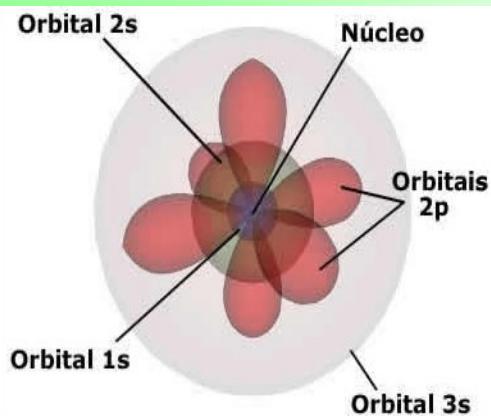


Cap. 7 – Átomos de um único elétron



átomo de hidrogênio



A solução da Equação de Schroedinger para átomos de único elétron resultou nas funções de ondas para energias $E_m = -Z^2 \cdot 13,6 \text{ eV} / n^2$ dados por:

$$\Psi_{n,l,ml}(r, \theta, \phi) = R_{n,l}(r) \cdot \Theta_{l,ml}(\theta) \cdot \Phi_{ml}(\phi)$$

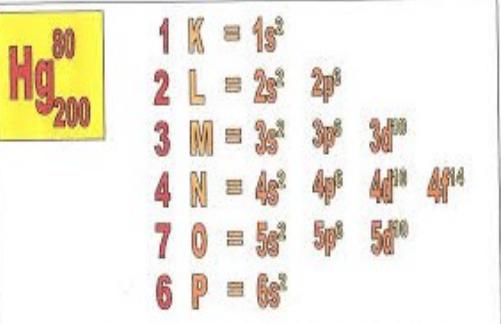
onde $m_l = -l, -l+1, \dots, 0, \dots, l-1, l$

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

Com I = 0,1,2,3....

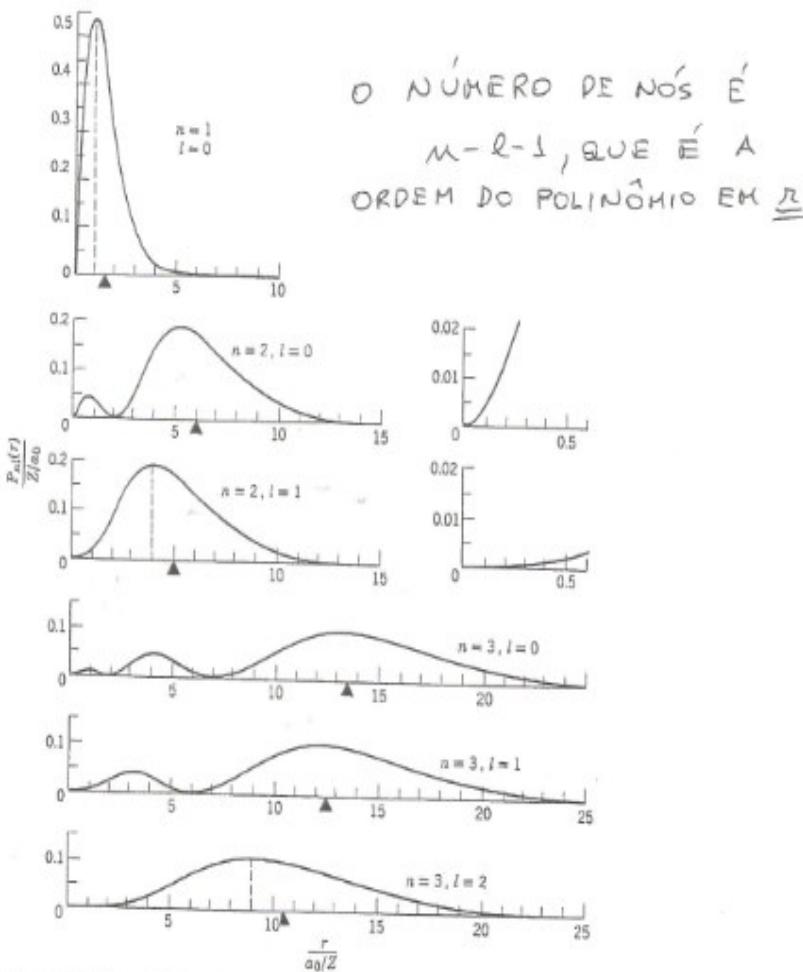
n é o número quântico principal, l ó número quântico orbital ou azimutal e m_l é o número quântico magnético.

