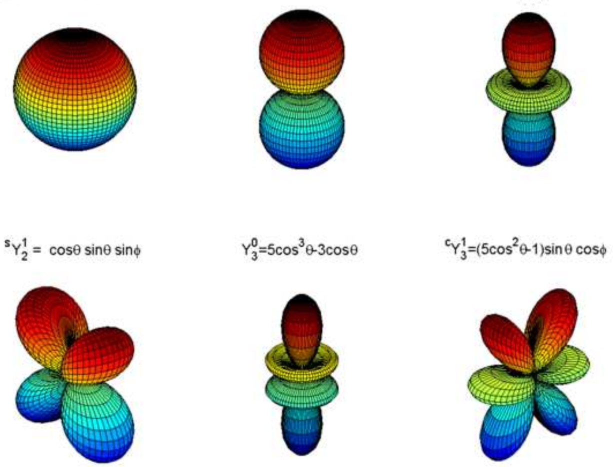
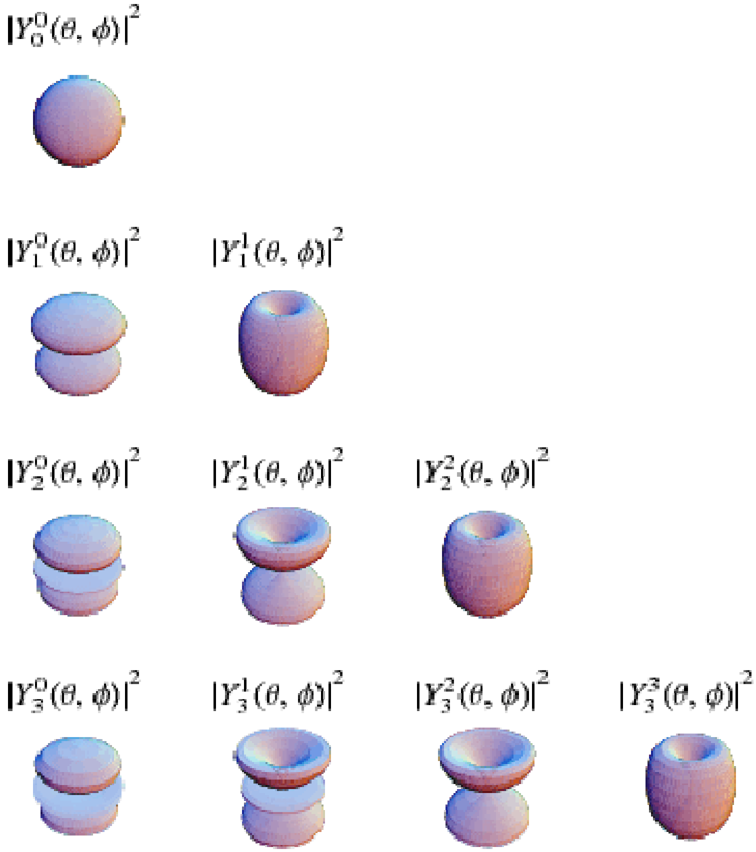
Harmônicos Esféricos

