More Hydrogen-like Wave Functions

The total spin free wavefunction for a one electron atom is given by

$$\psi_{n l m}(r,\theta,\phi) = R_{nl}(r) Y_l^m(\theta,\phi) = R_{nl}(r)\Theta_{l m}(\theta)\Phi_m(\phi)$$

with the spherical harmonic written as a product of $\Theta_{lm}(\theta) \& \Phi_m(\phi)$

$$Y_l^m(\theta,\phi) = \Theta_{l m}(\theta)\Phi_m(\phi)$$

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

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

δ_m is a phase factor which is not universally agreed upon. We will choose it to be $(-1)^m$ when $m > 0$ and +1 when $m < 0$. This is often called the Condon-Shortly choice of phase and is sometimes written as the requirement that $Y_l^{-m} = (-1)^m \left(Y_l^m\right)^*$.

The radial functions are

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

in which

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

and

$$a_0 = \frac{4\pi\varepsilon_0\hbar^2}{\mu e^2}$$

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

The functions in $r, \theta,$ and ϕ are separately normalized to unity and mutually orthogonal

$$\int_0^{2\pi} \Phi_m^*(\phi)\Phi_m(\phi)\,d\phi = 1$$

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

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

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

except for $n = n'$, $\mathrm{l} = \mathrm{l}'$, and $m = m'$.

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

$\ell = 0$, s orbitals:

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

$\ell = 1$, p orbitals:

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

$$\Theta_{1\pm1}(\theta) = \mathrm{m}\frac{\sqrt{3}}{2}\sin\theta$$

$\ell = 2$, d orbitals:

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

$$\Theta_{2\pm1}(\theta) = \mathrm{m}\frac{\sqrt{15}}{2}\sin\theta\cos\theta$$

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

$\ell = 3$, f orbitals:

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

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

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

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

$\ell = 4$, g orbitals:

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

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

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

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

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

$\ell = 5$, h orbitals:

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

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

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

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

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

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

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:

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

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

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

n = 4, N shell:

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

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

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

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

n = 5, *O* shell:

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

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

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

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

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

n = 6, *P* shell:

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

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

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

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

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

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