

Mathematica for spherical harmonics

Spherical harmonics are built in functions.

Arguments are l, m, θ, ϕ

Here, for example, are the $l=4$ harmonics for $m=0-4$

```
Table[SphericalHarmonicY[4, m,  $\theta$ ,  $\phi$ ], {m, 0, 4}] // TableForm
```

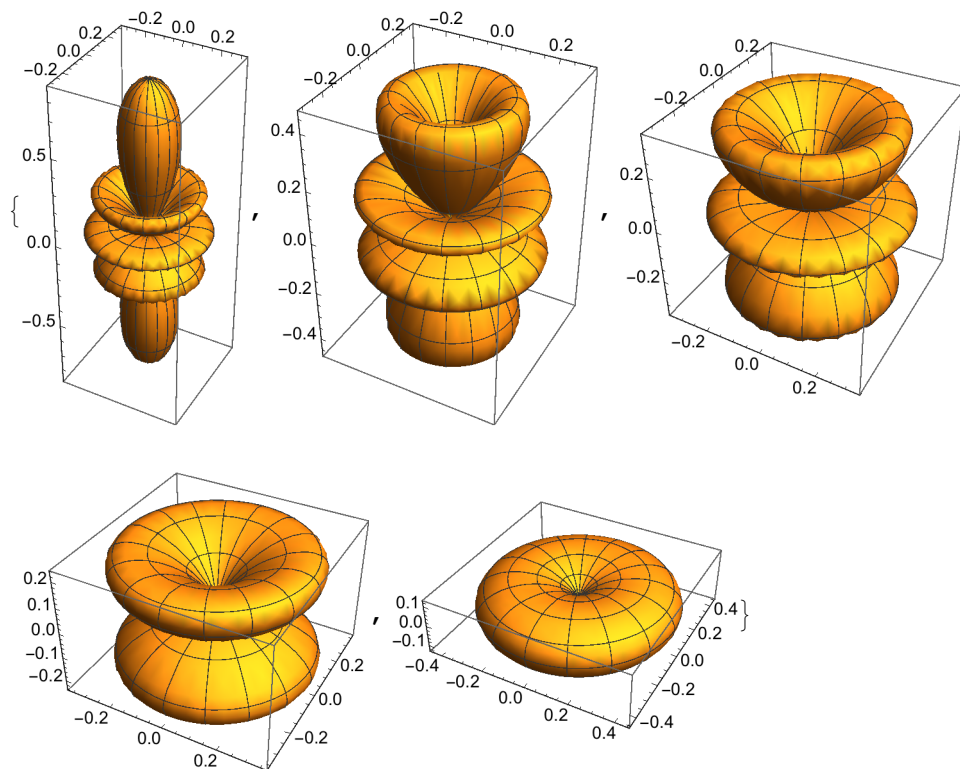
$$\begin{aligned} & \frac{3}{16} \frac{(3 - 30 \cos[\theta]^2 + 35 \cos[\theta]^4)}{\sqrt{\pi}} \\ & - \frac{3}{8} e^{i\phi} \sqrt{\frac{5}{2\pi}} \cos[\theta] (-3 + 7 \cos[\theta]^2) \sin[\theta] \\ & \frac{3}{8} e^{2i\phi} \sqrt{\frac{5}{2\pi}} (-1 + 7 \cos[\theta]^2) \sin[\theta]^2 \\ & - \frac{3}{8} e^{3i\phi} \sqrt{\frac{35}{\pi}} \cos[\theta] \sin[\theta]^3 \\ & \frac{3}{16} e^{4i\phi} \sqrt{\frac{35}{2\pi}} \sin[\theta]^4 \end{aligned}$$

Spherical plot visualizes their shape in angular space.

The distance of the surface from the origin at a given θ, ϕ is the function being plotted.

The absolute value removes the ϕ dependence, so one only sees the θ dependence.