TABLE 3.7
Some Spherical Harmonics

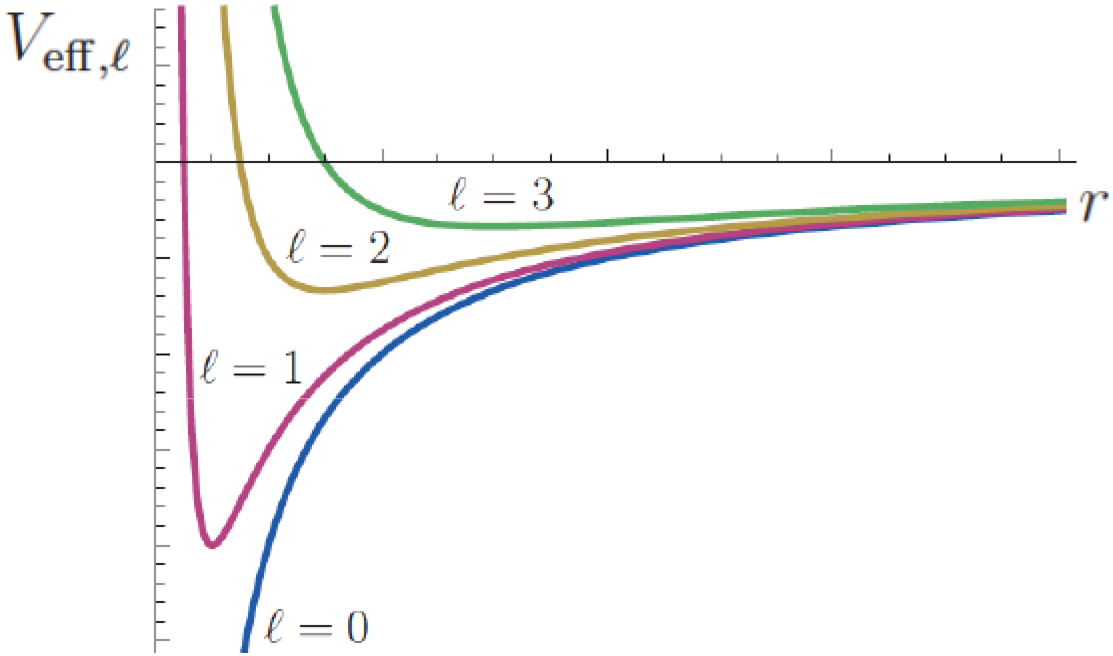
Symbol	Polar	Cartesian	Normalization Constant
Y_{00}	1	1	$\frac{1}{2}(1/\pi)^{1/2}$
Y_{10}	$\cos\theta$	z/r	$\frac{1}{2}(3/\pi)^{1/2}$
$Y_{1\pm1}$	$\mp(\sin\theta)e^{\pm i\phi}$	$\mp(x \pm iy)/r$	$\frac{1}{2}(3/2\pi)^{1/2}$
Y_{20}	$(3\cos^2\theta - 1)$	$(3z^2 - r^2)/r^2$	$\frac{1}{4}(5/\pi)^{1/2}$
$Y_{2\pm1}$	$\mp(\sin\theta)(\cos\theta)e^{\pm i\phi}$	$\mp z(x \pm iy)r^2$	$\frac{1}{2}(15/2\pi)^{1/2}$
$Y_{2\pm2}$	$(\sin^2\theta)e^{\pm 2i\phi}$	$(x \pm iy)^2/r^2$	$\frac{1}{4}(15/2\pi)^{1/2}$
Y_{30}	$(5\cos^3\theta - 3\cos\theta)$	$z(5z^2 - 3r^2)/r^3$	$\frac{1}{4}(7/\pi)^{1/2}$
$Y_{3\pm1}$	$\mp\sin\theta(5\cos^2\theta - 1)e^{\pm i\phi}$	$\mp(x \pm iy)(5z^2 - r^2)/r^3$	$\frac{1}{8}(21/\pi)^{1/2}$
$Y_{3\pm2}$	$(\sin^2\theta)(\cos\theta)e^{\pm 2i\phi}$	$z(x \pm iy)^2/r^3$	$\frac{1}{4}(105/2\pi)^{1/2}$
$Y_{3\pm3}$	$\mp(\sin^3\theta)e^{\pm 3i\phi}$	$\mp(x \pm iy)^3/r^3$	$\frac{1}{8}(35/\pi)^{1/2}$

Douglas, Bodie E. and Hollingsworth, Charles A. *Symmetry in Bonding and Spectra – An Introduction* (Orlando, Florida: Academic Press, Inc., 1985) p. 88.





Átomo de H: Potencial Efetivo



$$V_{\text{eff}}(r) = -\frac{e^2}{4\pi\epsilon_0 r} + \frac{\hbar^2 l(l+1)}{2\mu r^2}$$

Funções de onda radiais - átomo H

$L_0^0 = 1$	$L_0^2 = 2$
$L_1^0 = -x + 1$	$L_1^2 = -6x + 18$
$L_2^0 = x^2 - 4x + 2$	$L_2^2 = 12x^2 - 96x + 144$
$L_0^1 = 1$	$L_0^3 = 6$
$L_1^1 = -2x + 4$	$L_1^3 = -24x + 96$
$L_2^1 = 3x^2 - 18x + 18$	$L_2^3 = 60x^2 - 600x + 1200$

