

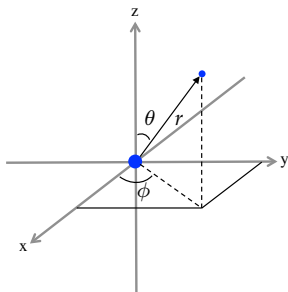
Estructura de la Materia

Átomo de Hidrógeno

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ÁTOMO DE HIDRÓGENO



$$\Psi(r, \theta, \phi) = R(r) \Theta(\theta) \Phi(\phi) \quad (1)$$

$$\hat{H} = -\frac{\hbar^2}{2\mu} \nabla^2 - \frac{kZe^2}{r} \quad (2)$$

$$\hat{H}\Psi(r, \theta, \phi) = E\Psi(r, \theta, \phi) \quad (3)$$

SOLUCIONES DE ÁTOMO DE HIDRÓGENO

$$\Psi_{n,l,m}(r, \theta, \phi) = \underbrace{R_{n,l}(r)}_{\text{radial}} \underbrace{\Theta_{l,m}(\theta) \Phi_m(\phi)}_{\text{angular}} \quad (4)$$

$$\Psi_{n,l,m}(r, \theta, \phi) = R_{n,l}(r) Y_{l,m}(\theta, \phi) \quad (5)$$

$$E_n = -\frac{1}{2} \frac{kZ^2 e^2}{n^2 a_0} \quad (6)$$

Números cuánticos

n	número cuántico principal (nivel de energía)	$n = 1, 2, 3, \dots$	
l	número cuántico asociado al momento angular orbital (forma del orbital)	$l = 0, 1, 2, \dots, n - 1$	$l = 0 \rightarrow s$ $l = 1 \rightarrow p$ $l = 2 \rightarrow d$ $l = 3 \rightarrow f$...
m	número cuántico asociado a la componente en z del mo- mento angular (orientación del orbital)	$m = -l, -l + 1, \dots, 0, \dots, l - 1, l$	

- Funciones radiales $R_{n,l}(r)$

$$R_{n,l}(r) = r^l e^{Zr/na_0} \sum_{j=0}^{n-l-1} C_j r^j \quad (7)$$

- Funciones angulares $Y_{l,m}(\theta, \phi)$

$$Y_{l,m}(\theta, \phi) = \left[\frac{2l+1}{4\pi} \frac{(l-|m|)!}{(l+|m|)!} \right]^{1/2} P_{l,m}(w) e^{im\phi} \quad (8)$$

$$P_{l,m}(w) = (1-w^2)^{|m|/2} \frac{d^{|m|}}{dw^{|m|}} P_l(w) \quad ; \quad w = \cos \theta$$

$$P_l(w) = \begin{cases} P_0(w) = 1 \\ P_1(w) = w \\ P_2(w) = \frac{1}{2}(3w^2 - 1) \\ P_3(w) = \frac{1}{2}(5w^3 - 3w) \dots \end{cases}$$

Funciones radiales del átomo de hidrógeno

n	l	$R_{n,l}(r)$
1	0	$2 \left(\frac{Z}{a_0}\right)^{3/2} e^{-Zr/a_0}$
2	0	$\frac{1}{2\sqrt{2}} \left(\frac{Z}{a_0}\right)^{3/2} \left(2 - \frac{Zr}{a_0}\right) e^{-Zr/2a_0}$
2	1	$\frac{1}{2\sqrt{6}} \left(\frac{Z}{a_0}\right)^{3/2} \left(\frac{Zr}{a_0}\right) e^{-Zr/2a_0}$
3	0	$\frac{2}{81\sqrt{3}} \left(\frac{Z}{a_0}\right)^{3/2} \left[2 \left(\frac{Zr}{a_0}\right)^2 - 18 \left(\frac{Zr}{a_0}\right) + 27\right] e^{-Zr/3a_0}$
3	1	$\frac{2\sqrt{2}}{81\sqrt{3}} \left(\frac{Z}{a_0}\right)^{3/2} \left[6 - \left(\frac{Zr}{a_0}\right)\right] \left(\frac{Zr}{a_0}\right) e^{-Zr/3a_0}$
3	2	$\frac{2\sqrt{2}}{81\sqrt{15}} \left(\frac{Z}{a_0}\right)^{3/2} \left(\frac{Zr}{a_0}\right)^2 e^{-Zr/3a_0}$