1. Para cada valor de n existem n valores de l possíveis.
 2. Para cada valor de l existem $(2l+1)$ valores de m_l possíveis.
 3. Para cada valores de n , existe um total de n^2 autofunções degeneradas.



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Há várias maneiras de se visualizar as funções de ondas ou a densidade de probabilidade a elas associadas. Como $|\Psi(r, \theta, \phi)|^2$ é uma função de 3 variáveis é útil considerar as várias dependências separadamente. Para isso, definimos:



$$P_{n,l}(r) dr = |R_{n,l}(r)|^2 4\pi r^2 dr$$

que é a densidade de probabilidade radial que expressa a probabilidade de se encontrar a partícula na casca esférica de raio interno r e raio externo $r+dr$.

O raio médio aumenta de forma similar ao modelo de Bohr:

$$\langle r \rangle = \int_0^\infty r P_{n,l}(r) dr$$

$$\langle r \rangle = n^2 a_0 \left\{ 1 + \frac{1}{2} \left[1 - \frac{l(l+1)}{n^2} \right] \right\}$$

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A dependência com ϕ de $|\Psi(r, \theta, \phi)|^2$ desaparece. Assim podemos verificar a dependência com θ apenas através de um gráfico polar de $\Theta_{lml}^*(\theta)\Theta_{lml}(\theta)$.

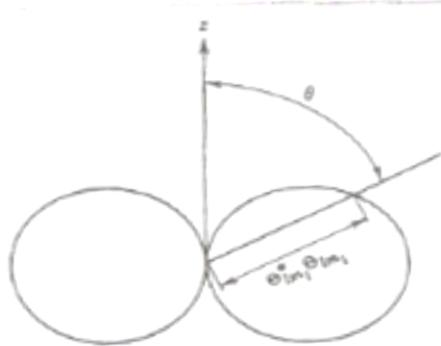


Figure 7-7 A polar diagram of the factor w determines the directional dependence of one-electron atom probability density.

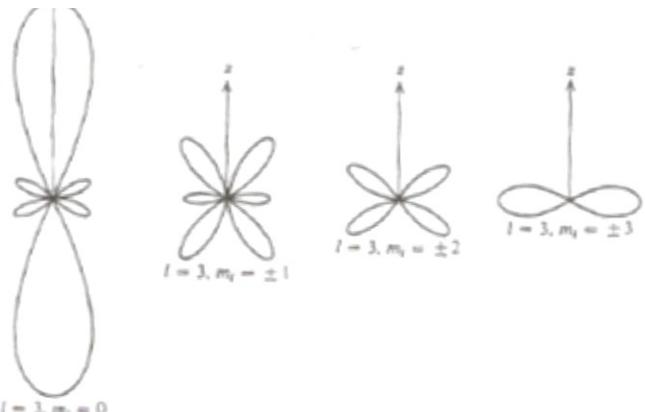


Figure 7-8 Polar diagrams of the directional dependence of the one-electron atom probability densities for $l = 3; m_l = 0, \pm 1, \pm 2, \pm 3$.

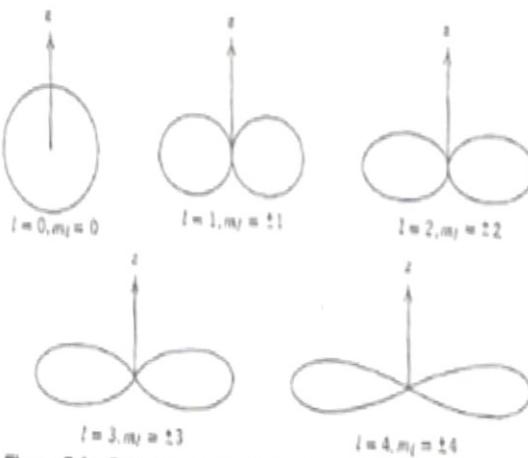


Figure 7-9 Polar diagrams of the directional dependence of the one-electron probability densities for $l = 0, 1, 2, 3, 4; m_l = \pm l$.

