Hydrogenlike Wave Functions

$$\psi_{n\ell m}(r,\vartheta,\varphi)=R_{n\ell}(r)\Theta_{\ell m}(\vartheta)\Phi_m(\varphi),$$

with

$$\Phi_m(\varphi)=\frac{1}{\sqrt{2\pi}}e^{im\varphi},$$

$$\Theta_{\ell m}(\vartheta)=\left\{\frac{(2\ell+1)(\ell-|m|)!}{2(\ell+|m|)!}\right\}^{\frac{1}{2}}P_\ell^{|m|}(\cos\vartheta),$$

and

$$R_{n\ell}(r)=-\left[\left(\frac{2Z}{na_0}\right)^3\frac{(n-\ell-1)!}{2n\{(n+\ell)!\}^3}\right]^{\frac{1}{2}}e^{-\frac{\rho}{2}}\rho^\ell L_{n+\ell}^{2\ell+1}(\rho),$$

in which

$$\rho=\frac{2Z}{na_0}$$

and

$$a_0=\frac{h^2}{4\pi^2\mu e^2}$$

and $L_{n+\ell}^{2\ell+1}(\rho)$ is an associated Laguerre polynomial.

$$\int_0^\infty\int_0^\pi\int_0^{2\pi}\psi^*_{n\ell m}(r,\vartheta,\varphi)\psi_{n\ell m}(r,\vartheta,\varphi)r^2\sin\vartheta d\varphi d\vartheta dr=1$$

The functions in $r,\vartheta,$ and φ are separately normalized to unity:

$$\int_0^{2\pi}\Phi^*_m(\varphi)\Phi_m(\varphi)d\varphi=1$$

$$\int_0^\pi\{\Theta_{\ell m}(\vartheta)\}^2\sin\vartheta d\vartheta=1$$

$$\int_0^\infty\{R_{n\ell}(r)\}^2r^2dr=1$$

They are also mutually orthogonal,

$$\int_0^\infty\int_0^\pi\int_0^{2\pi}\psi^*_{n\ell m}(r,\vartheta,\varphi)\psi_{n'\ell'm'}(r,\vartheta,\varphi)r^2\sin\vartheta d\varphi d\vartheta dr=\delta_{nn'}\delta_{\ell\ell'}\delta_{mm'}$$

vanishing, except for $n=n',\ \ell=\ell',$ and $m=m'.$

The Wave Functions $\Theta_{\ell m}(\vartheta)$

(The associated Legendre functions normalized to unity)

$\ell = 0$, s orbitals:

$$\Theta_{00}(\vartheta) = \frac{\sqrt{2}}{2}$$

$\ell = 1$, p orbitals:

$$\Theta_{10}(\vartheta) = \frac{\sqrt{6}}{2}\cos\vartheta$$

$$\Theta_{1\pm1}(\vartheta) = \frac{\sqrt{3}}{2}\sin\vartheta$$

$\ell = 2$, d orbitals:

$$\Theta_{20}(\vartheta) = \frac{\sqrt{10}}{4}\left(3\cos^2\vartheta - 1\right)$$

$$\Theta_{2\pm1}(\vartheta) = \frac{\sqrt{15}}{2}\sin\vartheta\cos\vartheta$$

$$\Theta_{2\pm2}(\vartheta) = \frac{\sqrt{15}}{4}\sin^2\vartheta$$

$\ell = 3$, f orbitals:

$$\Theta_{30}(\vartheta) = \frac{3\sqrt{14}}{4}\left(\frac{5}{3}\cos^3\vartheta - \cos\vartheta\right)$$

$$\Theta_{3\pm1}(\vartheta) = \frac{\sqrt{42}}{8}\sin\vartheta\left(5\cos^2\vartheta - 1\right)$$

$$\Theta_{3\pm2}(\vartheta) = \frac{\sqrt{105}}{4}\sin^2\vartheta\cos\vartheta$$

$$\Theta_{3\pm3}(\vartheta) = \frac{\sqrt{70}}{8}\sin^3\vartheta$$

$\ell = 4$, g orbitals:

$$\Theta_{40}(\vartheta) = \frac{9\sqrt{2}}{16}\left(\frac{35}{3}\cos^4\vartheta - 10\cos^2\vartheta + 1\right)$$

$$\Theta_{4\pm1}(\vartheta) = \frac{9\sqrt{10}}{8}\sin\vartheta\left(\frac{7}{3}\cos^3\vartheta - \cos\vartheta\right)$$

$$\Theta_{4\pm2}(\vartheta) = \frac{3\sqrt{5}}{8}\sin^2\vartheta\left(7\cos^2\vartheta - 1\right)$$

$$\Theta_{4\pm3}(\vartheta) = \frac{3\sqrt{70}}{8}\sin^3\vartheta\cos\vartheta$$

$$\Theta_{4\pm4}(\vartheta) = \frac{3\sqrt{35}}{16}\sin^4\vartheta$$

continued

The Wave Functions $\Theta_{\ell m}(\vartheta)$ - *continued*

$\ell = 5,\ h$ orbitals:

$$\Theta_{50}(\vartheta) = \frac{15\sqrt{22}}{16}\left(\frac{21}{5}\cos^5\vartheta - \frac{14}{3}\cos^3\vartheta + \cos\vartheta\right)$$

$$\Theta_{5\pm1}(\vartheta) = \frac{\sqrt{165}}{16}\sin\vartheta\left(21\cos^4\vartheta - 14\cos^2\vartheta + 1\right)$$

$$\Theta_{5\pm2}(\vartheta) = \frac{\sqrt{1155}}{8}\sin^2\vartheta\left(3\cos^3\vartheta - \cos\vartheta\right)$$

$$\Theta_{5\pm3}(\vartheta) = \frac{\sqrt{770}}{32}\sin^3\vartheta\left(9\cos^2\vartheta - 1\right)$$

$$\Theta_{5\pm4}(\vartheta) = \frac{3\sqrt{385}}{16}\sin^4\vartheta\cos\vartheta$$

$$\Theta_{5\pm5}(\vartheta) = \frac{3\sqrt{154}}{32}\sin^5\vartheta$$

The Hydrogenlike Radial Wave Functions

n = 1, K shell:

$\ell = 0,\ 1s$ $\qquad R_{10}(r) = (Z/a_0)^{\frac{3}{2}} \bullet 2e^{-\frac{\rho}{2}}$

n = 2, L shell:

$\ell = 0, 2s$ $\qquad R_{20}(r) = \frac{(Z/a_0)^{\frac{3}{2}}}{2\sqrt{2}}(2-\rho)e^{-\frac{\rho}{2}}$

$\ell = 1, 2p$ $\qquad R_{21}(r) = \frac{(Z/a_0)^{\frac{3}{2}}}{2\sqrt{6}}\rho e^{-\frac{\rho}{2}}$

n = 3, M shell:

$\ell = 0, 3s$ $\qquad R_{30}(r) = \frac{(Z/a_0)^{\frac{3}{2}}}{9\sqrt{3}}\left(6 - 6\rho + \rho^2\right)e^{-\frac{\rho}{2}}$

$\ell = 1, 3p$ $\qquad R_{31}(r) = \frac{(Z/a_0)^{\frac{3}{2}}}{9\sqrt{6}}(4-\rho)\rho e^{-\frac{\rho}{2}}$

