Construction of the Electronic Angular Wave Functions and Probability Distributions of the Hydrogen Atom

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Goal: This document illustrates a method by which one may generate and present graphs of the probability distributions of the angular electronic wave function for the hydrogen atom "from scratch". No attempt is made to derive this wave function.

Objectives:

After completing this exercise, students should be able to:

1. Separately evaluate and graphically display the 2 different angular functions of that are used in constructing the angular electronic wave function for the hydrogen atom, given the quantum numbers $l$ and $m$.

2. Construct and plot the probability distribution of the angular electronic wave function of the hydrogen atom, given any values of the quantum numbers $l$ and $m$.

3. Describe why the quantum number $m$ may only have values that range from $-l$ to $l$, according to the associated Legendre polynomial used in constructing the angular electronic wave function of the hydrogen atom.

4. Construct and plot the probability distributions of the angular electronic wave functions of the hydrogen atom that are traditionally displayed for functions having $m \neq 0$.

Introduction:

In general, the wavefunction for the angular portion of the electronic wavefunction in the Hydrogen atom is given by:

$$Y(\theta, \phi) = N_{lm} P_{\ell}^{m} (\cos \theta) e^{im\phi}$$
Where \( Y(\theta, \phi) \) is the angular electronic wavefunction of the H-atom, \( N_{lm} \) is a normalization constant, \( P_l^{m}(\cos \theta) \) is an **associated** Legendre polynomial, and \( e^{im\phi} \) is an exponential function containing an imaginary component. In this document we will construct each portion of the angular electronic wavefunction of the H-atom and explore some of the properties of each portion.

**Legendre Polynomials:**

We begin by studying the Legendre polynomials and show how they are obtained and examine their properties. To find the associated Legendre polynomials, \( P_l^{m}(\cos \theta) \), we first need to know how to construct the Legendre polynomials, \( P_l(\cos \theta) \). The Legendre polynomial is a built-in Mathcad function. For example, to call the Legendre polynomial that is 2nd order in \( x \), you would type Leg(2,x). You can observe the characteristics of the first five Legendre polynomials below in Graph 1. Note carefully the shape of each curve and identify the function type of each line, e.g. linear. Be sure to identify the order of the polynomial with the curve function type.

![Graph 1: The First 5 Legendre Polynomials](image)

Alternatively, the \( l \)th Laguerre polynomial may be generated from the following expression:

\[
\frac{1}{2^l l!} \frac{d^l}{dx^l} \left( x^2 - 1 \right)^l
\]

Expression 1
The Legendre polynomial which is \( l \)th order in \( x \) can be generated by substituting the appropriate value for \( l \) into the above expression. For example, the 2nd order Legendre polynomial is generated by substituting \( l = 2 \) into equation 1. Notice that the variable \( l \) is highlighted in equation 1 (and expression 1, below) but the numeral 1 is not highlighted.

**Question 1:** Evaluate expression 1 for \( l = 5 \) by replacing each " \( l \)" with "5" in expression (1) above. In the expression for the derivative, replace the \( l \) in the lower portion of the derivative expression with a 5 first -- the \( l \) in the upper portion will then automatically be changed as well. Once you have completed this, highlight the above expression, click on "Symbolics" and then "Simplify".

Mathcad should have returned the following polynomial, which is equal to the built-in Mathcad function, \( \text{Leg}(5,x) \):

\[
\frac{63}{8} x^5 - \frac{35}{4} x^3 + \frac{15}{8} x
\]

We're going to check to see if we have generated the 5th order Legendre polynomial using expression 1. Define \( F(x) \) and \( G(x) \) as the 5th Legendre polynomial as follows:

\[
F(x) := \text{Leg}(5,x) \quad G(x) := \frac{63}{8} x^5 - \frac{35}{4} x^3 + \frac{15}{8} x
\]

Here is a plot of both \( F(x) \) and \( G(x) \):
The similarity of these curves strongly suggest \( F(x) \) and \( G(x) \) are the same function!

**Question 2:**

a. Use Expression 1 to find the 0th, 1st, 2nd, 3rd, and 4th order Legendre polynomial. You should be aware that Mathcad will not evaluate the zeroth derivatives. However, because the zeroth derivative of any function, \( f(x) \), is simply \( f(x) \), finding the zeroth derivative of a function is trivial.

b. What order in \( x \) is the 1st Legendre polynomial? What about the 4th Legendre polynomial? In general, what order in \( x \) is the \( l \)th Legendre polynomial?

c. Using the Expression 1 and Mathcad's built-in Legendre polynomial function, generate a graph that displays overlay plots of the 3rd Legendre polynomial generated by these two methods (See Graph 2, above).

