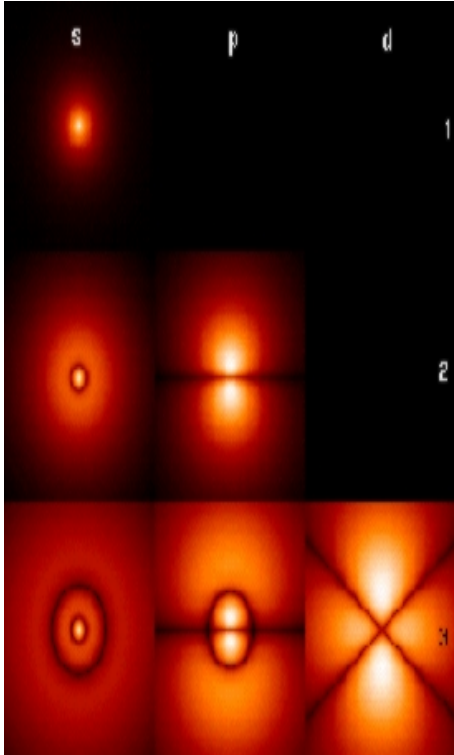


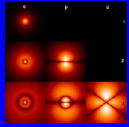
Átomos hidrogenoides

TEMA: ÁTOMOS HIDROGENOIDES

Introducción



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I.A. Hamiltoniano

- Átomos hidrogenoides \Rightarrow Un solo electrón. Ej. H, He⁺, Li²⁺, ...
- Hamiltoniano del sistema

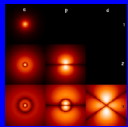
$$\hat{H}(x, y, z) = -\frac{\hbar^2}{2\mu} \left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} \right) - k \frac{Ze^2}{\underbrace{\sqrt{x^2 + y^2 + z^2}}_r}$$

- Partículas puntuales
- Nucleo fijo origen coordenadas $m_{\text{nucleo}} \gg m_e$

$$\mu = \frac{m_{\text{nucleo}} m_e}{m_{\text{nucleo}} + m_e} \simeq m_e$$

- Coordenadas polares esféricas

$$\hat{H}(r, \theta, \phi) = -\frac{\hbar^2}{2\mu} \left(\frac{1}{r^2} \frac{\partial}{\partial r} r^2 \frac{\partial}{\partial r} \right) + \frac{\hat{L}^2(\theta, \phi)}{2\mu r^2} - k \frac{Ze^2}{r}$$



I.A. Hamiltoniano: números cuánticos

- Funciones propias $\Rightarrow \hat{H}\psi_{n,l,m}(r, \theta, \phi) = E\psi_{n,l,m}(r, \theta, \phi)$

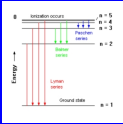
$$\psi_{n,l,m}(r, \theta, \phi) = \underbrace{R_{n,l}(r)}_{\text{radial}} \underbrace{Y_l^m(\theta, \phi)}_{\text{angular}}$$