Funciones angulares del átomo de hidrógeno

l	m	$Y_{l,m}(\theta, \phi) = \Theta_{l,m}(\theta) \Phi_m(\phi)$
0	0	$(1/4\pi)^{1/2}$
1	0	$(3/4\pi)^{1/2} \cos \theta$
1	1	$(3/8\pi)^{1/2} \operatorname{sen} \theta e^{i\phi}$
1	-1	$(3/8\pi)^{1/2} \operatorname{sen} \theta e^{-i\phi}$
2	0	$(5/16\pi)^{1/2} (3 \cos^2 \theta - 1)$
2	1	$(15/8\pi)^{1/2} \operatorname{sen} \theta \cos \theta e^{i\phi}$
2	-1	$(15/8\pi)^{1/2} \operatorname{sen} \theta \cos \theta e^{-i\phi}$
2	2	$(15/32\pi)^{1/2} \operatorname{sen}^2 \theta e^{2i\phi}$
2	-2	$(15/32\pi)^{1/2} \operatorname{sen}^2 \theta e^{-2i\phi}$

Funciones del hidrógeno

n	l	m	$\Psi_{n,l,m}(r, \theta, \phi) = R_{n,l}(r) Y_{l,m}(\theta, \phi)$	Orbital
1	0	0	$\Psi_{1,0,0}(r, \theta, \phi) = R_{1,0}(r) Y_{0,0}(\theta, \phi)$	Ψ_{1s}
2	0	0	$\Psi_{2,0,0}(r, \theta, \phi) = R_{2,0}(r) Y_{0,0}(\theta, \phi)$	Ψ_{2s}
2	1	0	$\Psi_{2,1,0}(r, \theta, \phi) = R_{2,1}(r) Y_{1,0}(\theta, \phi)$	Ψ_{2p_0}
2	1	1	$\Psi_{2,1,1}(r, \theta, \phi) = R_{2,1}(r) Y_{1,1}(\theta, \phi)$	Ψ_{2p_1}
2	1	-1	$\Psi_{2,1,-1}(r, \theta, \phi) = R_{2,1}(r) Y_{1,-1}(\theta, \phi)$	$\Psi_{2p_{-1}}$
3	0	0	$\Psi_{3,0,0}(r, \theta, \phi) = R_{3,0}(r) Y_{0,0}(\theta, \phi)$	Ψ_{3s}
3	1	0	$\Psi_{3,1,0}(r, \theta, \phi) = R_{3,1}(r) Y_{1,0}(\theta, \phi)$	Ψ_{3p_0}
3	1	1	$\Psi_{3,1,1}(r, \theta, \phi) = R_{3,1}(r) Y_{1,1}(\theta, \phi)$	Ψ_{3p_1}
3	1	-1	$\Psi_{3,1,-1}(r, \theta, \phi) = R_{3,1}(r) Y_{1,-1}(\theta, \phi)$	$\Psi_{3p_{-1}}$
3	2	0	$\Psi_{3,2,0}(r, \theta, \phi) = R_{3,2}(r) Y_{2,0}(\theta, \phi)$	Ψ_{3d_0}
3	2	1	$\Psi_{3,2,1}(r, \theta, \phi) = R_{3,2}(r) Y_{2,1}(\theta, \phi)$	Ψ_{3d_1}
3	2	-1	$\Psi_{3,2,-1}(r, \theta, \phi) = R_{3,2}(r) Y_{2,-1}(\theta, \phi)$	$\Psi_{3d_{-1}}$
3	2	2	$\Psi_{3,2,2}(r, \theta, \phi) = R_{3,2}(r) Y_{2,2}(\theta, \phi)$	Ψ_{3d_2}
3	2	-2	$\Psi_{3,2,-2}(r, \theta, \phi) = R_{3,2}(r) Y_{2,-2}(\theta, \phi)$	$\Psi_{3d_{-2}}$

NIVELES DE ENERGÍA DEL ÁTOMO DE HIDRÓGENO

$$E_n = -\frac{1}{2} \frac{kZ^2 e^2}{n^2 a_0}$$

$n \rightarrow$ número cuántico principal

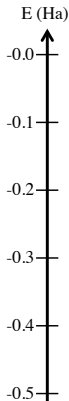
E (Ha)