It is actually the associated Legendre polynomials that are used in the constructing the \( P_l^m(\cos \theta) \) portion of the angular electronic orbitals of the H-atom. The \( m \)th associated Legendre polynomial of order \( l \) is generated using Expression 2:

\[
\frac{(-1)^m}{2^l l!} \left( 1 - x^2 \right)^{l - 1/2} \frac{d^l}{dx^l} \frac{1}{1 - 2x + x^2}^{l - 1} \tag{Expression 2}
\]

You may have guessed that the values of \( l \) and \( m \) which are substituted into Expression 2 are the values for \( l \) and \( m \) of the atomic orbital you wish to construct (where \( l \) is the orbital angular momentum quantum number and \( m \) is the magnetic quantum number). Recall that for any value of \( l \), \( m \) can take on values from \(-l\) to \(+l\). Let's use Expression 2 to find the associated Legendre polynomial that is used to construct part of a \( 2p_{\pm1} \) orbital. To do this, we substitute \( l = 1 \) and \( m = 1 \) into expression 2 above. You may want to copy and paste expression 2 into the space below. Notice again, that \( l \) and \( m \) are highlighted in the above expression, but numerals are not. Then highlight this expression you have generated, choose "Symbolics", "Simplify" from the toolbar. If you get \(-(1-x^2)^{1/2}\) as your answer, you have evaluated the the expression correctly.

**Question 3:**

a. Find the 2nd associated Legendre polynomial of order 2, and the 2nd associated Legendre polynomial of order 3.

b. Use expression 2 to find the second Legendre polynomial, \( P_2(x) \), by setting \( m = 0 \). You should note that when \( m = 0 \), the associated Legendre polynomial reduces to the Legendre polynomial.
Legendre polynomial.

C. Carefully examine expression 2. If $m = 0$, what order polynomial will be generated for a given value of $l$?

C. Again, carefully examine expression 2. What order polynomial will be generated if $l = m$? What order polynomial will be generated if $m > l$? For a given value of $l$, what is the maximum value of $m$ that will give a non-zero associated Legendre polynomial?

D. According to your answer in part c, why must it be that $m \leq l$? Use this fact to explain why the values of the quantum number $m$ are allowed to vary from $-l$ to $l$.

Finally, we notice that the associated Legendre polynomial is defined in terms of $\theta$, which is the angle of displacement from the vertical (z) axis. Specifically, the associated Legendre polynomial is defined as $P_l^m(\cos \theta)$. To construct the associated Legendre polynomial in this form, we simply substitute $\cos \theta = x$ into the appropriate associated Legendre polynomial. Because $x = \cos \theta$ and because $\theta$ varies from 0 to $\pi$, we note that $\cos(0) = 1$ and $\cos(\pi) = -1$.

Thus, the form of an associated Legendre polynomial, $P_l^m(\cos \theta)$, from 0 to $\pi$ should be similar in form to the associated Legendre polynomial, $P_l^m(x)$, from 1 to -1. Let’s explore this similarity in a bit more detail. First, define $l = 2$ and $m = 1$ (to what type of orbital does this correspond?):

\[ l := 2 \quad m := 1 \]

Now find the appropriate associated Legendre polynomial, by substituting the appropriate values for $l$ and $m$ into expression 2: and symbolically evaluating:

\[
\frac{(-1)^{|l|} |l|}{2^{2-l} \cdot 2!} \left(1 - x^2\right)^{|l|} \frac{d^{2+|l|}}{dx^{2+|l|}}(x^2 - 1)^2
\]

Did you find this polynomial to be equal to $-3 \left(1 - x^2\right)^2 \cdot x$? If not, try again until you do.

Define this as $P(x)$ and $PC(\theta)$, making the substitution $x = \cos \theta$ for the latter.

\[
P(x) := -3 \left(1 - x^2\right)^2 \cdot x \quad PC(\theta) := -3 \left(1 - \cos(\theta)^2\right)^2 \cdot \cos(\theta)
\]

We now graph $P(x)$ vs. $x$ (Graph 3a) and $PC(\theta)$ vs. $\cos(\theta)$ (Graph 3b).
**Question 4:**

a. To what type of orbital does \( l = 1 \) and \( m = 0 \) correspond?

b. Generate graphs similar to those of Graph 3a and 3b to compare \( P(x) \) to \( PC(\theta) \) for any \( s \) orbital. Repeat for any \( p \) orbital.

