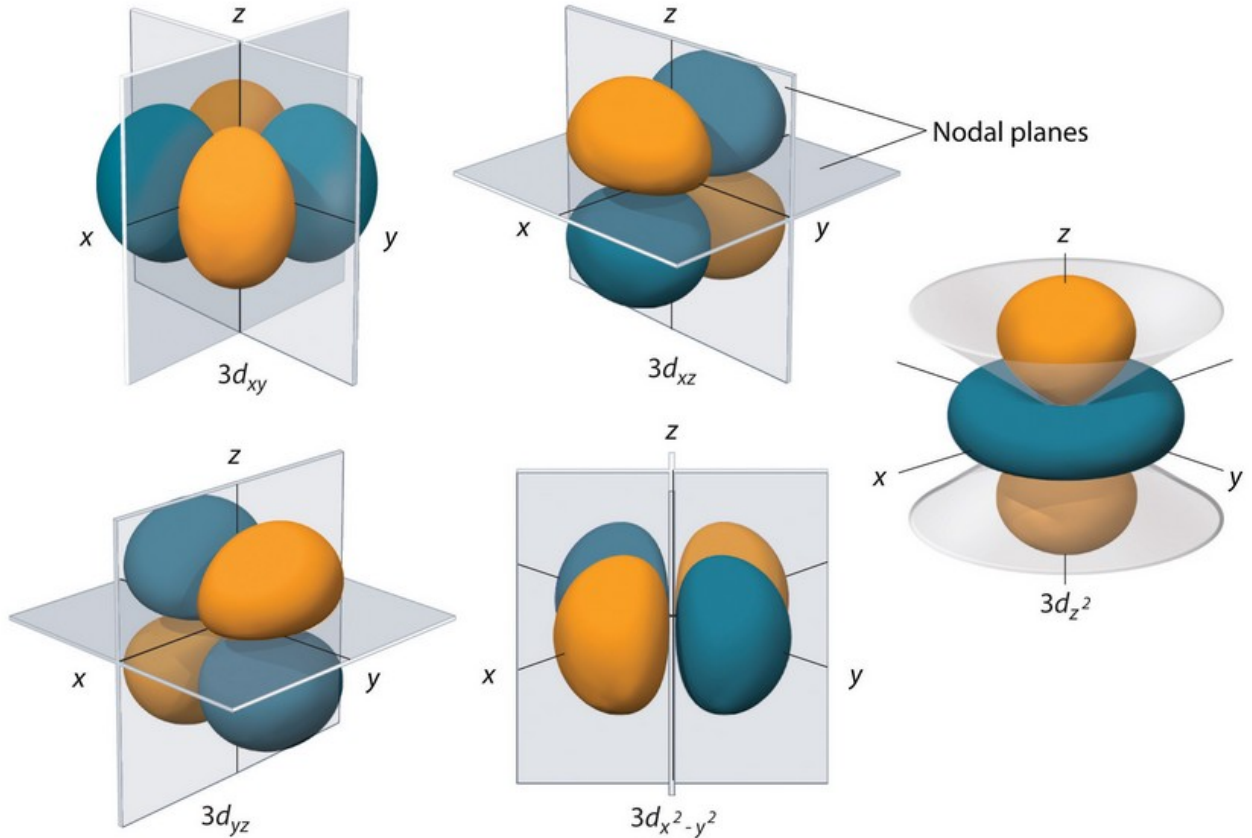
# Distribuição eletrônica na subcamada p

- Somente os orbitais  $s$  são esfericamente simétricos
- Quando  $l$  aumenta, aumenta também o número de orbitais na subcamada
- O orbital fica mais complexo, com o surgimento de planos nodais
- A subcamada  $2p$  tem  $l = 1$ , com três valores de  $m$  ( $-1$ ,  $0$ , e  $+1$ ), logo três orbitais



# Distribuição eletrônica na subcamada d

- A subcamada 3d tem  $l = 2$ , com três valores de  $m$  (-2, -1, 0, +1 e +2), logo cinco orbitais



# Visualizando os orbitais quânticos

Revista Brasileira de Ensino de Física, vol. 41, n° 4, e20190073 (2019)  
[www.scielo.br/rbef](http://www.scielo.br/rbef)  
DOI: <http://dx.doi.org/10.1590/1806-9126-RBEF-2019-0073>

Articles



Licença Creative Commons

## A smooth path to plot hydrogen atom via Monte Carlo method

Pedro Henrique Fernandes Lobo<sup>\*</sup>, Everaldo Arashiro<sup>1</sup>, Alcides Castro e Silva<sup>2</sup>, Carlos Felipe Saraiva Pinheiro<sup>2</sup>

