

The first few wavefunctions of one-electron atoms

WCC

The wavefunctions are most-commonly expressed as complex eigenstates of L_z or as real-valued functions that point along directions in space. The complex ones are typically preferred in physics, and are the energy eigenstates of gas-phase atoms, with or without a static, uniform magnetic field. The real-valued functions are typically preferred in chemistry, where symmetry breaking from chemical bonding makes the energy eigenstates more-closely resemble the real-valued functions.

First, we can write some of the lowest-energy complex wavefunctions. The general case is given by

$$\psi_{n,L,M}(\mathbf{r}) = \sqrt{\left(\frac{2Z}{na_0}\right)^{3+2L} \frac{(n-L-1)!}{(n+L)! 2^n}} e^{-Zr/(na_0)} r^L \mathcal{L}_{n-L-1}^{2L+1}\left[\frac{2Z}{na_0}r\right] Y_{LM}(\boldsymbol{\omega}) \quad (1)$$

where $\mathcal{L}_n^a[x]$ is the generalized Laguerre polynomial in x (we are using the convention adopted by, for example, Mathematica).

orbital	$\psi_{n,L,M}(\mathbf{r})$
$1s (M_L = 0)$	$\sqrt{\frac{Z^3}{\pi a_0^3}} e^{-Zr/a_0}$
$2s (M_L = 0)$	$\frac{1}{4} \sqrt{\frac{Z^5}{2\pi a_0^5}} (r - 2\frac{a_0}{Z}) e^{-Zr/(2a_0)}$
$2p (M_L = \pm 1)$	$\mp \frac{1}{8} \sqrt{\frac{Z^5}{\pi a_0^5}} r e^{-Zr/(2a_0)} \sin(\theta) e^{\pm i\phi}$
$2p (M_L = 0)$	$\frac{1}{4} \sqrt{\frac{Z^5}{2\pi a_0^5}} r e^{-Zr/(2a_0)} \cos(\theta)$
$3s (M_L = 0)$	$\frac{2}{81} \sqrt{\frac{Z^7}{3\pi a_0^7}} \left(r^2 - 9\frac{a_0}{Z} r + \frac{27}{2} \left(\frac{a_0}{Z}\right)^2\right) e^{-Zr/(3a_0)}$
$3p (M_L = \pm 1)$	$\mp \frac{1}{81} \sqrt{\frac{Z^7}{\pi a_0^7}} (r - 6\frac{a_0}{Z}) r e^{-Zr/(3a_0)} \sin(\theta) e^{\pm i\phi}$
$3p (M_L = 0)$	$\frac{1}{81} \sqrt{\frac{2Z^7}{\pi a_0^7}} (r - 6\frac{a_0}{Z}) r e^{-Zr/(3a_0)} \cos(\theta)$
$3d (M_L = \pm 2)$	$\frac{1}{162} \sqrt{\frac{Z^7}{\pi a_0^7}} r^2 e^{-Zr/(3a_0)} \sin^2(\theta) e^{\pm i2\phi}$
$3d (M_L = \pm 1)$	$\mp \frac{1}{81} \sqrt{\frac{Z^7}{\pi a_0^7}} r^2 e^{-Zr/(3a_0)} \sin(\theta) \cos(\theta) e^{\pm i\phi}$
$3d (M_L = 0)$	$\frac{1}{81} \sqrt{\frac{Z^7}{6\pi a_0^7}} r^2 e^{-Zr/(3a_0)} (3 \cos^2(\theta) - 1)$
$4s (M_L = 0)$	$\frac{1}{1536} \sqrt{\frac{Z^9}{\pi a_0^9}} \left(r^3 - 24\frac{a_0}{Z} r^2 + 144 \left(\frac{a_0}{Z}\right)^2 r - 192 \left(\frac{a_0}{Z}\right)^3\right) e^{-Zr/(4a_0)}$
$4p (M_L = \pm 1)$	$\mp \frac{1}{512} \sqrt{\frac{Z^9}{10\pi a_0^9}} \left(r^2 - 20\frac{a_0}{Z} r + 80 \left(\frac{a_0}{Z}\right)^2\right) r e^{-Zr/(4a_0)} \sin(\theta) e^{\pm i\phi}$
$4p (M_L = 0)$	$\frac{1}{512} \sqrt{\frac{Z^9}{5\pi a_0^9}} \left(r^2 - 20\frac{a_0}{Z} r + 80 \left(\frac{a_0}{Z}\right)^2\right) r e^{-Zr/(4a_0)} \cos(\theta)$
$4d (M_L = \pm 2)$	$\frac{1}{1024} \sqrt{\frac{Z^9}{6\pi a_0^9}} (r - 12\frac{a_0}{Z}) r^2 e^{-Zr/(4a_0)} \sin^2(\theta) e^{\pm i2\phi}$
$4d (M_L = \pm 1)$	$\mp \frac{1}{512} \sqrt{\frac{Z^9}{6\pi a_0^9}} (r - 12\frac{a_0}{Z}) r^2 e^{-Zr/(4a_0)} \sin(\theta) \cos(\theta) e^{\pm i\phi}$
$4d (M_L = 0)$	$\frac{1}{3072} \sqrt{\frac{Z^9}{\pi a_0^9}} (r - 12\frac{a_0}{Z}) r^2 e^{-Zr/(4a_0)} (3 \cos^2(\theta) - 1)$
$4f (M_L = \pm 3)$	$\mp \frac{1}{6144} \sqrt{\frac{Z^9}{\pi a_0^9}} r^3 e^{-Zr/(4a_0)} \sin^3(\theta) e^{\pm i3\phi}$
$4f (M_L = \pm 2)$	$\frac{1}{1024} \sqrt{\frac{Z^9}{6\pi a_0^9}} r^3 e^{-Zr/(4a_0)} \sin^2(\theta) \cos(\theta) e^{\pm i2\phi}$
$4f (M_L = \pm 1)$	$\mp \frac{1}{2048} \sqrt{\frac{Z^9}{15\pi a_0^9}} r^3 e^{-Zr/(4a_0)} (5 \cos^2(\theta) - 1) \sin(\theta) e^{\pm i\phi}$
$4f (M_L = 0)$	$\frac{1}{3072} \sqrt{\frac{Z^9}{5\pi a_0^9}} r^3 e^{-Zr/(4a_0)} (5 \cos^2(\theta) - 3) \cos(\theta)$