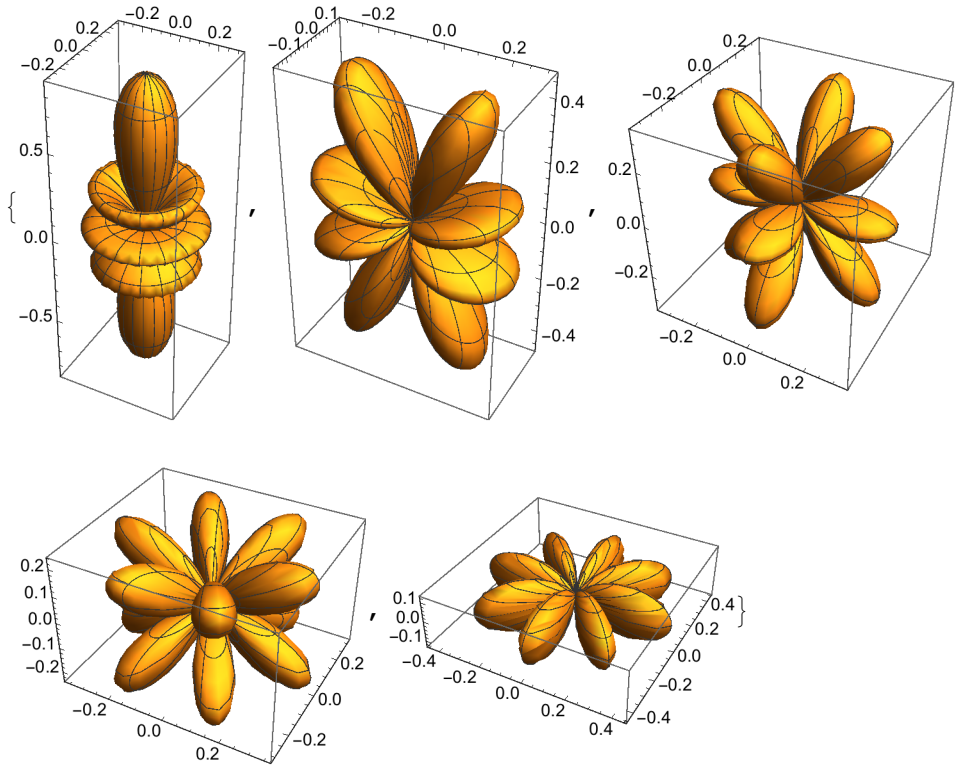
```
Table[SphericalPlot3D[  
  {Abs[SphericalHarmonicY[4, m,  $\theta$ ,  $\phi$ ]]}, { $\theta$ , 0, Pi}, { $\phi$ , 0, 2 Pi}], {m, 0, 4}]
```



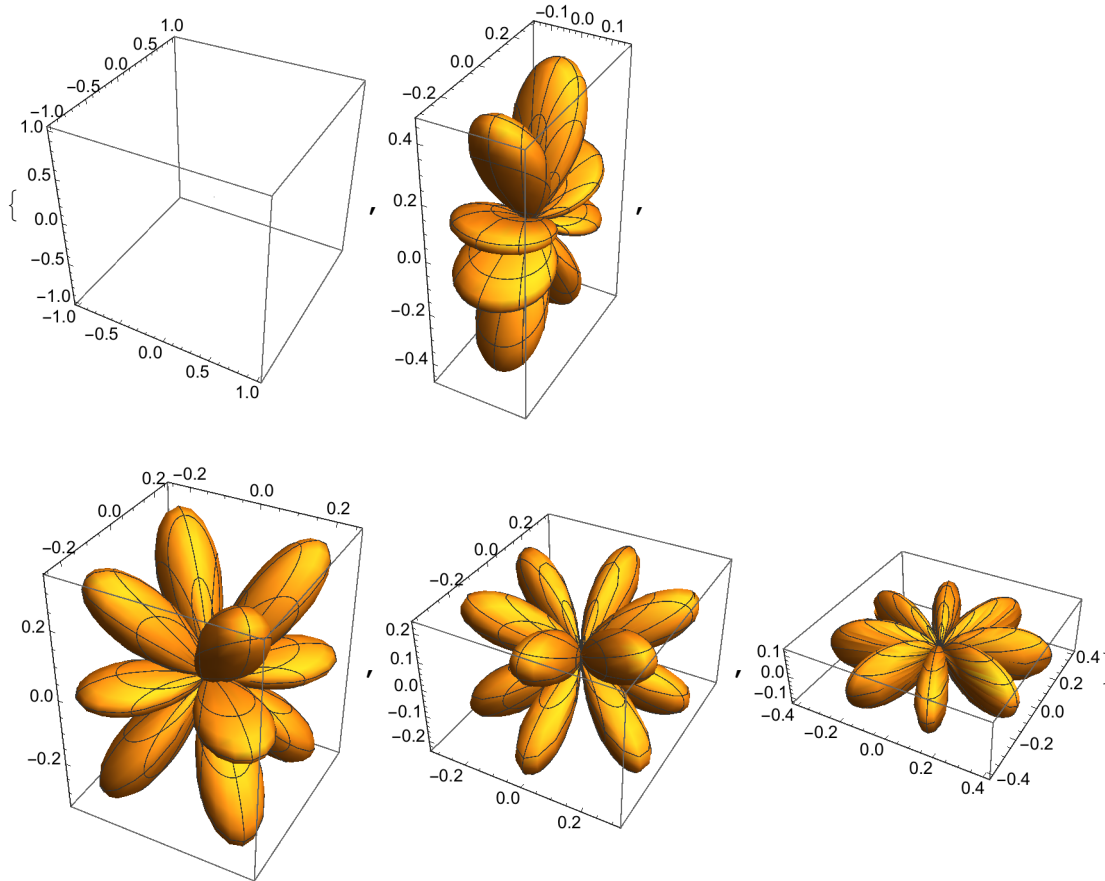
To see the ϕ dependence one can take either the real or imaginary part.