- Origen de los números cuánticos

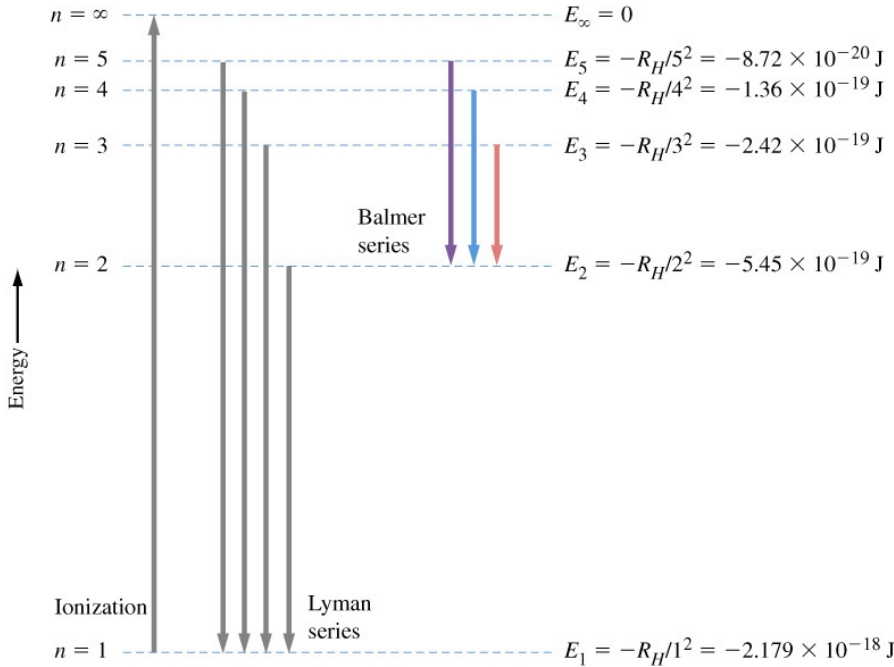
- $\psi(r, \theta, \phi) = \psi(r, \theta + 2\pi, \phi)$
- $\psi(r, \theta, \phi) = \psi(r, \theta, \phi + 2\pi)$
- $\lim_{r \rightarrow \infty} \psi(r, \theta, \phi) = 0$

- Valores discretos

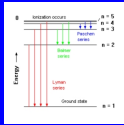
- $n = 1, 2, 3, \dots \Rightarrow \hat{H}\psi = E\psi \Rightarrow E = -\frac{\mu e^4 k^2 Z^2}{2\hbar^2 n^2}$
- $l = 0, 1, 2, \dots, n-1 \Rightarrow \hat{L}^2\psi = L^2\psi \Rightarrow L^2 = l(l+1)\hbar^2$
- $m = -l, -l+1, \dots, 0, \dots, l-1, l \Rightarrow \hat{L}_z\psi = L_z\psi \Rightarrow L_z = m\hbar$



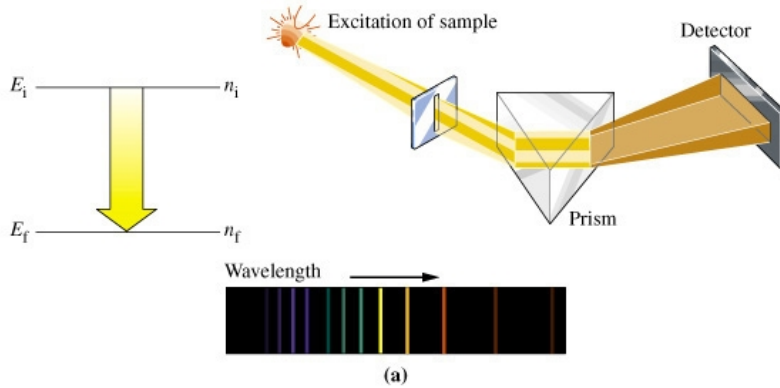
I.B. Niveles de energía



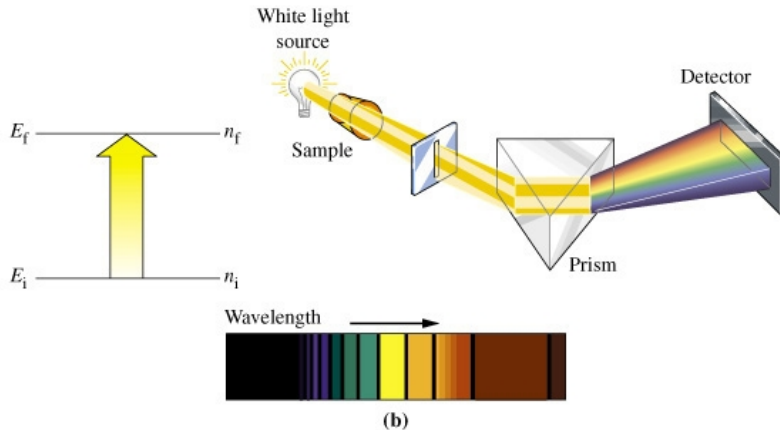
$$E_n = - \underbrace{\frac{\mu e^4 k^2 Z^2}{2 \hbar^2}}_{R_H} \frac{1}{n^2}$$