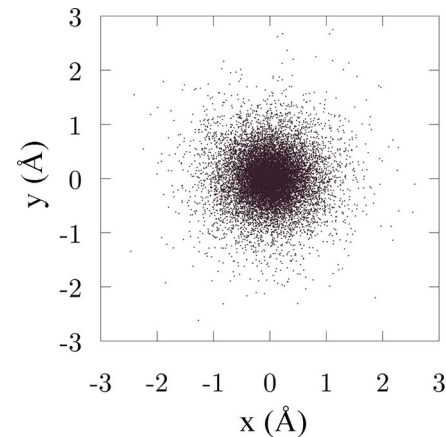
<sup>1</sup>Universidade Federal do Rio Grande, Instituto de Matemática, Estatística e Física, Av. Itália km 8 Carreiros, Rio Grande, RS, Brasil

<sup>2</sup>Universidade Federal de Ouro Preto, Instituto de Ciências, Exatas e Biológicas, Departamento de Física, Ouro Preto, MG, Brasil.

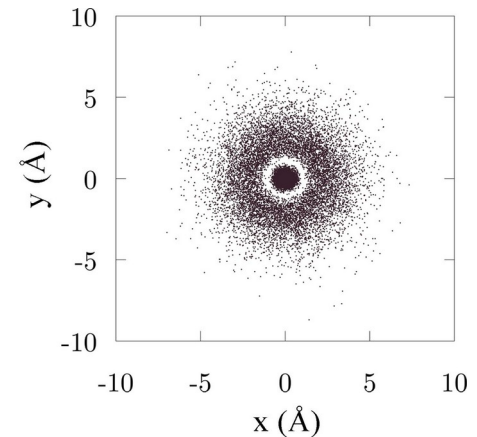
Received on March 30, 2019; Revised on May 16, 2019; Accepted on May 25, 2019.

In this paper, we show how to build a basic computer program using the Monte Carlo method to display the hydrogen atomic orbitals. For this, in a heuristic way, we applied a von Neumann acceptance-rejection method in simple problems of potential wells, and we end with the hydrogen orbitals representation. In this technique, we spread points uniformly on the 1D and 2D charts of probability density distributions, then we filtered points under these “curves or surfaces”, and we extended this logic to 3D cases. Throughout the work, we also made some comments to help beginner students better understand the term “wave function” present in the Schrödinger equation. Also, we made all source code available at a third-party platform, for any purpose under the MIT license.

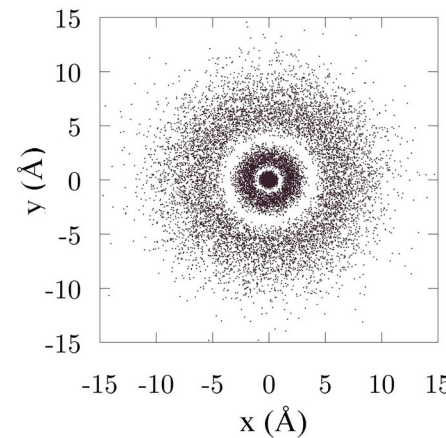
**Keywords:** hydrogen atom, quantum mechanics, Monte Carlo method, Neumann acceptance-rejection method.



