The Hydrogen Atom

The solutions are given as: $\left|\psi_{nlm_l}\right\rangle = R(r)\Theta(\theta)\Phi(\phi)$

where we've found already that,

$$\Phi(\phi) = e^{im_l\phi}$$

$$\Theta(\theta) = \varepsilon\sqrt{\frac{(2l+1)}{4\pi}\frac{\left(l-|m_l|\right)!}{\left(l+|m_l|\right)!}}P_l^{m_l}\left(\cos\theta\right); \quad \varepsilon = \begin{cases} (-1)^{m_l} & m_l \geq 0 \\ 1 & m_l \leq 0 \end{cases}$$

The Hydrogen Atom

In the solution for $\Theta(\theta)$ we have:

$$P_l^{m_l}(\cos\theta) = \left(1-\cos^2\theta\right)^{\frac{|m_l|}{2}} \left(\frac{d}{d\cos\theta}\right)^{|m_l|} P_l(\cos\theta)$$

which are the associated Legendre functions and

$$P_l(\cos\theta) = \frac{1}{2^l l!}\left(\frac{d}{d\cos\theta}\right)^l \left(\cos^2\theta - 1\right)^l$$

are the Legendre polynomials of degree *l*.

The Hydrogen Atom

In normalized angular solutions are called the Spherical Harmonics

$$Y_l^{m_l}(\theta,\phi)=\varepsilon\sqrt{\frac{(2l+1)}{4\pi}\frac{(l-|m_l|)!}{(l+|m_l|)!}}e^{im\phi}P_l^{m_l}(\cos\theta)$$

The Hydrogen Atom

In non-normalized radial solutions are

$$R(r) = \frac{u(r)}{r} = \frac{1}{r}\left(\frac{r}{an}\right)^{l+1} e^{-\frac{r}{an}} v(r)$$

where

$$v(r) = L_{n-l-1}^{2l+1}\left(\tfrac{2r}{na}\right) = (-1)^{2l+1}\left(\tfrac{na}{2}\right)^{2l+1}\left(\tfrac{d}{dr}\right)^{2l+1} L_{n+2l}\left(\tfrac{2r}{na}\right)$$

are the associated Laguerre functions and

$$L_{n+2l}\left(\tfrac{2r}{na}\right) = e^{\frac{2r}{na}}\left(\tfrac{na}{2}\right)^{n+2l}\left(\tfrac{d}{dr}\right)^{n+2l}\left(e^{-\frac{2r}{na}}\left(\tfrac{2r}{na}\right)^{n+2l}\right)$$

are the Laguerre polynomials.

The Hydrogen Atom

We normalize the solutions according to:

$$P = 1 = \int \psi^* \psi \, d^3 r = \int_0^{2\pi} \int_0^{\pi} \int_0^{\infty} \psi^* \psi \, r^2 \, dr \sin\theta \, d\theta d\phi$$

The normalized wavefunctions for the one electron atom are given as

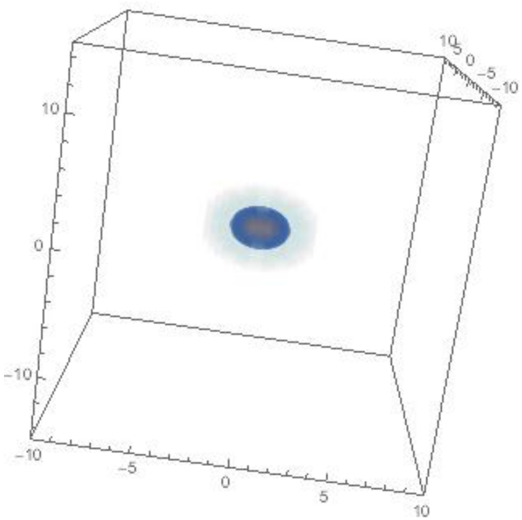
$$\left| \psi_{nlm_l} \right\rangle = \sqrt{\left(\tfrac{2}{na}\right)^3 \frac{(n-l-1)!}{2n\left[(n+l)!\right]^3}} \, e^{-\frac{r}{na}} \left(\tfrac{2r}{na}\right)^l \left[L_{n-l-1}^{2l+1}\left(\tfrac{2r}{na}\right) \right] Y_l^{m_l}(\theta,\phi)$$