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A dependência global de $|\Psi(r, \theta, \phi)|^2$ com r e θ é mostrada através de “nuvens” de probabilidade tridimensionais.

Table 7-2 Some Eigenfunctions for the One-Electron Atom

Quantum Numbers			Eigenfunctions
n	l	m_l	
1	0	0	$\psi_{100} = \frac{1}{\sqrt{\pi}} \left(\frac{Z}{a_0}\right)^{3/2} e^{-Zr/a_0}$
2	0	0	$\psi_{200} = \frac{1}{4\sqrt{2\pi}} \left(\frac{Z}{a_0}\right)^{3/2} \left(2 - \frac{Zr}{a_0}\right) e^{-Zr/2a_0}$
2	1	0	$\psi_{210} = \frac{1}{4\sqrt{2\pi}} \left(\frac{Z}{a_0}\right)^{3/2} \frac{Zr}{a_0} e^{-Zr/2a_0} \cos \theta$
2	1	± 1	$\psi_{21\pm 1} = \frac{1}{8\sqrt{\pi}} \left(\frac{Z}{a_0}\right)^{3/2} \frac{Zr}{a_0} e^{-Zr/2a_0} \sin \theta e^{\pm i\phi}$
3	0	0	$\psi_{300} = \frac{1}{81\sqrt{6\pi}} \left(\frac{Z}{a_0}\right)^{3/2} \left(27 - 18\frac{Zr}{a_0} + 2\frac{Z^2 r^2}{a_0^2}\right) e^{-Zr/3a_0}$
3	1	0	$\psi_{310} = \frac{\sqrt{2}}{81\sqrt{\pi}} \left(\frac{Z}{a_0}\right)^{3/2} \left(6 - \frac{Zr}{a_0}\right) \frac{Zr}{a_0} e^{-Zr/3a_0} \cos \theta$
3	1	± 1	$\psi_{31\pm 1} = \frac{1}{81\sqrt{\pi}} \left(\frac{Z}{a_0}\right)^{3/2} \left(6 - \frac{Zr}{a_0}\right) \frac{Zr}{a_0} e^{-Zr/3a_0} \sin \theta e^{\pm i\phi}$
3	2	0	$\psi_{320} = \frac{1}{81\sqrt{6\pi}} \left(\frac{Z}{a_0}\right)^{3/2} \frac{Z^2 r^2}{a_0^2} e^{-Zr/3a_0} (3 \cos^2 \theta - 1)$
3	2	± 1	$\psi_{32\pm 1} = \frac{1}{81\sqrt{\pi}} \left(\frac{Z}{a_0}\right)^{3/2} \frac{Z^2 r^2}{a_0^2} e^{-Zr/3a_0} \sin \theta \cos \theta e^{\pm i\phi}$
3	2	± 2	$\psi_{32\pm 2} = \frac{1}{162\sqrt{\pi}} \left(\frac{Z}{a_0}\right)^{3/2} \frac{Z^2 r^2}{a_0^2} e^{-Zr/3a_0} \sin^2 \theta e^{\pm 2i\phi}$

Table 7-1 Possible Values of l and m_l for $n = 1, 2, 3$

n	1	2	3
l	0	0	0
m_l	0	0	-1, 0, +1
Number of degenerate eigenfunctions for each l	1	1	3
Number of degenerate eigenfunctions for each n	1	4	9