**The \( \phi \)-dependent Function of the Angular Electronic Wave Function:**

We now turn to the \( \phi \)-dependent portion of the angular electronic wavefunction of the H-atom, which is quite easy to construct in Mathcad. The form of this function is given below:

\[
\Phi(\phi) = \frac{1}{\sqrt{2\pi}} e^{im\phi}
\]

Recall that possible values for \( m = 0, 1, 2 \ldots \) for the solutions to the \( \Phi \) portion of the angular wavefunction. We'll define \( m = 1 \) below:

\[
m := 1
\]

Now we define \( \Phi(\phi) \):

\[
\Phi(\phi) := \frac{1}{\sqrt{2\pi}} e^{i m \phi}
\]

Although \( \Phi \) is not real when \( m \neq 0 \), we can get some idea of the behavior of this function by graphing its real and imaginary components separately:
**Question 5:**

a. Why is $\Phi(\phi)$ real when $m = 0$?

b. $\Phi(\phi)$ is an exponential function of $\phi$, but the real and imaginary portions appear to vary cosinusoidally and sinusoidally, respectively. Why? HINT: Recall Euler’s theorem.

c. What changes do you observe in the real and imaginary portions of $\Phi(\phi)$ when you change the value of $m$?

d. What would you expect the probability distribution of $\Phi(\phi)$ to look like? Why?

**The Normalization Constant:**

Finally, we turn to the normalization constant, $N_{l,m}$. $N_{l,m}$ depends upon $l$ and $m$, we need to define these numbers (Keep in mind you need to define these appropriately so that the associated Legendre polynomial does not vanish (see questions 3c and 3d, above):

\[
\begin{align*}
\mathbf{l} &:= 1 \\
\mathbf{m} &:= 0
\end{align*}
\]

The normalization constant is:

\[
N := \frac{1}{\left[ \frac{(2l + 1) \cdot (1 - |m|)!}{2 \cdot (1 + |m|)!} \right]^2}
\]

$N = 1.225$

Let’s check to see if $PC(\theta)$ is normalized:

\[
PC(\theta) := -3 \left( 1 - \cos(\theta) \right)^2 \cdot \cos(\theta)
\]
\[ \int_{0}^{\pi} PC(\theta) \cdot PC(\theta) \cdot \sin(\theta) \, d\theta = 2.4 \]

The function is not normalized. We need to make the wavefunction normalized. (Why is it important to have the wavefunction normalized?)

If we include the normalization constant, is this function normalized?

\[ \int_{0}^{\pi} N \cdot PC(\theta) \cdot N \cdot PC(\theta) \cdot \sin(\theta) \, d\theta = 3.6 \]

**Question 6**: Check that PC(\(\theta\)) is normalized for \(l=1, m=0\).

**Construction of the Entire Wave Function and Probability Distribution:**

We can now construct the full angular electronic wavefunction for the H-atom. Let's do this for a 2p_z orbital, for which \(l = 1\) and \(m = 0\). We first define \(l\) and \(m\) below:

\[ l := 1 \quad m := 0 \]

The normalization constant is then:

\[ N = \left[ \frac{(2l + 1) \cdot (1 - |m|) !}{2 \cdot (l + |m|) !} \right]^{1/2} \]

\[ N = 1.225 \]

The appropriate associated Legendre polynomial is defined as \(P(m, l, x)\), using expression 2:

\[ P(m, l, x) := \frac{(-1)^{|m|}}{2^l \cdot l !} \cdot (1 - x^2)^l \cdot \frac{d^{|m|}}{dx^{|m|}} \left( x^2 - 1 \right)^l \]
Now we can put it all together in the angular wavefunction, which we define as \( \Psi(\theta, \phi, l, m) \):

\[
\Psi(\theta, \phi, l, m) := \frac{(2l + 1) \cdot (1 - |m|)!}{4\pi (1 + |m|)!} \cdot P(l, m, \cos(\theta)) \cdot \exp(i m \phi)
\]

Equation 3

where \( l \) and \( m \) are the familiar quantum numbers, \( \theta \) is the angle displaced from the z-axis, and \( \phi \) is an angle that is swept out within the xy plane.