NIVELES DE ENERGÍA DEL ÁTOMO DE HIDRÓGENO

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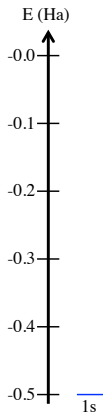
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NIVELES DE ENERGÍA DEL ÁTOMO DE HIDRÓGENO

$$E_n = -\frac{1}{2} \frac{kZ^2 e^2}{n^2 a_0}$$

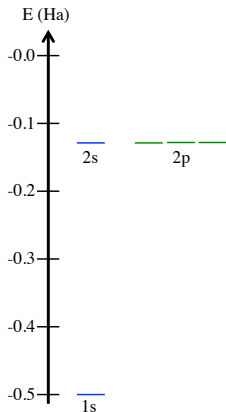
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NIVELES DE ENERGÍA DEL ÁTOMO DE HIDRÓGENO

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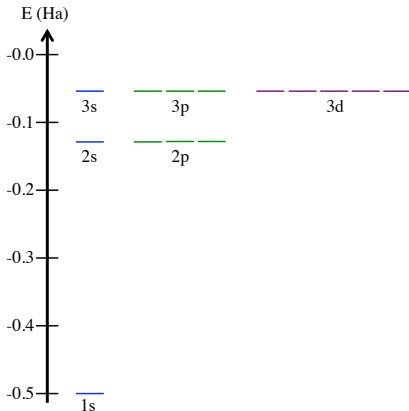
$n \rightarrow$ número cuántico principal



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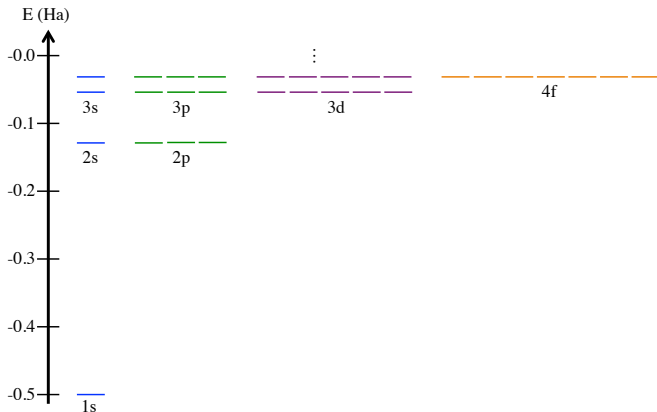
$n \rightarrow$ número cuántico principal



NIVELES DE ENERGÍA DEL ÁTOMO DE HIDRÓGENO

$$E_n = -\frac{1}{2} \frac{kZ^2 e^2}{n^2 a_0}$$

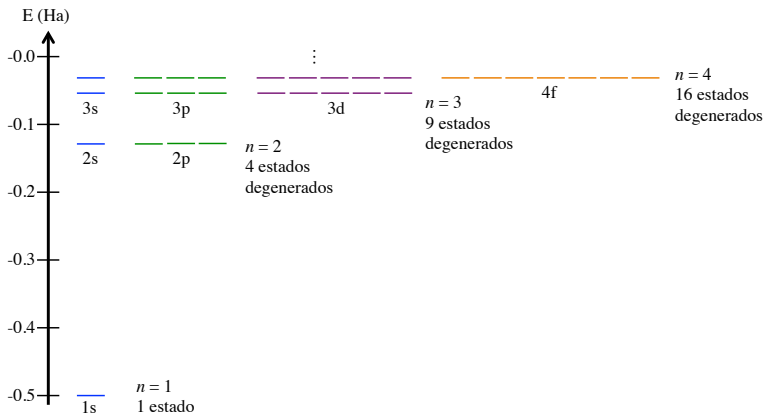
$n \rightarrow$ número cuántico principal