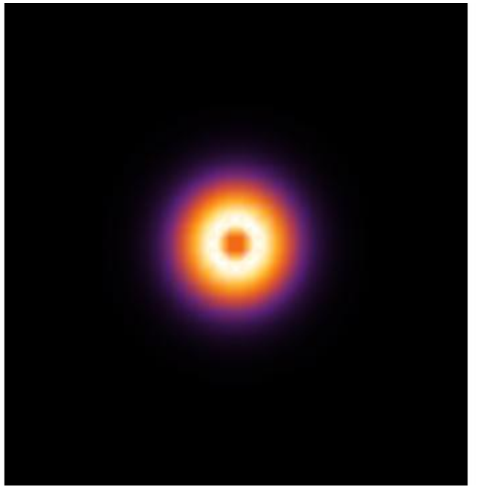
where the following conditions apply:

$$n = 1,2,3,\ldots$$
$$l = 0,1,2,3,\ldots,(n-1)$$
$$-l \le m_l \le l$$

The 1S Orbital in a Hydrogen Atom

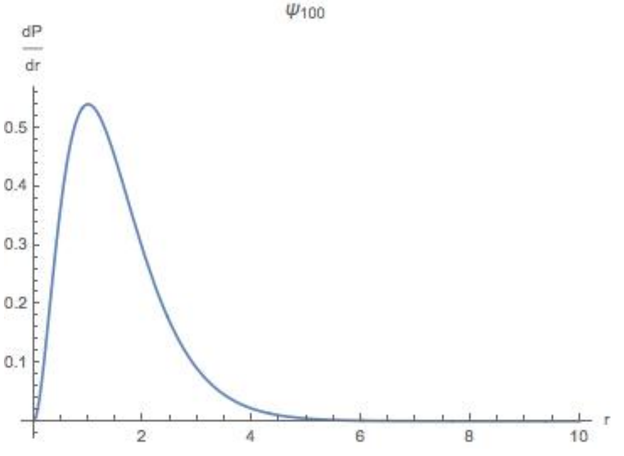
$$\left|\psi_{100}\right\rangle = \frac{1}{\sqrt{\pi a^3}} e^{-\frac{r}{a}}$$





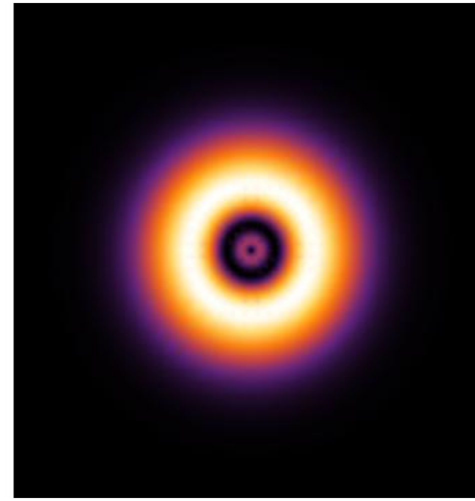
The radial probability function

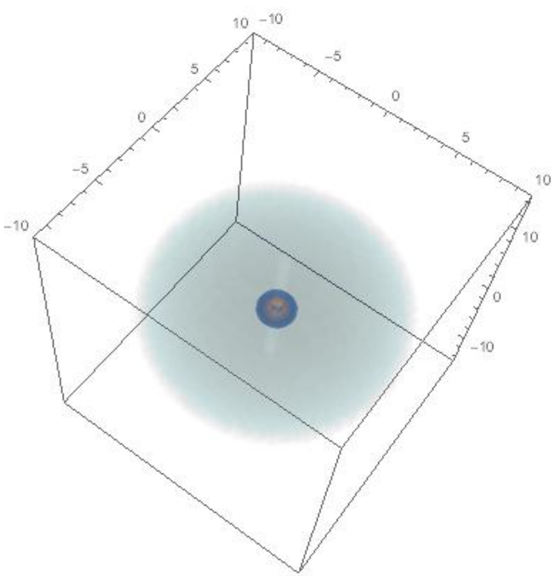
$$\frac{dP}{dr} = 4\pi r^2 \psi^* \psi$$



The 2S Orbital in Hydrogen Atom

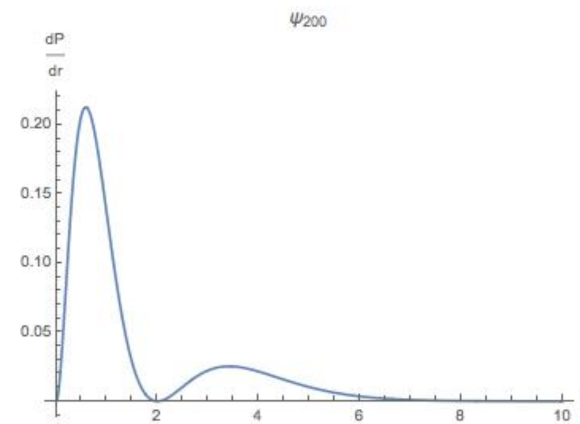
$$\left|\psi_{200}\right\rangle = \frac{1}{\sqrt{\pi a^3}}\left(1-\frac{r}{2a}\right)e^{-\frac{r}{2a}}$$