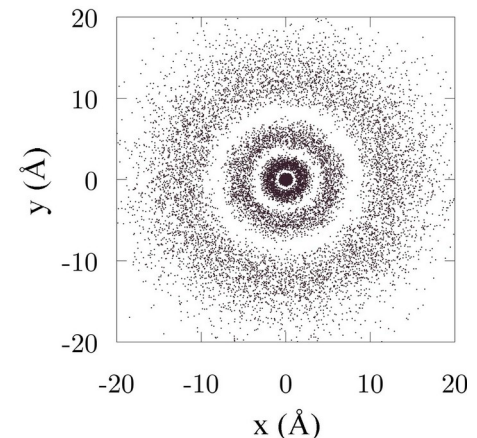
(a)  $n, l, m = (1, 0, 0)$



(b)  $n, l, m = (2, 0, 0)$

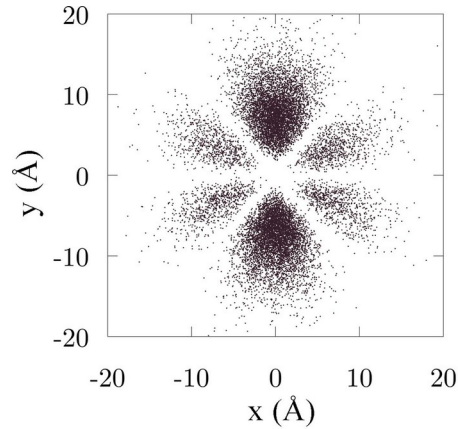


(c)  $n, l, m = (3, 0, 0)$

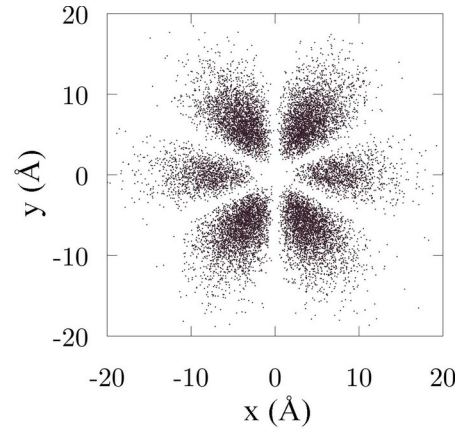


(d)  $n, l, m = (4, 0, 0)$

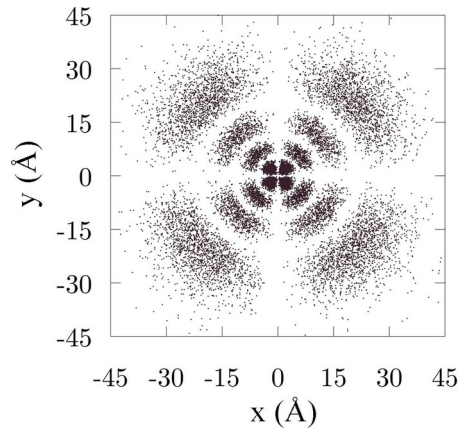
# Visualizando os orbitais quânticos



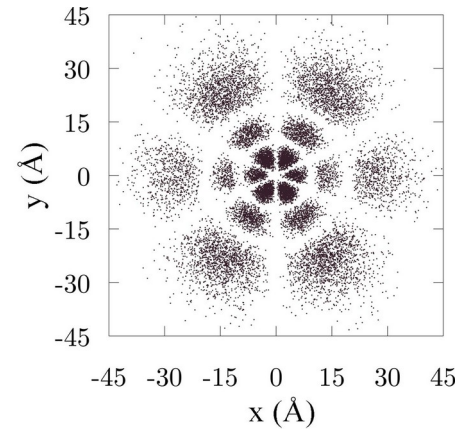
(a)  $n, l, m = (4, 3, 0)$



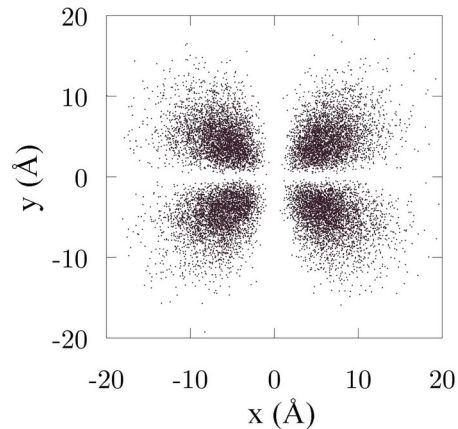
(b)  $n, l, m = (4, 3, 1)$



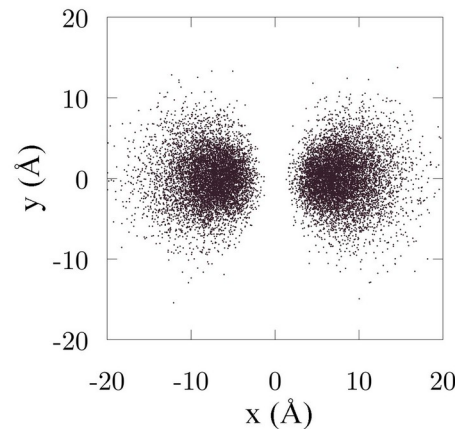
(a)  $n, l, m = (6, 2, 1)$



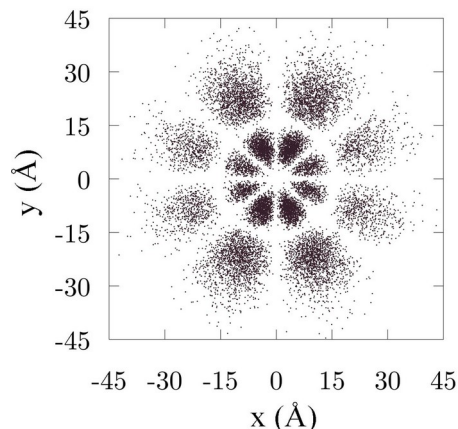
(b)  $n, l, m = (6, 3, 1)$



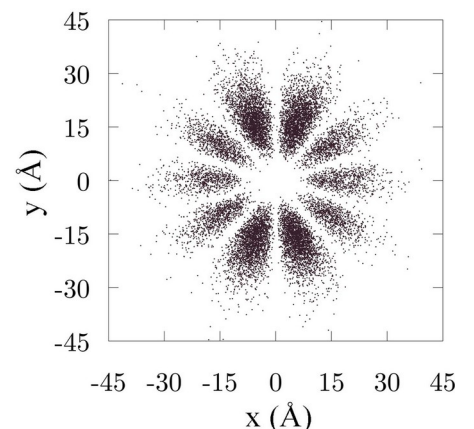
(c)  $n, l, m = (4, 3, 2)$



(d)  $n, l, m = (4, 3, 3)$



(c)  $n, l, m = (6, 4, 1)$



(d)  $n, l, m = (6, 5, 1)$