NIVELES DE ENERGÍA DEL ÁTOMO DE HIDRÓGENO

$$E_n = -\frac{1}{2} \frac{kZ^2 e^2}{n^2 a_0}$$

$n \rightarrow$ número cuántico principal



ANÁLISIS DE LA PARTE RADIAL

$\Psi \rightarrow$ Contiene toda la información del sistema

No tiene significado físico

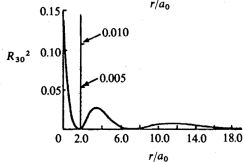
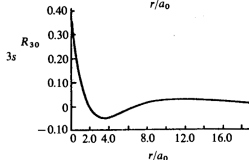
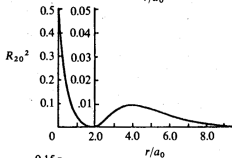
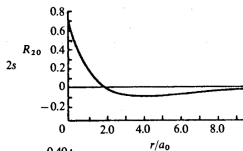
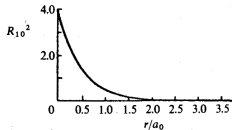
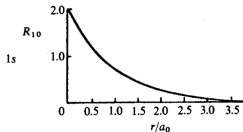
$|\Psi|^2 \rightarrow$ Densidad de probabilidad(ρ)

$$\rho(r, \theta, \phi) = |\Psi(r, \theta, \phi)|^2 = |R(r)|^2 |\Theta(\theta)|^2 |\Phi(\phi)|^2 \quad (9)$$

$$\rho(r, \theta, \phi) = |\Psi(r, \theta, \phi)|^2 = \underbrace{|R(r)|^2}_{\text{radial}} |Y(\theta, \phi)|^2 \quad (10)$$

- $R_{n,l}(r)$ es función de la distancia al núcleo
- $R_{n,l}(r)$ depende de los números cuánticos n y l
- Número de nodos, penetración de las funciones y funciones difusas o localizadas

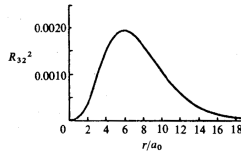
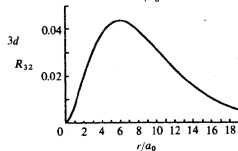
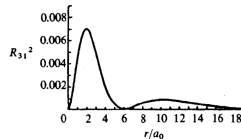
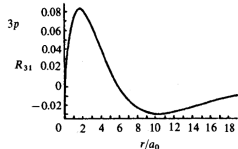
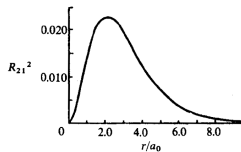
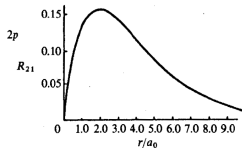
Funciones 1s, 2s y 3s:



- En las funciones s la ρ es distinta de cero en el origen, su valor disminuye al aumentar n
- Nodos \rightarrow están asociados con cambios de signo en la función:

$$ns \rightarrow n - 1 \text{ nodos}$$

Funciones 2p, 3p, 3d:



- En las funciones p y d la ρ es cero en el origen
- El número de nodos depende de n y l para cualquier tipo de función:
número de nodos = $n - l - 1$ nodos

FUNCIÓN DE DISTRIBUCIÓN RADIAL

$$\int_{-\infty}^{\infty} |\Psi|^2 d\tau = 1 \quad (11)$$

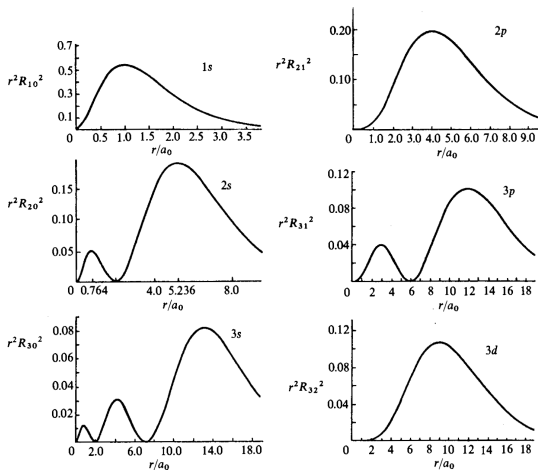
$$\int_0^{\infty} \int_0^{\pi} \int_0^{2\pi} |R(r)|^2 |\Theta(\theta)|^2 |\Phi(\phi)|^2 r^2 \operatorname{sen} \theta d\phi d\theta dr = 1 \quad (12)$$

$$\int_0^{\infty} |R(r)|^2 r^2 dr \int_0^{\pi} \int_0^{2\pi} |\Theta(\theta)|^2 |\Phi(\phi)|^2 \operatorname{sen} \theta d\phi d\theta = 1 \quad (13)$$