The radial wavefunctions, $R_{n,L}(r)$ are normalized according to $\int dr r^2 |R_{n,L}(r)|^2 = 1$ and the first few are given by

$$\begin{aligned}
R_{n,L} & \quad \text{radial wavefunction} \\
R_{1,0}(r) &= 2\sqrt{\frac{Z^3}{a_0^3}} e^{-Zr/a_0} \\
R_{2,0}(r) &= \frac{1}{2}\sqrt{\frac{Z^5}{2a_0^5}} \left(r - 2\frac{a_0}{Z}\right) e^{-Zr/(2a_0)} \\
R_{2,1}(r) &= \frac{1}{2}\sqrt{\frac{Z^5}{6a_0^5}} r e^{-Zr/(2a_0)} \\
R_{3,0}(r) &= \frac{4}{81}\sqrt{\frac{Z^7}{3a_0^7}} \left(r^2 - 9\frac{a_0}{Z}r + \frac{27}{2}\left(\frac{a_0}{Z}\right)^2\right) e^{-Zr/(3a_0)} \\
R_{3,1}(r) &= \frac{2}{81}\sqrt{\frac{2Z^7}{3a_0^7}} r \left(r - 6\frac{a_0}{Z}\right) e^{-Zr/(3a_0)} \\
R_{3,2}(r) &= \frac{2}{81}\sqrt{\frac{2Z^7}{15a_0^7}} r^2 e^{-Zr/(3a_0)} \\
R_{4,0}(r) &= \frac{1}{768}\sqrt{\frac{Z^9}{a_0^9}} \left(r^3 - 24\frac{a_0}{Z}r^2 + 144\left(\frac{a_0}{Z}\right)^2 r - 192\left(\frac{a_0}{Z}\right)^3\right) e^{-Zr/(4a_0)} \\
R_{4,1}(r) &= \frac{1}{256}\sqrt{\frac{Z^9}{15a_0^9}} r \left(r^2 - 20\frac{a_0}{Z}r + 80\left(\frac{a_0}{Z}\right)^2\right) e^{-Zr/(4a_0)} \\
R_{4,2}(r) &= \frac{1}{768}\sqrt{\frac{Z^9}{5a_0^9}} r^2 \left(r - 12\frac{a_0}{Z}\right) e^{-Zr/(4a_0)} \\
R_{4,3}(r) &= \frac{1}{768}\sqrt{\frac{Z^9}{35a_0^9}} r^3 e^{-Zr/(4a_0)}
\end{aligned}$$