Here they are:

```
Table[SphericalPlot3D[Re[SphericalHarmonicY[4, m,  $\theta$ ,  $\phi$ ]],
  { $\theta$ , 0, Pi}, { $\phi$ , 0, 2 Pi}, PlotRange -> All], {m, 0, 4}]
```



```
Table[SphericalPlot3D[Im[SphericalHarmonicY[4, m,  $\theta$ ,  $\phi$ ]],
  { $\theta$ , 0, Pi}, { $\phi$ , 0, 2 Pi}, PlotRange -> All], {m, 0, 4}]
```



The $m=0$ spherical harmonic is purely real

```
FunctionExpand[SphericalHarmonicY[4, 0,  $\theta$ ,  $\phi$ ]]
```

$$\frac{3 \left(3 - 30 \cos^2[\theta] + 35 \cos^4[\theta] \right)}{16 \sqrt{\pi}}$$

The spherical harmonics can be written in terms of the associated Legendre polynomials as:

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

So it follows that for $m=0$, it can be written in terms of the standard Legendre polynomials, which are real

```
FunctionExpand[SphericalHarmonicY[1, 0,  $\theta$ ,  $\phi$ ]]
```

$$\frac{\sqrt{1+2\cos^2[\theta]} \text{LegendreP}[1, \cos[\theta]]}{2 \sqrt{\pi}}$$

As you will learn in quantum mechanics (or may have learned in chemistry) the orbitals are spherical harmonics

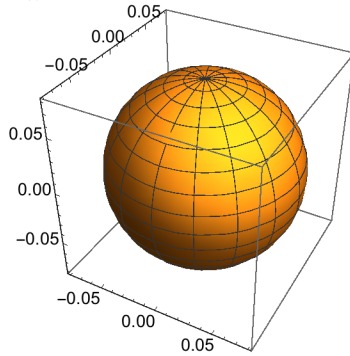
The s orbital is $l=0$, p is $l=1$, d is $l=2$ and so on

```
Table[{StringForm["l=``", l], StringForm["m=±``, m], FullSimplify[
  Abs[SphericalHarmonicY[l, m, θ, φ]]^2, Assumptions → θ ∈ Reals && φ ∈ Reals],
  SphericalPlot3D[Abs[SphericalHarmonicY[l, m, θ, φ]]^2, {θ, 0, Pi},
    {φ, 0, 2 Pi}, PlotRange → All]}, {l, 0, 3}, {m, 0, 1}] // TableForm
```

$$l=0$$

$$m=\pm 0$$

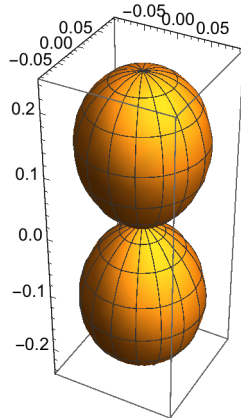
$$\frac{1}{4\pi}$$



$$l=1$$

$$m=\pm 0$$

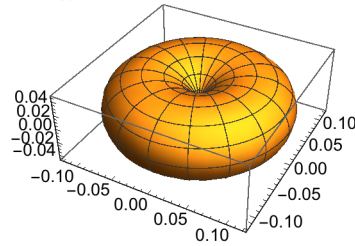
$$\frac{3 \cos[\theta]^2}{4\pi}$$



$$l=1$$

$$m=\pm 1$$

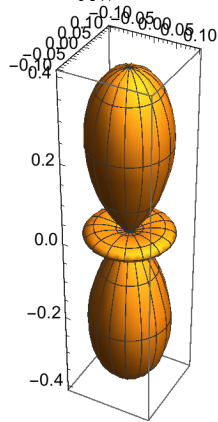
$$\frac{3 \sin[\theta]^2}{8\pi}$$



$$l=2$$

$$m=\pm 0$$

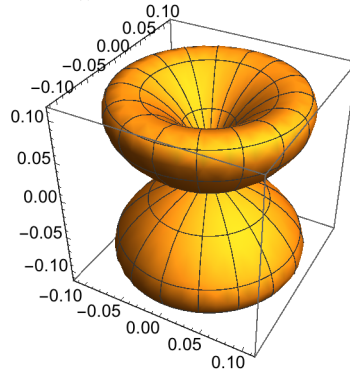
$$\frac{5 (1 + 3 \cos[2\theta])^2}{64\pi}$$