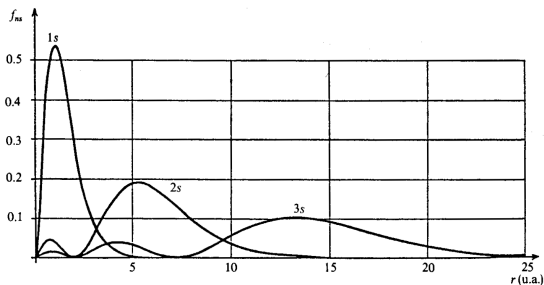
Si la parte angular está normalizada:

$$\int_0^{\infty} \underbrace{|R(r)|^2 r^2}_{\text{función de distribución radial}} dr = 1 \quad (14)$$

Funciones de distribución radial:



- Orbitales difusos → Que tan extendida se vuelve la función
- Este comportamiento es más evidente al cambiar de nivel de energía (n)



$$3s > 2s > 1s$$

El orbital 3s es más difuso que el 2s y este a su vez es más difuso que el 1s

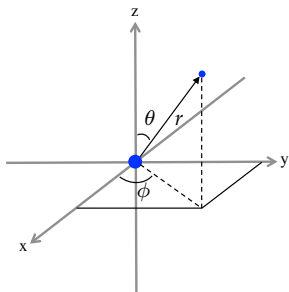
ANÁLISIS DE LA PARTE ANGULAR

$$\Psi_{n,l,m}(r, \theta, \phi) = R_{n,l}(r) \underbrace{\Theta_{l,m}(\theta) \Phi_m(\phi)}_{\text{angular}} \quad (15)$$

$$\Psi_{n,l,m}(r, \theta, \phi) = R_{n,l}(r) Y_{l,m}(\theta, \phi) \quad (16)$$

n	l	m	$\Psi_{n,l,m}(r, \theta, \phi) = R_{n,l}(r) Y_{l,m}(\theta, \phi)$	Orbital
1	0	0	$\Psi_{1,0,0}(r, \theta, \phi) = R_{1,0}(r) (1/4\pi)^{1/2}$	Ψ_{1s}
2	0	0	$\Psi_{2,0,0}(r, \theta, \phi) = R_{2,0}(r) (1/4\pi)^{1/2}$	Ψ_{2s}
2	1	0	$\Psi_{2,1,0}(r, \theta, \phi) = R_{2,1}(r) (3/4\pi)^{1/2} \cos \theta$	Ψ_{2p_0}
2	1	1	$\Psi_{2,1,1}(r, \theta, \phi) = R_{2,1}(r) (3/8\pi)^{1/2} \sen \theta e^{i\phi}$	Ψ_{2p_1}
2	1	-1	$\Psi_{2,1,-1}(r, \theta, \phi) = R_{2,1}(r) (3/8\pi)^{1/2} \sen \theta e^{-i\phi}$	$\Psi_{2p_{-1}}$

- Las funciones son imaginarias excepto cuando $m = 0$
- Para eliminar la parte imaginaria hay que hacer combinaciones lineales



$$r, \theta, \phi \rightarrow x, y, z$$

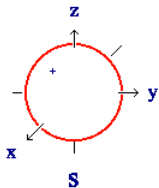
$$z = r \cos \theta \tag{17}$$

$$y = r \sin \theta \sin \phi \tag{18}$$

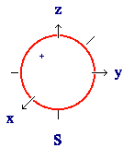
$$x = r \sin \theta \cos \phi \tag{19}$$

Función s:

- $l = 0, m = 0$
- $Y_{0,0}(\theta, \phi) = (1/4\pi)^{1/2}$
- $Y_{0,0}(\theta, \phi)$ no depende de θ ni de $\phi \rightarrow$ se define una esfera



$Y_{0,0}(\theta, \phi)$

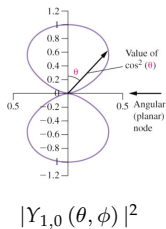
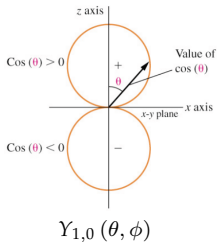