$\ell = 2, 3d$ $\qquad R_{32}(r) = \frac{(Z/a_0)^{\frac{3}{2}}}{9\sqrt{30}}\rho^2 e^{-\frac{\rho}{2}}$

continued

The Hydrogenlike Radial Wave Functions (Continued)

n = 4, N shell:

$$\ell = 0, 4s \qquad R_{40}(r) = \frac{(Z/a_0)^{\frac{3}{2}}}{96}\left(24 - 36\rho + 12\rho^2 - \rho^3\right)e^{-\frac{\rho}{2}}$$

$$\ell = 1, 4p \qquad R_{41}(r) = \frac{(Z/a_0)^{\frac{3}{2}}}{32\sqrt{15}}\left(20 - 10\rho + \rho^2\right)\rho e^{-\frac{\rho}{2}}$$

$$\ell = 2, 4d \qquad R_{42}(r) = \frac{(Z/a_0)^{\frac{3}{2}}}{96\sqrt{5}}(6 - \rho)\rho^2 e^{-\frac{\rho}{2}}$$

$$\ell = 3, 4f \qquad R_{43}(r) = \frac{(Z/a_0)^{\frac{3}{2}}}{96\sqrt{35}}\rho^3 e^{-\frac{\rho}{2}}$$

n = 5, O shell:

$$\ell = 0, 5s \qquad R_{50}(r) = \frac{(Z/a_0)^{\frac{3}{2}}}{300\sqrt{5}}\left(120 - 240\rho + 120\rho^2 - 20\rho^3 + \rho^4\right)e^{-\frac{\rho}{2}}$$

$$\ell = 1, 5p \qquad R_{51}(r) = \frac{(Z/a_0)^{\frac{3}{2}}}{150\sqrt{30}}\left(120 - 90\rho + 18\rho^2 - \rho^3\right)\rho e^{-\frac{\rho}{2}}$$

$$\ell = 2, 5d \qquad R_{52}(r) = \frac{(Z/a_0)^{\frac{3}{2}}}{150\sqrt{70}}\left(42 - 14\rho + \rho^2\right)\rho^2 e^{-\frac{\rho}{2}}$$

$$\ell = 3, 5f \qquad R_{53}(r) = \frac{(Z/a_0)^{\frac{3}{2}}}{300\sqrt{70}}(8 - \rho)\rho^3 e^{-\frac{\rho}{2}}$$

$$\ell = 4, 5g \qquad R_{54}(r) = \frac{(Z/a_0)^{\frac{3}{2}}}{900\sqrt{70}}\rho^4 e^{-\frac{\rho}{2}}$$

continued)

The Hydrogenlike Radial Wave Functions (Continued)

n = 6, *P* shell:

$$\ell = 0, 6s \qquad R_{60}(r) = \frac{(Z/a_0)^{\frac{3}{2}}}{2160\sqrt{6}}\left(720 - 1800\rho + 1200\rho^2 - 300\rho^3 + 30\rho^4 - \rho^5\right)e^{-\frac{\rho}{2}}$$

$$\ell = 1, 6p \qquad R_{61}(r) = \frac{(Z/a_0)^{\frac{3}{2}}}{432\sqrt{210}}\left(840 - 840\rho + 252\rho^2 - 28\rho^3 + \rho^4\right)\rho e^{-\frac{\rho}{2}}$$

$$\ell = 2, 6d \qquad R_{62}(r) = \frac{(Z/a_0)^{\frac{3}{2}}}{864\sqrt{105}}\left(336 - 168\rho + 24\rho^2 - \rho^3\right)\rho^2 e^{-\frac{\rho}{2}}$$

$$\ell = 3, 6f \qquad R_{63}(r) = \frac{(Z/a_0)^{\frac{3}{2}}}{2592\sqrt{35}}\left(72 - 18\rho + \rho^2\right)\rho^3 e^{-\frac{\rho}{2}}$$

$$\ell = 4, 6g \qquad R_{64}(r) = \frac{(Z/a_0)^{\frac{3}{2}}}{12960\sqrt{7}}(10 - \rho)\rho^4 e^{-\frac{\rho}{2}}$$

$$\ell = 5, 6h \qquad R_{65}(r) = \frac{(Z/a_0)^{\frac{3}{2}}}{12960\sqrt{77}}\rho^5 e^{-\frac{\rho}{2}}$$