$$l=2$$

$$m=\pm 1$$

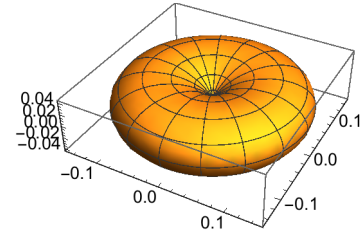
$$\frac{15 \sin[2\theta]^2}{32\pi}$$



$$l=2$$

$$m=\pm 2$$

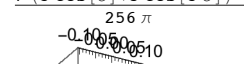
$$\frac{15 \sin[\theta]^4}{32\pi}$$



$$l=3$$

$$m=\pm 0$$

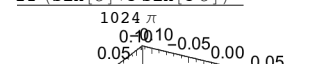
$$\frac{7 (3 \cos[\theta] + 5 \cos[3\theta])^2}{256\pi}$$



$$l=3$$

$$m=\pm 1$$

$$\frac{21 (\sin[\theta] + 5 \sin[3\theta])^2}{1024\pi}$$

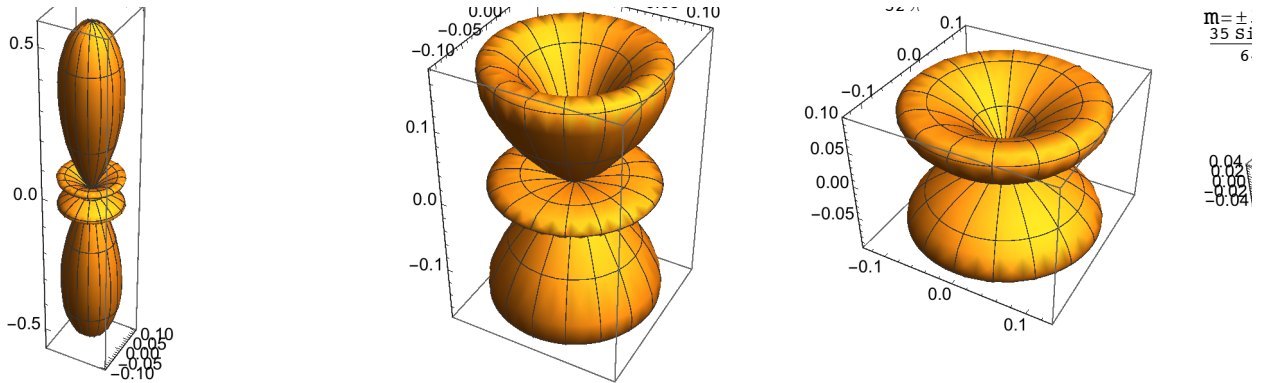


$$l=3$$

$$m=\pm 2$$

$$\frac{105 \cos[\theta]^2 \sin[\theta]^4}{32\pi}$$





Note that this is only the angular part of the hydrogen wave function, the radial part is based on the associated Laguerre polynomials.

We won't discuss the Laguerre polynomials as they aren't as widespread as the spherical harmonics. All we'll say for now is that the radial part of the hydrogen Schrodinger equation takes the form of the associated Laguerre differential equation, for which the associated Laguerre polynomials are the solution. In *Mathematica* the associated Laguerre polynomials can be called as `LaguerreL[λ, ν, x]` ($= L_{\lambda}^{\nu}[x]$)

The radial wave function (including the overall normalization) looks like,

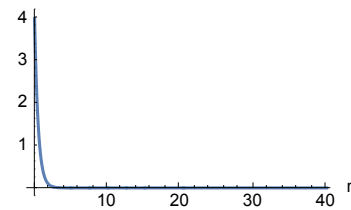
`R[r_, n_, l_] :=`

$$\sqrt{\left(\frac{2}{n}\right)^3 \frac{(n-l-1)!}{2n*(n+1)!}} \left(2 \frac{r}{n}\right)^l \text{Exp}[-r/n] \text{LaguerreL}[n-l-1, 2l+1, 2 \frac{r}{n}] /. n \rightarrow 2 /. l \rightarrow 0$$