$|Y_{0,0}(\theta, \phi)|^2$

- No hay nodos en la función (planos nodales)
- La probabilidad de encontrar al electrón es independiente de la dirección

Función p:

- $l = 1, m = 0$
- $Y_{1,0}(\theta, \phi) = (3/4\pi)^{1/2} \cos \theta$



- Función p_z
- Hay un plano nodal
- La probabilidad de encontrar al electrón es mayor sobre el eje z

Función p :

- $l = 1, m = 1 \quad \rightarrow \quad Y_{1,1}(\theta, \phi) = (3/8\pi)^{1/2} \text{sen } \theta e^{i\phi}$
- $l = 1, m = -1 \quad \rightarrow \quad Y_{1,-1}(\theta, \phi) = (3/8\pi)^{1/2} \text{sen } \theta e^{-i\phi}$

Se hacen combinaciones lineales:

$$Y_{p+}(\theta, \phi) = \frac{1}{\sqrt{2}} [Y_{1,1} + Y_{1,-1}] \quad (20)$$

$$Y_{p-}(\theta, \phi) = \frac{1}{i\sqrt{2}} [Y_{1,1} - Y_{1,-1}] \quad (21)$$

Además, la función exponencial compleja se puede escribir como:

$$e^{i\phi} = \cos \phi + i \text{sen } \phi \quad (22)$$

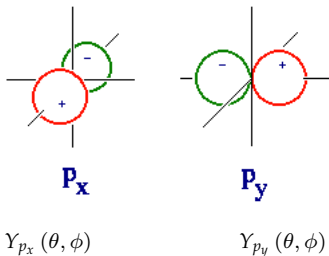
$$e^{i\phi} + e^{-i\phi} = \cos \phi + i \text{sen } \phi + \cos \phi - i \text{sen } \phi = 2 \cos \phi \quad (23)$$

$$e^{i\phi} - e^{-i\phi} = \cos \phi + i \text{sen } \phi - \cos \phi + i \text{sen } \phi = 2i \text{sen } \phi \quad (24)$$

$$\begin{aligned}
Y_{p+}(\theta, \phi) &= \frac{1}{\sqrt{2}} [Y_{1,1} + Y_{1,-1}] \\
&= \frac{1}{\sqrt{2}} \left[\left(\frac{3}{8\pi} \right)^{1/2} \text{sen } \theta e^{i\phi} + \left(\frac{3}{8\pi} \right)^{1/2} \text{sen } \theta e^{-i\phi} \right] \\
&= \frac{1}{\sqrt{2}} \left(\frac{3}{8\pi} \right)^{1/2} \text{sen } \theta [e^{i\phi} + e^{-i\phi}] \\
&= \frac{1}{2} \left(\frac{3}{4\pi} \right)^{1/2} \text{sen } \theta [2 \cos \phi] \\
&= \left(\frac{3}{4\pi} \right)^{1/2} \text{sen } \theta \cos \phi \\
&= Y_{p_x}(\theta, \phi)
\end{aligned} \tag{25}$$

$$\begin{aligned}
Y_{p-}(\theta, \phi) &= \frac{1}{i\sqrt{2}} [Y_{1,1} - Y_{1,-1}] \\
&= \frac{1}{i\sqrt{2}} \left[\left(\frac{3}{8\pi}\right)^{1/2} \text{sen } \theta e^{i\phi} - \left(\frac{3}{8\pi}\right)^{1/2} \text{sen } \theta e^{-i\phi} \right] \\
&= \frac{1}{i\sqrt{2}} \left(\frac{3}{8\pi}\right)^{1/2} \text{sen } \theta [e^{i\phi} - e^{-i\phi}] \\
&= \frac{1}{2i} \left(\frac{3}{4\pi}\right)^{1/2} \text{sen } \theta [2i \text{sen } \phi] \\
&= \left(\frac{3}{4\pi}\right)^{1/2} \text{sen } \theta \text{sen } \phi \\
&= Y_{p_y}(\theta, \phi)
\end{aligned} \tag{26}$$

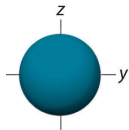
Funciones p_x y p_y :