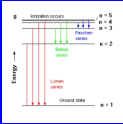
I.B. Niveles de energía: espectroscopía



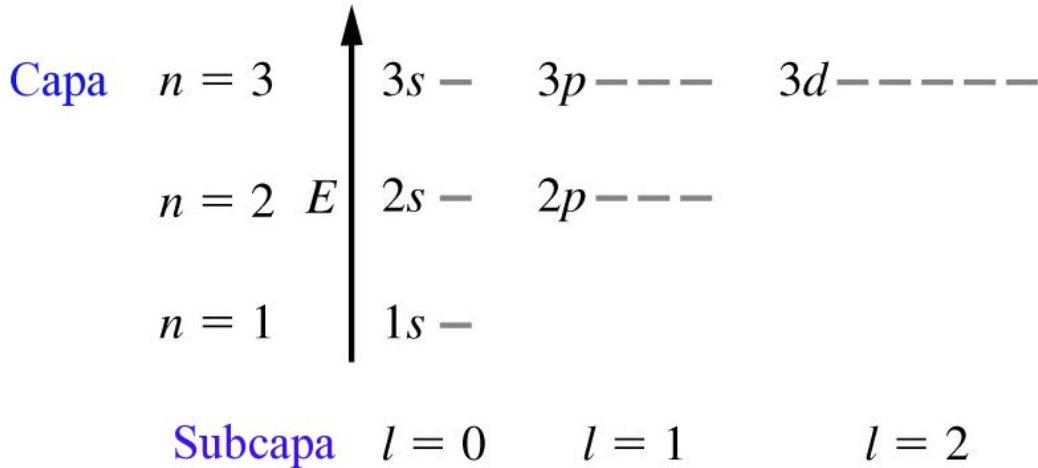
- Emisión



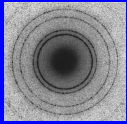
- Absorción



I.B. Niveles de energía: capas y subcapas



- Degeneración subcapa $\Rightarrow 2l + 1$
- Degeneración capa $\Rightarrow \sum_{l=0}^{n-1} (2l + 1)$



I.C. Orbitales atómicos

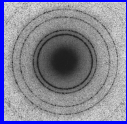
- Densidad de probabilidad

$$|\Psi_{n,l,m}(r, \theta, \phi)|^2 = \underbrace{|R_{n,l}(r)|^2}_{\text{radial}} \underbrace{|Y_l^m(\theta, \phi)|^2}_{\text{angular}}$$

- Funciones radiales

n	l	$R_{n,l}(r)$
1	0	$2 \left(\frac{Z}{a'_o}\right)^{3/2} e^{-Zr/a'_o}$
2	0	$\frac{1}{2\sqrt{2}} \left(\frac{Z}{a'_o}\right)^{3/2} \left(2 - \frac{Zr}{a'_o}\right) e^{-Zr/2a'_o}$
2	1	$\frac{1}{2\sqrt{6}} \left(\frac{Z}{a'_o}\right)^{3/2} \frac{Zr}{a'_o} e^{-Zr/2a'_o}$