Alguns Polinômios associados de Laguerre

$R_{10} = 2a^{-3/2}\exp(-r/a)$
$R_{20} = \frac{1}{\sqrt{2}} a^{-3/2}\left(1 - \frac{1}{2}\frac{r}{a}\right)\exp(-r/2a)$
$R_{21} = \frac{1}{\sqrt{24}} a^{-3/2}\frac{r}{a}\exp(-r/2a)$
$R_{30} = \frac{2}{\sqrt{27}} a^{-3/2}\left(1 - \frac{2}{3}\frac{r}{a} + \frac{2}{27}\left(\frac{r}{a}\right)^2\right)\exp(-r/3a)$
$R_{31} = \frac{8}{27\sqrt{6}} a^{-3/2}\left(1 - \frac{1}{6}\frac{r}{a}\right)\left(\frac{r}{a}\right)\exp(-r/3a)$
$R_{32} = \frac{4}{81\sqrt{30}} a^{-3/2}\left(\frac{r}{a}\right)^2\exp(-r/3a)$
$R_{40} = \frac{1}{4} a^{-3/2}\left(1 - \frac{3}{4}\frac{r}{a} + \frac{1}{8}\left(\frac{r}{a}\right)^2 - \frac{1}{192}\left(\frac{r}{a}\right)^3\right)\exp(-r/4a)$
$R_{41} = \frac{\sqrt{5}}{16\sqrt{3}} a^{-3/2}\left(1 - \frac{1}{4}\frac{r}{a} + \frac{1}{80}\left(\frac{r}{a}\right)^2\right)\frac{r}{a}\exp(-r/4a)$
$R_{42} = \frac{1}{64\sqrt{5}} a^{-3/2}\left(1 - \frac{1}{12}\frac{r}{a}\right)\left(\frac{r}{a}\right)^2\exp(-r/4a)$
$R_{43} = \frac{1}{768\sqrt{35}} a^{-3/2}\left(\frac{r}{a}\right)^3\exp(-r/4a)$

$$R_{nl}(r) = L_{n-l-1}^{2l+1}(2\lambda_n r)(\lambda_n r)^{l+1}\frac{e^{-\lambda_n r}}{r}$$

$$\lambda_n . n = (a_B)^{-1}$$

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

$$R_{n0}(r) \propto e^{-\lambda_n r} \to R_{n0}(r=0) = \text{const}$$

Átomos H: Funções de onda radias

$$R_{10} = 2a^{-3/2}\exp(-r/a)$$

$$R_{20} = \frac{1}{\sqrt{2}}a^{-3/2}\left(1-\frac{1}{2}\frac{r}{a}\right)\exp(-r/2a)$$

$$R_{21} = \frac{1}{\sqrt{24}}a^{-3/2}\frac{r}{a}\exp(-r/2a)$$

$$R_{30} = \frac{2}{\sqrt{27}}a^{-3/2}\left(1-\frac{2}{3}\frac{r}{a}+\frac{2}{27}\left(\frac{r}{a}\right)^2\right)\exp(-r/3a)$$

$$R_{31} = \frac{8}{27\sqrt{6}}a^{-3/2}\left(1-\frac{1}{6}\frac{r}{a}\right)\left(\frac{r}{a}\right)\exp(-r/3a)$$

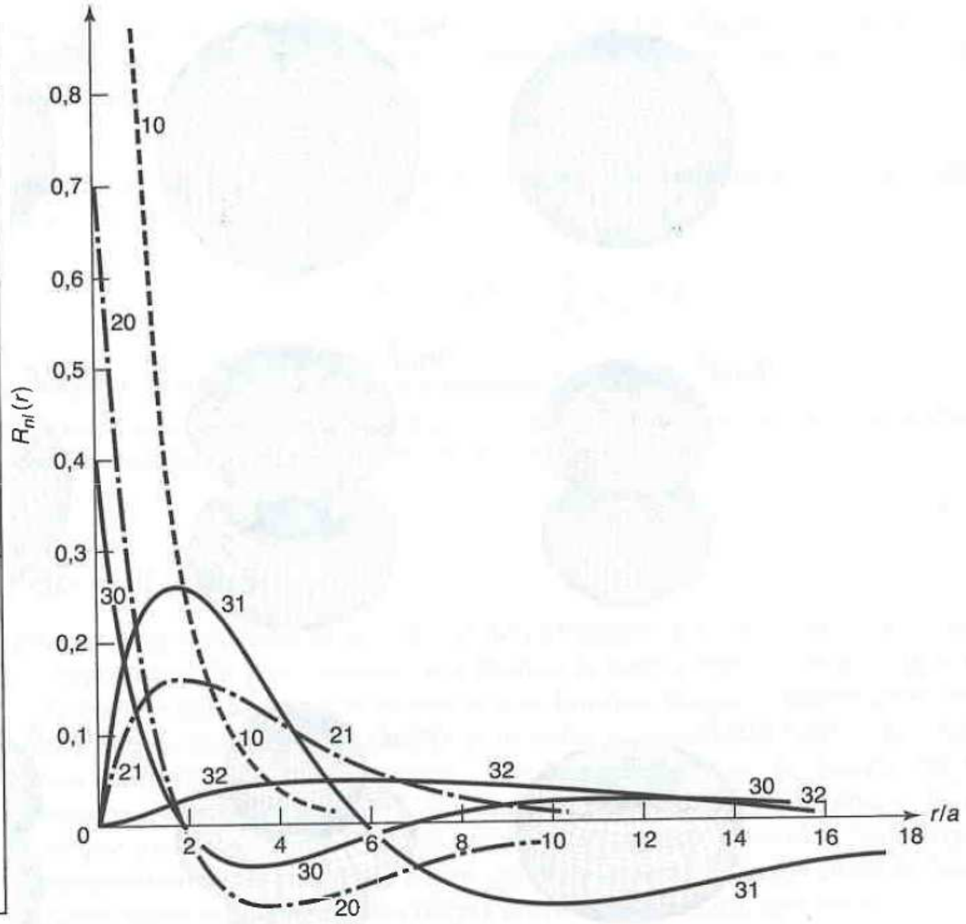
$$R_{32} = \frac{4}{81\sqrt{30}}a^{-3/2}\left(\frac{r}{a}\right)^2\exp(-r/3a)$$