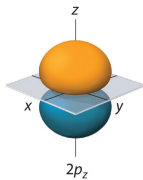
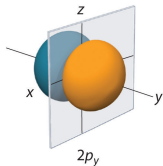
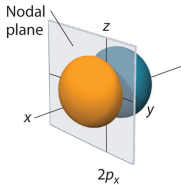
- Cada una tiene un plano nodal
- $|Y|^2 \rightarrow$ La probabilidad de encontrar al electrón es mayor sobre los ejes x y y respectivamente

Planos nodales:

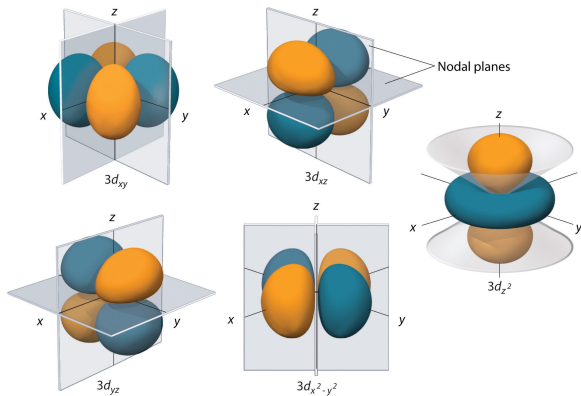
- La función s ($l = 0$) no tiene planos nodales



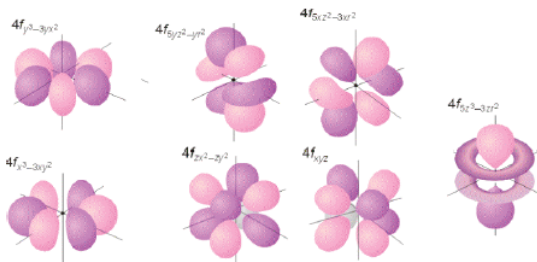
- Las funciones p ($l = 1$) tienen 1 plano nodal



- Las funciones d ($l = 2$) tienen 2 planos nodales



- Las funciones f ($l = 3$) tienen 3 planos nodales



- Las funciones angulares ($Y_{l,m}(\theta, \phi)$) tienen l planos nodales
- Las funciones radiales ($R_{n,l}(\theta, \phi)$) tienen $n - l - 1$ planos nodales
- Las funciones totales ($\Psi_{n,l,m}(\theta, \phi)$) tienen $n - 1$ planos nodales

$$\underbrace{\Psi_{n,l,m}(r, \theta, \phi)}_{n-1} = \underbrace{R_{n,l}(r)}_{n-l-1} \underbrace{Y_{l,m}(\theta, \phi)}_l$$

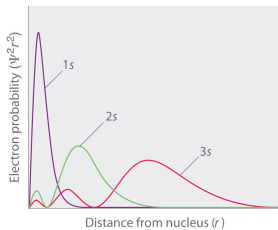
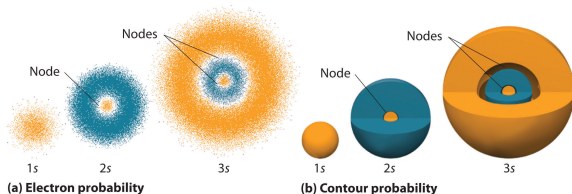
FUNCIONES DE ONDA REALES