The real-valued, Cartesian-friendly “chemist’s wavefunctions” are

orbital	$\psi(\mathbf{r})$
$1s$	$\sqrt{\frac{Z^3}{\pi a_0^3}} e^{-Zr/a_0}$
$2s$	$\frac{1}{4} \sqrt{\frac{Z^5}{2\pi a_0^5}} (r - 2\frac{a_0}{Z}) e^{-Zr/(2a_0)}$
$2p_x$	$\frac{1}{4} \sqrt{\frac{Z^5}{2\pi a_0^5}} x e^{-Zr/(2a_0)}$
$2p_y$	$\frac{1}{4} \sqrt{\frac{Z^5}{2\pi a_0^5}} y e^{-Zr/(2a_0)}$
$2p_z$	$\frac{1}{4} \sqrt{\frac{Z^5}{2\pi a_0^5}} z e^{-Zr/(2a_0)}$
$3s$	$\frac{2}{81} \sqrt{\frac{Z^7}{3\pi a_0^7}} \left(r^2 - 9\frac{a_0}{Z}r + \frac{27}{2} \left(\frac{a_0}{Z}\right)^2\right) e^{-Zr/(3a_0)}$
$3p_x$	$\frac{1}{81} \sqrt{\frac{2Z^7}{\pi a_0^7}} \left(r - 6\frac{a_0}{Z}\right) x e^{-Zr/(3a_0)}$
$3p_y$	$\frac{1}{81} \sqrt{\frac{2Z^7}{\pi a_0^7}} \left(r - 6\frac{a_0}{Z}\right) y e^{-Zr/(3a_0)}$
$3p_z$	$\frac{1}{81} \sqrt{\frac{2Z^7}{\pi a_0^7}} \left(r - 6\frac{a_0}{Z}\right) z e^{-Zr/(3a_0)}$
$3d_{3z^2-r^2}$	$\frac{1}{81} \sqrt{\frac{Z^7}{6\pi a_0^7}} \left(3z^2 - r^2\right) e^{-Zr/(3a_0)}$
$3d_{zx}$	$\frac{1}{81} \sqrt{\frac{2Z^7}{\pi a_0^7}} zx e^{-Zr/(3a_0)}$
$3d_{zy}$	$\frac{1}{81} \sqrt{\frac{2Z^7}{\pi a_0^7}} zy e^{-Zr/(3a_0)}$
$3d_{xy}$	$\frac{1}{81} \sqrt{\frac{2Z^7}{\pi a_0^7}} xy e^{-Zr/(3a_0)}$
$3d_{x^2-y^2}$	$\frac{1}{81} \sqrt{\frac{Z^7}{2\pi a_0^7}} \left(x^2 - y^2\right) e^{-Zr/(3a_0)}$
$4s$	$\frac{1}{1536} \sqrt{\frac{Z^9}{\pi a_0^9}} \left(r^3 - 24\frac{a_0}{Z}r^2 + 144 \left(\frac{a_0}{Z}\right)^2 r - 192 \left(\frac{a_0}{Z}\right)^3\right) e^{-Zr/(4a_0)}$
$4p_x$	$\mp \frac{1}{512} \sqrt{\frac{Z^9}{5\pi a_0^9}} \left(r^2 - 20\frac{a_0}{Z}r + 80 \left(\frac{a_0}{Z}\right)^2\right) x e^{-Zr/(4a_0)}$
$4p_y$	$\mp \frac{1}{512} \sqrt{\frac{Z^9}{5\pi a_0^9}} \left(r^2 - 20\frac{a_0}{Z}r + 80 \left(\frac{a_0}{Z}\right)^2\right) y e^{-Zr/(4a_0)}$
$4p_z$	$\mp \frac{1}{512} \sqrt{\frac{Z^9}{5\pi a_0^9}} \left(r^2 - 20\frac{a_0}{Z}r + 80 \left(\frac{a_0}{Z}\right)^2\right) z e^{-Zr/(4a_0)}$
$4d_{3z^2-r^2}$	$\frac{1}{3072} \sqrt{\frac{Z^9}{\pi a_0^9}} \left(r - 12\frac{a_0}{Z}\right) \left(3z^2 - r^2\right) e^{-Zr/(4a_0)}$