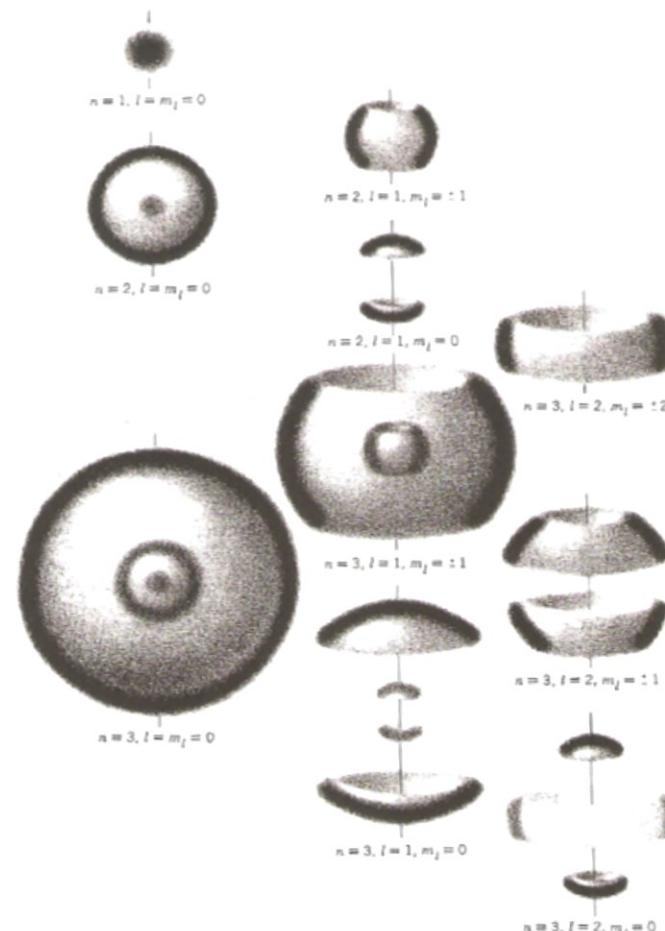


Figure 7-10 An artist's conception of the three-dimensional appearance of several one-electron atom probability density functions. For each of the drawings a line represents the z axis. If all the probability densities for a given n and l are combined, the result is spherically symmetrical.

Cap. 7 – Átomos de um único elétron – Momento Angular Orbital

Os números quânticos l e m_l estão ambos relacionados ao momento angular do elétron.

$$\langle L^2 \rangle = l(l + 1)\hbar^2$$

$$\langle L_x \rangle = 0$$

$$\langle L_z \rangle = m_l \hbar$$

$$\langle L_y \rangle = 0$$

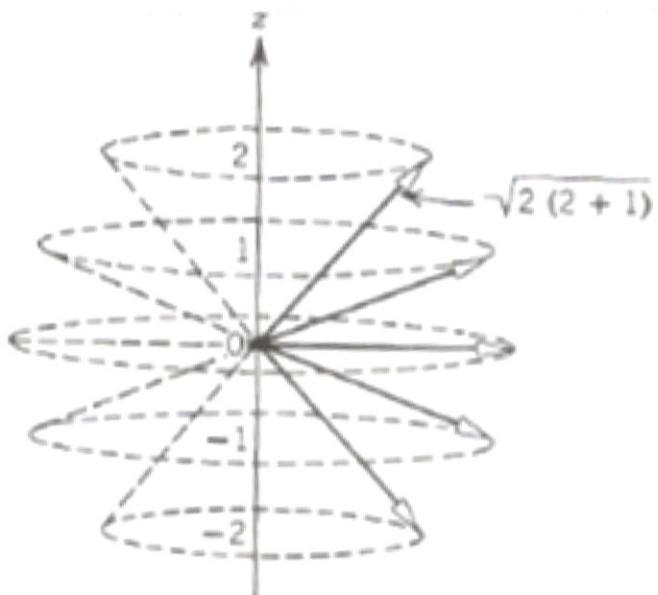


Figure 7-12 Representing the angular momentum vectors (measured in units of \hbar) for the possible states with $l = 2$. In each state the vector is equally likely to be found anywhere on a cone symmetrical about the z axis. It has a definite magnitude and z component but does not have a definite x or y component.