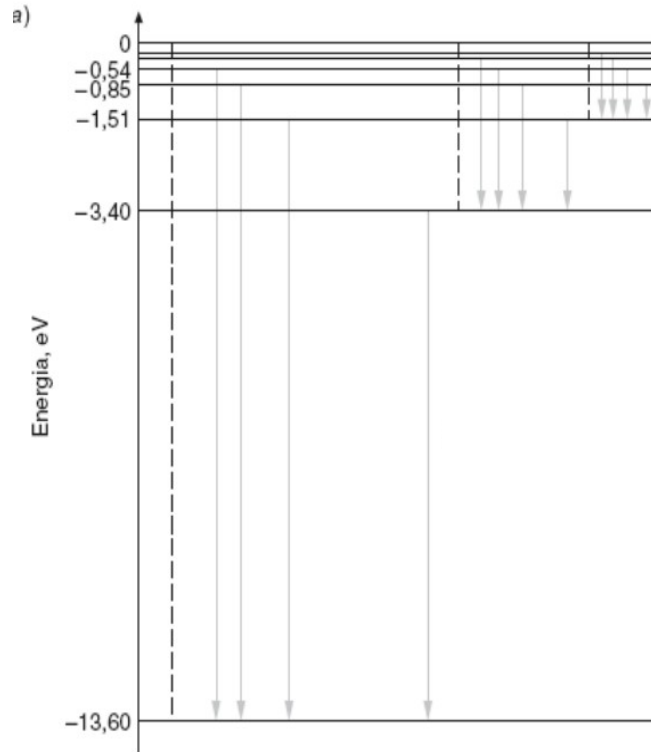


# Bohr Vs Schrödinger

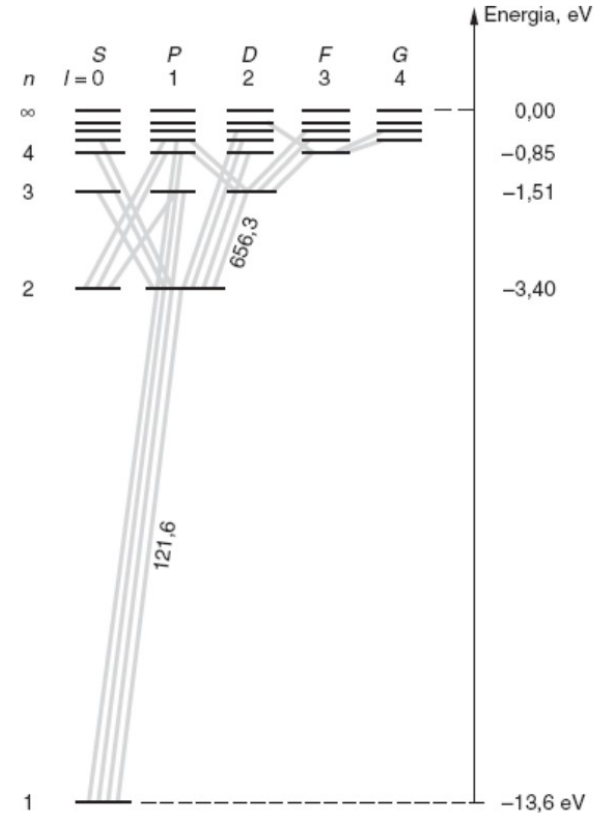
- Comparando os dois modelos (antiga e nova mecânica quântica)
- **Primeiro:** O modelo de Schrödinger não prevê órbitas bem definidas para os elétrons. A função de onda só nos dá probabilidades no espaço
- **Segundo:** A quantização do momento angular no modelo de Schrödinger é diferente do proposto por Bohr
- **Terceiro:** Os números quânticos aparecem naturalmente na solução das equações diferenciais, enquanto que Bohr impôs as quantizações por postulados
- **Quarto:** Apesar de bem mais complicado, o modelo de Schrödinger leva a uma melhor compreensão sobre o átomo quando comparado com o modelo de Bohr, como veremos em **física moderna 2**