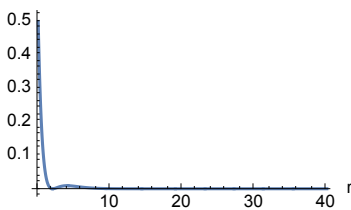
Note: Here I have set the Bohr radius (a combination of physical constants with units of length) to 1.

```
Table[{StringForm["n=~", n], StringForm["l=~", l],
  FullSimplify[Abs[R[r, n, l]]^2, Assumptions -> r ∈ Reals],
  Plot[Abs[R[r, n, l]]^2, {r, 0, 40}, AxesLabel -> {"r", "|R(r)|^2"}, PlotRange -> All]},
{n, 1, 4}, {l, 0, n - 1}] // TableForm
```

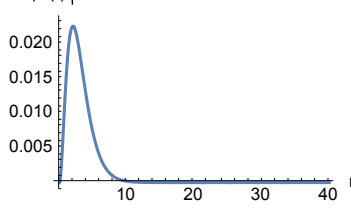
n=1
l=0
 $\frac{1}{4} e^{-2 r}$
 $|R(r)|^2$



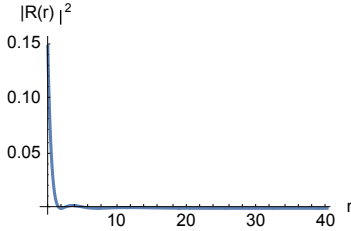
n=2
l=0
 $\frac{1}{8} e^{-r} (-2 + r)^2$
 $|R(r)|^2$



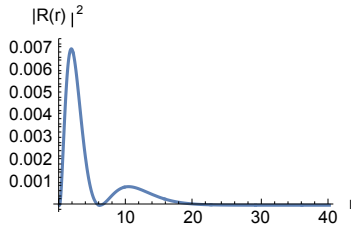
n=2
l=1
 $\frac{1}{24} e^{-r} r^2$
 $|R(r)|^2$



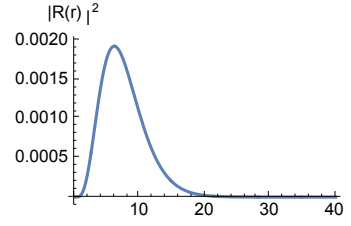
n=3
l=0
 $\frac{2 e^{-2 r/3} (27 + 2 (-9 + r) r)^2}{6561}$
 $|R(r)|^2$



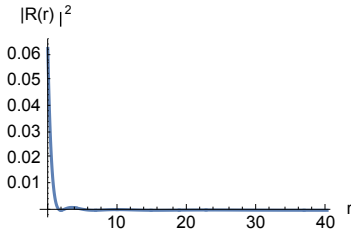
n=3
l=1
 $\frac{8 e^{-2 r/3} (-6 + r)^2 r^2}{19683}$
 $|R(r)|^2$



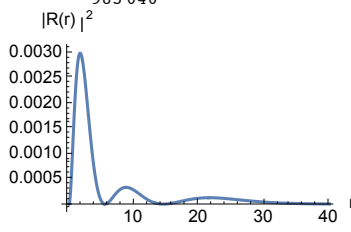
n=3
l=2
 $\frac{8 e^{-2 r/3}}{98415}$
 $|R(r)|^2$



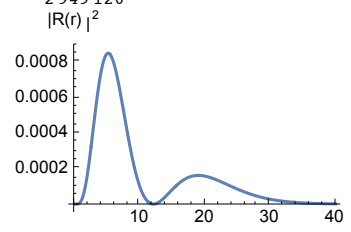
n=4
l=0
 $\frac{e^{-r/2} (-192 + (-12 + r)^2 r)^2}{589824}$
 $|R(r)|^2$



n=4
l=1
 $\frac{e^{-r/2} r^2 (80 + (-20 + r) r)^2}{983040}$
 $|R(r)|^2$



n=4
l=2
 $\frac{e^{-r/2} (-12 + r)^2}{2949120}$
 $|R(r)|^2$



n=4
l=3
 $\frac{e^{-r/2}}{2064}$
 $|R(r)|^2$

0.0003
0.0003
0.0003
0.0003
0.0003
0.0003
0.0003

Together with the spherical harmonics, the hydrogen atom wave function is,

$$\psi_{nlr}(r, \theta, \phi) = R_{nl}(r) Y_l^m(\theta, \phi)$$

(Sometimes the normalization is kept separate)