$$R_{40} = \frac{1}{4}a^{-3/2}\left(1-\frac{3}{4}\frac{r}{a}+\frac{1}{8}\left(\frac{r}{a}\right)^2-\frac{1}{192}\left(\frac{r}{a}\right)^3\right)\exp(-r/4a)$$

$$R_{41} = \frac{\sqrt{5}}{16\sqrt{3}}a^{-3/2}\left(1-\frac{1}{4}\frac{r}{a}+\frac{1}{80}\left(\frac{r}{a}\right)^2\right)\frac{r}{a}\exp(-r/4a)$$

$$R_{42} = \frac{1}{64\sqrt{5}}a^{-3/2}\left(1-\frac{1}{12}\frac{r}{a}\right)\left(\frac{r}{a}\right)^2\exp(-r/4a)$$

$$R_{43} = \frac{1}{768\sqrt{35}}a^{-3/2}\left(\frac{r}{a}\right)^3\exp(-r/4a)$$



Funções de onda do átomo de H

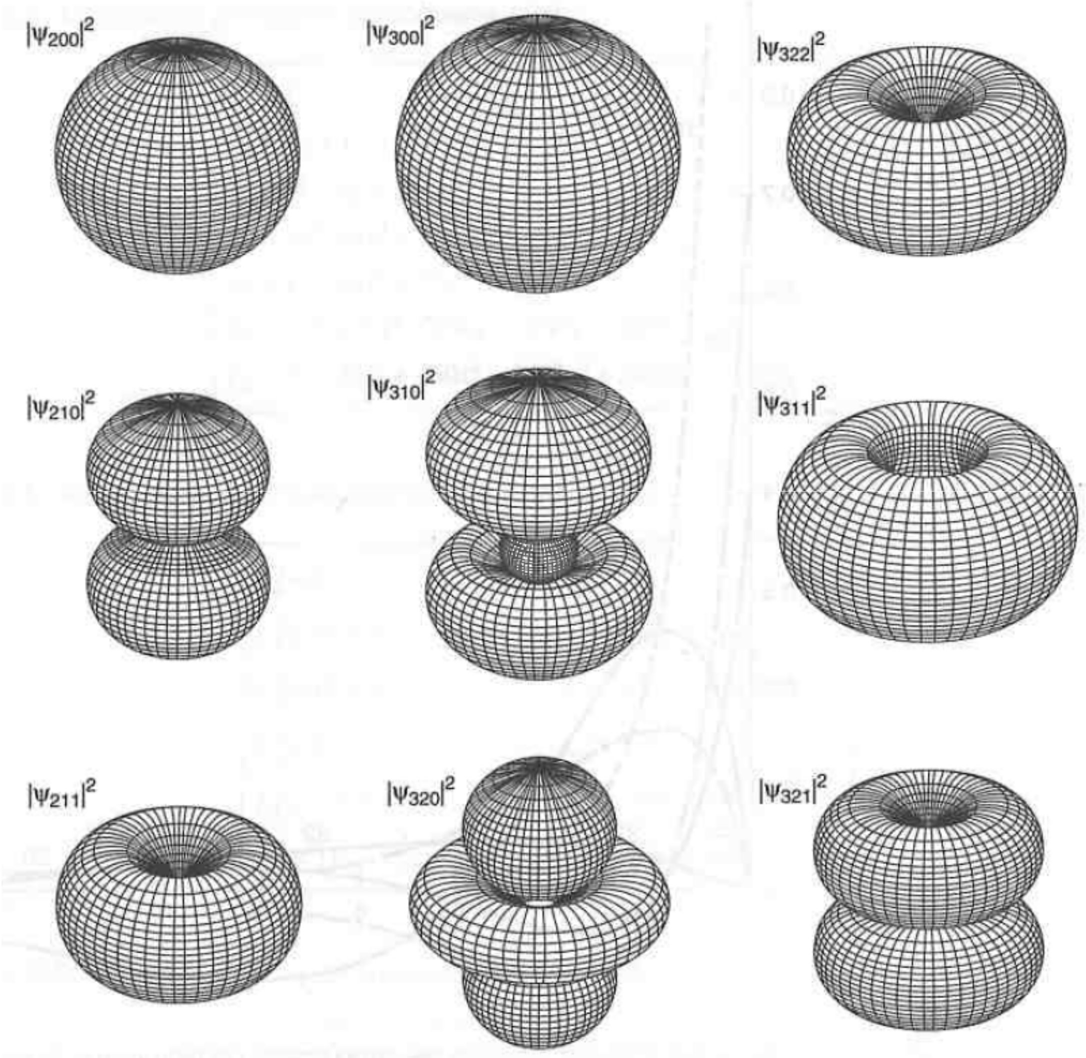
$$|\Psi_{nlm}(r)|^2$$

$$E_n = \frac{E_1}{n^2} = \frac{13.6 \text{ eV}}{n^2}$$

$$n = 0, 1, 2, ...$$

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

$$-l \leq m \leq l$$

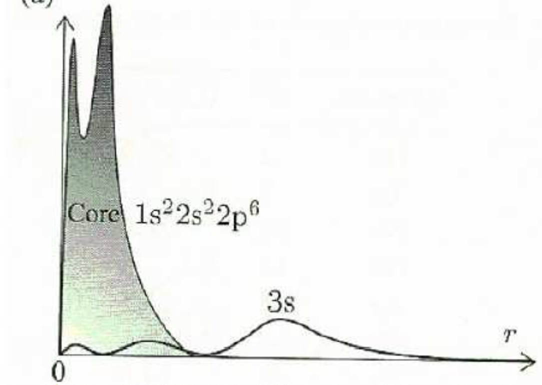


Blindagem e “camadas fechadas”

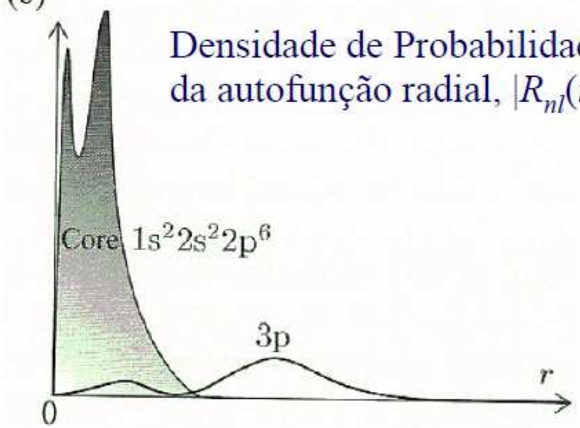
$$Z_{\text{eff}} = Z - \sigma$$