# Bohr Vs Schrödinger

## Níveis do átomo de Bohr

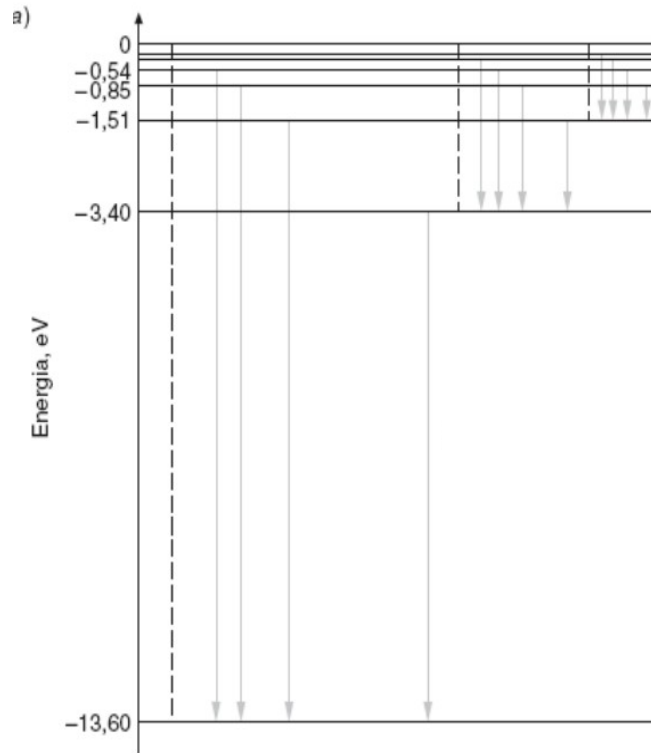


## Níveis do átomo de Schrödinger

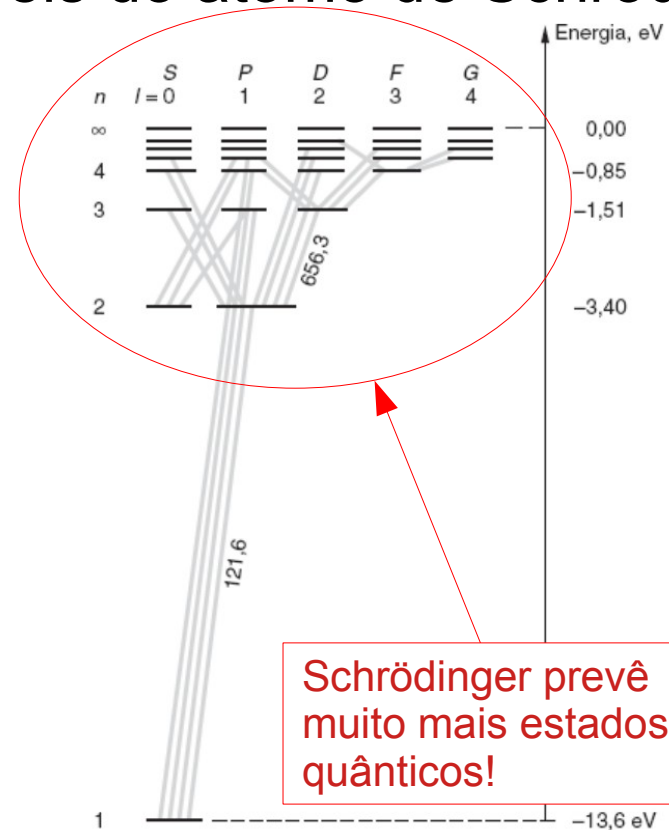


# Bohr Vs Schrödinger

## Níveis do átomo de Bohr



## Níveis do átomo de Schrödinger



# Em física moderna 2...

- O que a degenerescência do modelo de Schrödinger esconde?
  - Momento magnético orbital
  - Momento magnético intrínseco
  - Acoplamento spin-órbita
  - A estrutura fina do espectro de emissão
  - Probabilidades de transição