$a'_o = \hbar^2 / k\mu e^2 = a_o m_e / \mu$



I.C. Orbitales atómicos: distribución radial

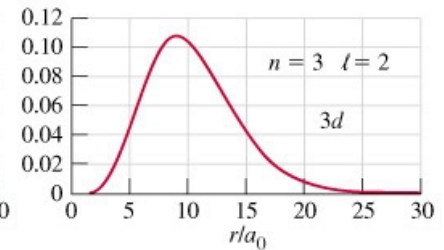
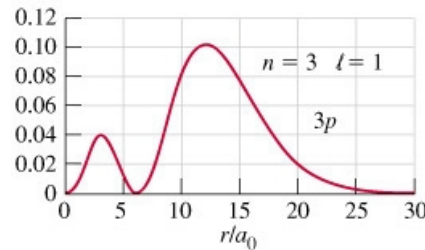
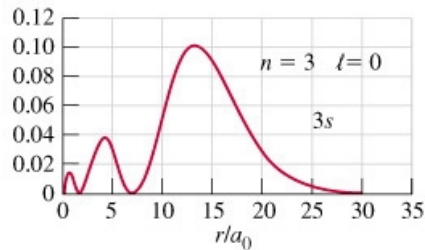
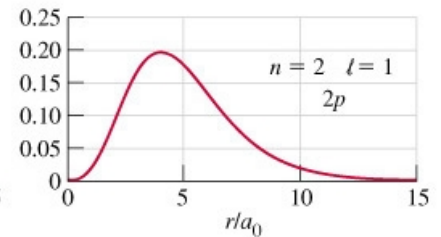
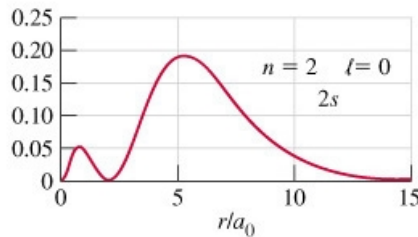
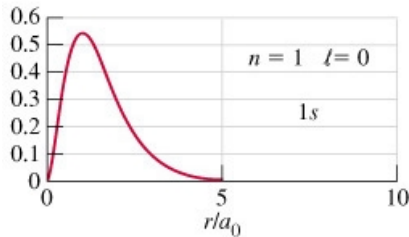
ÁTOMOS HIDROGENOIDES

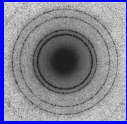
I. Ec. de Schrödinger para átomos hidrógenoides



- Función de distribución radial $\Rightarrow |R_{n,l}(r)|^2 r^2$

$$P(r \in (a, b)) = \int_a^b |R_{n,l}(r)|^2 r^2 dr$$

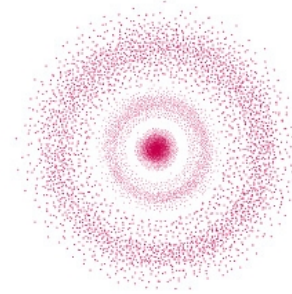
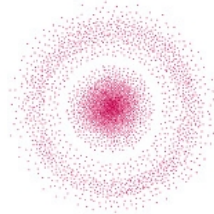
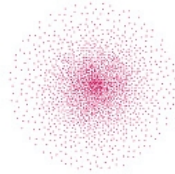
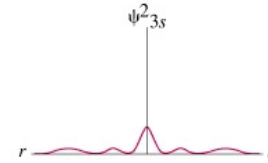
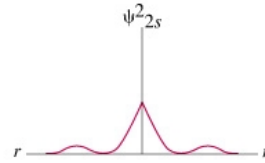
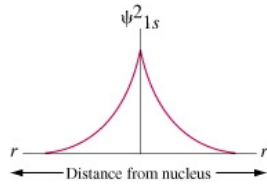




I.C. Orbitales atómicos: orbitales s

ÁTOMOS HIDROGENOIDES

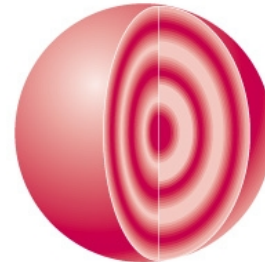
I. Ec. de Schrödinger para átomos hidrógenoides