Exemplo: Na ($Z = 11$): $1s^2\, 2s^2\, 2p^6\, 3s^1 \equiv [\text{Ne}]\, 3s^1$

(a)



(b)



Densidade de Probabilidade da autofunção radial, $|R_{nl}(r)|^2 r^2$

Table 7.1 Values of $Z_{\text{eff}} = Z - \sigma$ for neutral ground-state atoms

	H							He
1*s*	1							1.6875
	Li	Be	B	C	N	O	F	Ne
1*s*	2.6906	3.6848	4.6795	5.6727	6.6651	7.6579	8.6501	9.6421
2*s*	1.2792	1.9120	2.5762	3.2166	3.8474	4.4916	5.1276	5.7584
			2.4214	3.1358	3.8340	4.4532	5.1000	5.7584
	Na	Mg	Al	Si	P	S	Cl	Ar
	10.6259	11.6089	12.5910	13.5754	14.5578	15.5409	16.5239	17.5075
	6.5714	7.3920	8.2136	9.0200	9.8250	10.6288	11.4304	12.2304
	6.8018	7.8258	8.9634	9.9450	10.9612	11.9770	12.9932	14.0082
	2.5074	3.3075	4.1172	4.9032	5.6418	6.3669	7.0683	7.7568
			4.0656	4.2852	4.8864	5.4819	6.1161	6.7641

from E. Clementi and D.L. Raimondi, Atomic screening constants from SCF functions. IBM Res. Note NJ-27 (1963).

Tabela Periódica