orbital	ψ(r)
$4d_{zx}$	$\frac{1}{512} \sqrt{\frac{Z^9}{3\pi a_0^9}} (r - 12\frac{a_0}{Z}) zx e^{-Zr/(4a_0)}$
$4d_{zy}$	$\frac{1}{512} \sqrt{\frac{Z^9}{3\pi a_0^9}} (r - 12\frac{a_0}{Z}) zy e^{-Zr/(4a_0)}$
$4d_{xy}$	$\frac{1}{512} \sqrt{\frac{Z^9}{3\pi a_0^9}} (r - 12\frac{a_0}{Z}) xy e^{-Zr/(4a_0)}$
$4d_{x^2-y^2}$	$\frac{1}{1024} \sqrt{\frac{Z^9}{3\pi a_0^9}} (r - 12\frac{a_0}{Z}) (x^2 - y^2) e^{-Zr/(4a_0)}$
$4f_{xyz}$	$\frac{1}{512} \sqrt{\frac{Z^9}{\pi a_0^9}} xyz e^{-Zr/(4a_0)}$
$4f_{z(x^2-y^2)}$	$\frac{1}{1024} \sqrt{\frac{Z^9}{\pi a_0^9}} z (x^2 - y^2) e^{-Zr/(4a_0)}$
$4f_{y(3x^2-y^2)}$	$\frac{1}{1024} \sqrt{\frac{Z^9}{6\pi a_0^9}} y (3x^2 - y^2) e^{-Zr/(4a_0)}$
$4f_{x(x^2-3y^2)}$	$\frac{1}{1024} \sqrt{\frac{Z^9}{6\pi a_0^9}} x (x^2 - 3y^2) e^{-Zr/(4a_0)}$
$4f_{x(4z^2-x^2-y^2)}$	$\frac{1}{1024} \sqrt{\frac{Z^9}{10\pi a_0^9}} x (4z^2 - x^2 - y^2) e^{-Zr/(4a_0)}$
$4f_{y(4z^2-x^2-y^2)}$	$\frac{1}{1024} \sqrt{\frac{Z^9}{10\pi a_0^9}} y (4z^2 - x^2 - y^2) e^{-Zr/(4a_0)}$
$4f_{z(2z^2-3x^2-3y^2)}$	$\frac{1}{1024} \sqrt{\frac{Z^9}{15\pi a_0^9}} z (2z^2 - 3x^2 - 3y^2) e^{-Zr/(4a_0)}$