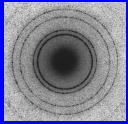
(a) 1s



(b) 2s



(c) 3s

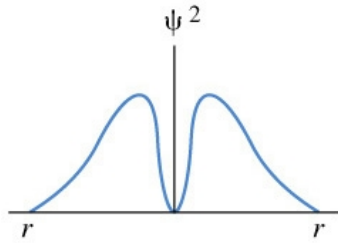


I.C. Orbitales atómicos: orbitales p

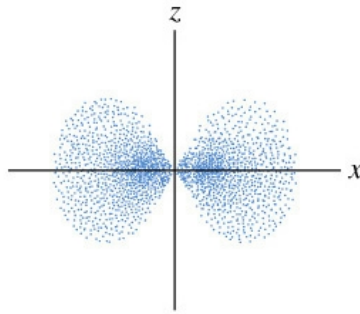
ÁTOMOS HIDROGENOIDES

I. Ec. de Schrödinger para átomos hidrógenoides

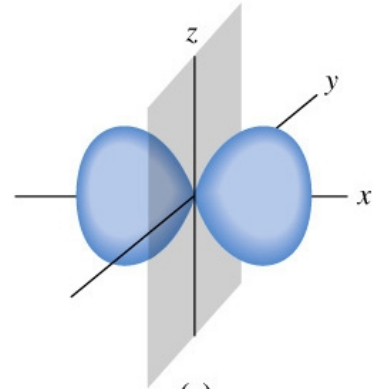
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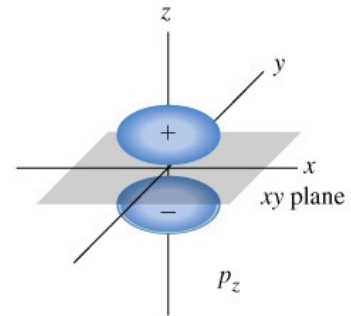
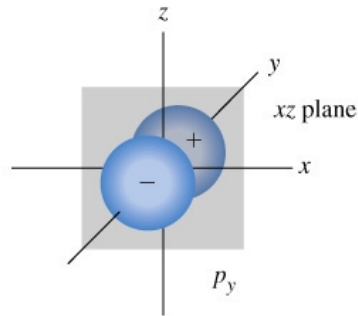
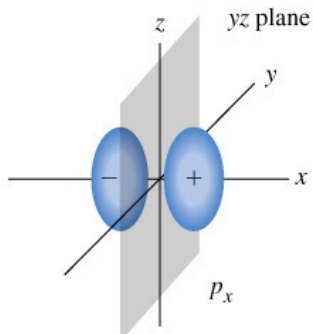
(a)

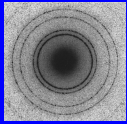


(b)



(c)



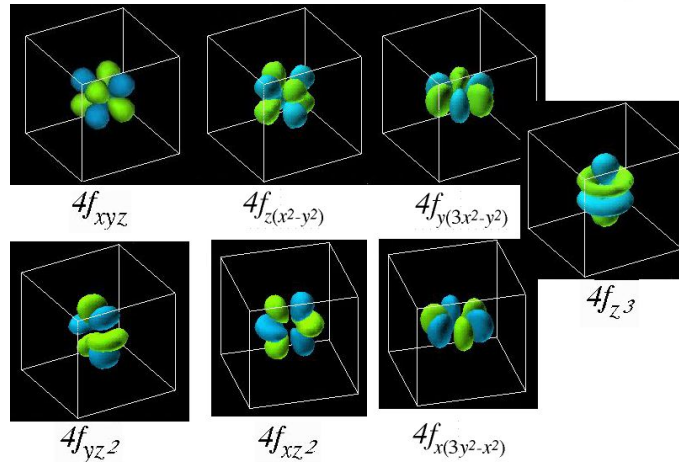
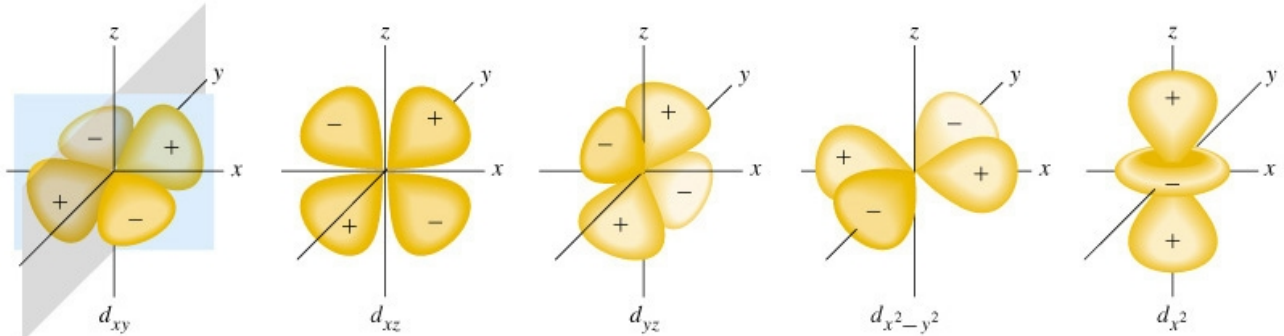