Tabla 3: Funciones de onda hidrogenoides reales

$\Psi_{n,l,m}(r, \theta, \phi) = R_{n,l}(r)Y_{l,m}(\theta, \phi)$
$1s = \frac{1}{\pi^{1/2}} \left(\frac{Z}{a_0} \right)^{3/2} e^{-Zr/a_0}$
$2s = \frac{1}{4(2\pi)^{1/2}} \left(\frac{Z}{a_0} \right)^{3/2} \left(2 - \frac{Zr}{a_0} \right) e^{-Zr/2a_0}$
$2p_z = \frac{1}{4(2\pi)^{1/2}} \left(\frac{Z}{a_0} \right)^{5/2} r e^{-Zr/2a_0} \cos \theta$
$2p_x = \frac{1}{4(2\pi)^{1/2}} \left(\frac{Z}{a_0} \right)^{5/2} r e^{-Zr/2a_0} \sin \theta \cos \phi$
$2p_y = \frac{1}{4(2\pi)^{1/2}} \left(\frac{Z}{a_0} \right)^{5/2} r e^{-Zr/2a_0} \sin \theta \sin \phi$
$3s = \frac{1}{81(3\pi)^{1/2}} \left(\frac{Z}{a_0} \right)^{3/2} \left(27 - 18 \frac{Zr}{a_0} + 2 \frac{Z^2 r^2}{a_0^2} \right) e^{-Zr/3a_0}$
$3p_z = \frac{2^{1/2}}{81\pi^{1/2}} \left(\frac{Z}{a_0} \right)^{5/2} \left(6 - \frac{Zr}{a_0} \right) r e^{-Zr/3a_0} \cos \theta$
$3p_x = \frac{2^{1/2}}{81\pi^{1/2}} \left(\frac{Z}{a_0} \right)^{5/2} \left(6 - \frac{Zr}{a_0} \right) r e^{-Zr/3a_0} \sin \theta \cos \phi$
$3p_y = \frac{2^{1/2}}{81\pi^{1/2}} \left(\frac{Z}{a_0} \right)^{5/2} \left(6 - \frac{Zr}{a_0} \right) r e^{-Zr/3a_0} \sin \theta \sin \phi$
$3d_{z^2} = \frac{1}{81(6\pi)^{1/2}} \left(\frac{Z}{a_0} \right)^{7/2} r^2 e^{-Zr/3a_0} (3 \cos^2 \theta - 1)$
$3d_{xz} = \frac{2^{1/2}}{81\pi^{1/2}} \left(\frac{Z}{a_0} \right)^{7/2} r^2 e^{-Zr/3a_0} \sin \theta \cos \theta \cos \phi$
$3d_{yz} = \frac{2^{1/2}}{81\pi^{1/2}} \left(\frac{Z}{a_0} \right)^{7/2} r^2 e^{-Zr/3a_0} \sin \theta \cos \theta \sin \phi$
$3d_{x^2-y^2} = \frac{1}{81(2\pi)^{1/2}} \left(\frac{Z}{a_0} \right)^{7/2} r^2 e^{-Zr/3a_0} \sin^2 \theta \cos 2\phi$
$3d_{xy} = \frac{1}{81(2\pi)^{1/2}} \left(\frac{Z}{a_0} \right)^{7/2} r^2 e^{-Zr/3a_0} \sin^2 \theta \sin 2\phi$

PARTE RADIAL Y PARTE ANGULAR

Para las funciones s:



(c) Radial probability

Para las demás funciones:

	$s (\ell = 0)$	$p (\ell = 1)$			$d (\ell = 2)$					$f (\ell = 3)$							
	$m = 0$	$m = 0$	$m = \pm 1$		$m = 0$	$m = \pm 1$		$m = \pm 2$		$m = 0$	$m = \pm 1$		$m = \pm 2$		$m = \pm 3$		
	s	p_z	p_x	p_y	d_{z^2}	d_{xz}	d_{yz}	d_{xy}	$d_{x^2-y^2}$	f_{z^3}	f_{xz^2}	f_{yz^2}	f_{xyz}	$f_z(x^2-y^2)$	$f_x(x^2-3y^2)$	$f_y(3x^2-y^2)$	
$n = 1$																	
$n = 2$																	
$n = 3$																	
$n = 4$																	
$n = 5$										
$n = 6$					
$n = 7$		



The Orbitron gallery of atomic orbitals



1s



2s



3s



4s



5s



6s



7s



$3d_{x^2-y^2}$



$3d_{yz}$



$3d_{zx}$



$3d_{xy}$



$3d_{z^2}$

2p_y



3p_y



4p_y



5p_y



6p_y



7p_y



$4f_{y(3x^2-y^2)}$



$4f_{x(3y^2-x^2)}$



$4f_{z^2}$



$4f_{yz}$



$4f_{zx}$



$4f_{xy}$



$4f_{x^2-3y^2}$



$5f_{y(3x^2-y^2)}$



$5f_{x(3y^2-x^2)}$



$5f_{z^2}$



$5f_{yz}$



$5f_{zx}$



$5f_{xy}$



$5f_{x^2-3y^2}$