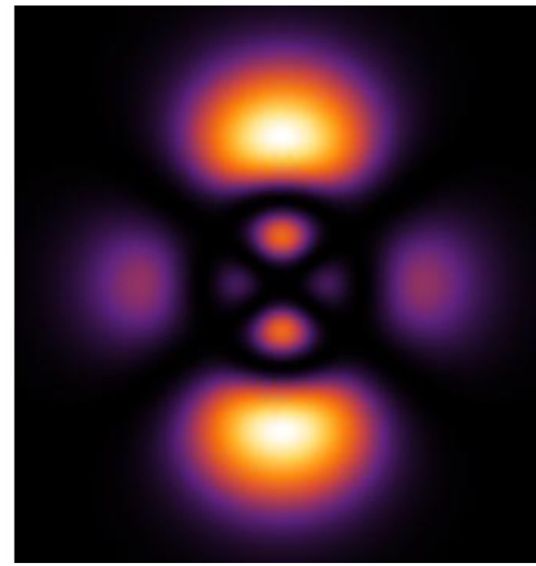
The radial probability function

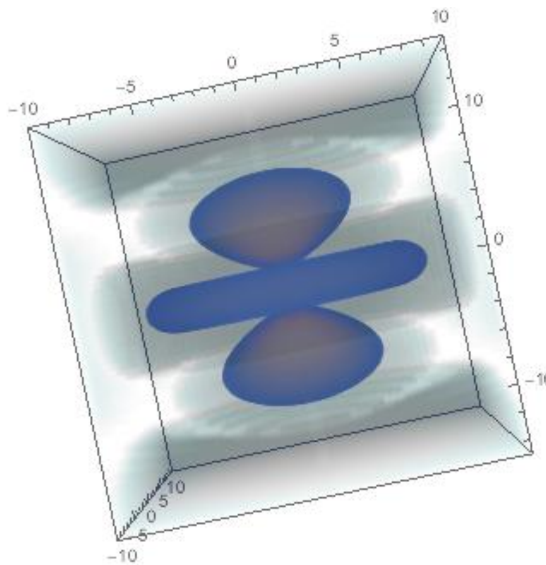
$$\frac{dP}{dr} = 4\pi r^2 \psi^* \psi$$

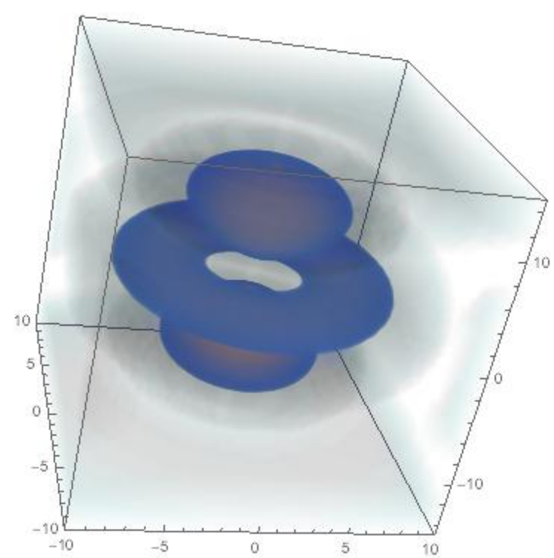


The $4D_0$ Orbital in a Hydrogen Atom

$$\left|\psi_{420}\right\rangle = \frac{1}{\sqrt{\pi a^3}}\left(\frac{1}{3062}\right)\left(20-\frac{r}{a}\right)\left(\frac{r}{a}\right)^2 e^{-\frac{r}{4a}}\left(3\cos^2\theta-1\right)$$







Orbital Labels for One-Electron Atoms

n	l	m_l	$Orbital$	degeneracy(n^2)	$Energy(eV)$
1	0	0	$1S$	1	–13.6
2	0 1	0 –1, 0, 1	$2S$ $2P_-$, $2P_0$, $2P_+$	4	–3.4
3	0 1 2	0 –1, 0, 1 –2, –1, 0, 1, 2	$3S$ $3P_-$, $3P_0$, $3P_+$ $3D_{-2}$, $3D_{-1}$, $3D_0$, $3D_{+1}$, $3D_{+2}$	9	–1.51
4	0 1 2 3	0 –1, 0, 1 –2, –1, 0, 1, 2 –3, –2, –1, 0, 1, 2, 3	$4S$ $4P_-$, $4P_0$, $4P_+$ $4D_{-2}$, $4D_{-1}$, $4D_0$, $4D_{+1}$, $4D_{+2}$ $4F_{-3}$, $4F_{-2}$, $4F_{-1}$, $4F_0$, $4F_{+1}$, $4F_{+2}$, $4F_{+3}$	16	–0.85