I.C. Orbitales atómicos: orbitales d y f

ÁTOMOS HIDROGENOIDES

I. Ec. de Schrödinger para átomos hidrógenoides

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I.D. El espín electrónico

- Medidas experimentales de desdoblamiento energético
- Dirac \Rightarrow Efectos relativistas \Rightarrow Momento angular intrínseco

$$\hat{S}^2 = \hat{S}_x^2 + \hat{S}_y^2 + \hat{S}_z^2$$

$$\hat{S}^2 f = s(s+1)\hbar^2 f; \quad s = 0, \frac{1}{2}, 1, \frac{3}{2}, \dots \left\{ \begin{array}{l} \text{bosones} \Rightarrow \text{entero} \\ \text{fermiones} \Rightarrow \text{semientero} \end{array} \right.$$

$$\hat{S}_z f = m_s \hbar f; \quad m_s = -s, -s+1, \dots, s-1, s$$

- $e^- \Rightarrow s = \frac{1}{2} \Rightarrow m_s = \pm \frac{1}{2} \Rightarrow \left\{ \begin{array}{l} \hat{S}_z \alpha = \frac{1}{2} \alpha \\ \hat{S}_z \beta = -\frac{1}{2} \beta \end{array} \right.$

$$\Psi_{n,l,m,m_s} = \Psi_{n,l,m}(r, \theta, \phi) S_{m_s}$$



I.D. El espín electrónico: Principio de Pauli

- Partículas indistinguibles $\left\{ \begin{array}{l} q_1 = (x_1, y_1, z_1, m_{s,1}) \\ q_2 = (x_2, y_2, z_2, m_{s,2}) \\ \vdots \\ q_n = (x_n, y_n, z_n, m_{s,n}) \end{array} \right.$

$$\begin{array}{ccc} \Psi(q_1, q_2, \dots, q_i, \dots, q_j, \dots, q_n) & & \Psi(q_1, q_2, \dots, q_j, \dots, q_i, \dots, q_n) \\ \downarrow & & \downarrow \\ |\Psi(q_1, q_2, \dots, q_i, \dots, q_j, \dots, q_n)|^2 & \equiv & |\Psi(q_1, q_2, \dots, q_j, \dots, q_i, \dots, q_n)|^2 \end{array}$$

- La función de onda de un sistema de electrones (fermiones) debe de ser antisimétrica con respecto al intercambio de dos electrones cualesquiera.

$$\Psi(q_1, q_2, \dots, q_i, \dots, q_j, \dots, q_n) = -\Psi(q_1, q_2, \dots, q_j, \dots, q_i, \dots, q_n)$$



I.D. El espín electrónico: Principio de Pauli

- Consecuencia. Si el e^- 2 tiene las mismas coordenadas que el e^- 1 entonces

$$\Psi(q_1, q_1, \dots, q_i, \dots, q_j, \dots, q_n) = -\Psi(q_1, q_1, \dots, q_i, \dots, q_j, \dots, q_n)$$

$$\Psi(q_1, q_1, \dots, q_i, \dots, q_j, \dots, q_n) = 0$$

$$|\Psi(q_1, q_1, \dots, q_i, \dots, q_j, \dots, q_n)|^2 = 0 \Rightarrow \text{repulsión de Pauli}$$