The first factor of Equation 3, \((2l+1)(1-|m|)! / 4\pi (1+|m|)!\) is the normalization constant for these orbitals. The second factor, \(P(l, m, \cos(\theta))\), is the associated Legendre polynomial in \( \theta \). The third factor, \(\exp(i m \phi)\), represents the portion of the wavefunction dependent upon \( \phi \). Notice that this portion of the wavefunction will yield imaginary results for any value of \( m > 0 \). However, because we are only interested in the probability distribution of this wavefunction, we will square \(\Psi(\theta, \phi, l, m)\) (multiply by its complex conjugate) or square linear combinations of wavefunctions (multiply them by their complex conjugates) with the same eigenvalues as \(\Psi(\theta, \phi, l, m)\).

Let's construct and display the probability distribution of the angular portion of the 2p\(_0\) orbital. To do so, we have to construct each of the three parts of Equation 3: The normalization constant, the associated Legendre polynomial transformed into a function of \( \theta \), and the function of \( \phi \). We define \( l \) and \( m \) for a 2p\(_0\) orbital:

\[
\begin{align*}
    l &= 1 \\
    m &= 0
\end{align*}
\]

NOTE: Define HERE the values for \( l \) and \( m \) that you want to use for the probability plots (see below).

First, we'll determine the normalization constant:

\[
N = \left( \frac{2l + 1}{4\pi (1 + |m|)!} \right)^{\frac{1}{2}}
\]

Next, we need to determine the associated Legendre polynomial that is part of the angular part of the wavefunction. This is Expression 2 from above, which allows us to determine the associated Legendre polynomial for specific values of the quantum numbers \( l \) and \( m \). Evaluate Expression 2 symbolically for the proper values of the \( l \) and \( m \) quantum numbers for a 2p\(_0\) orbital.
\[
\frac{(-1)^m}{2^l \cdot l!} \cdot (1 - x^2)^{\frac{l}{2}} \cdot \frac{d^{l+m}}{dx^{l+m}}(x^2 - 1)^l
\]
Expression 2

Did you find the value to be \( x \)? Good! Now be sure to cut and paste your answer into the space at the right hand side of the definition below to define \( P(x) \):

\[
P(x) \equiv x
\]

**NOTE:** Define HERE the associated Legendre polynomial that you want to use for the probability plots (see below). Simply cut and paste from your simplified expression 2 (above).

Later on, we'll make the substitution, \( x = \cos \theta \) to transform \( P(x) \) to \( P(\cos(\theta)) \). This is simply done by writing \( P(\cos(\theta)) \), which will allow Mathcad to do the substitution for us. This will come in handy with some of the more complicated Legendre polynomials. In the case for \( l = 1 \) and \( m = 0 \), however, you should note that \( P(\cos(\theta)) = \cos(\theta) \).

Now we define the function for \( \Phi(\phi) \):

\[
\Phi(\phi) \equiv \frac{1}{\sqrt{2\pi}} e^{im\phi}
\]

Now that we have each portion angular wavefunction defined, we can define \( \Psi(\theta, \phi) \) as a product of \( N \), \( P(\cos(\theta)) \), and \( \Phi(\phi) \):

\[
\Psi(\theta, \phi) \equiv N \cdot P(\cos(\theta)) \cdot \Phi(\phi)
\]

Multiplying each wavefunction by its complex conjugate and setting that equal to \( r \) allows us to visualize the angular part of the wavefunction in three dimensions. Here, \( r \) is not the distance from the nucleus. Rather, it is related to the probability of finding the electron at a location specified by the angles \((\theta, \phi)\) in space. To display the probability distribution of the wavefunction, we will multiply \( \psi(\theta, \phi) \) by its complex conjugate. In addition, the substitutions \( x = r \sin \theta \cos \phi \), \( y = r \sin \theta \sin \phi \) and \( z = r \cos \theta \) are also made, where \( r = \Psi^* \Psi \). The transformation of variables is done so we can display the wavefunction in Cartesian coordinates.

Denoting the complex conjugate of a function is done in Mathcad by placing a bar over the function. This is done by underlining the function you wish to take the complex conjugate of and typing a quote ("), or (Shift '),.
\[ X(\theta, \phi) := (\Psi(\theta, \phi) \cdot \overline{\Psi(\theta, \phi)}) \cdot \sin(\theta) \cdot \cos(\phi) \]

\[ Y(\theta, \phi) := (\Psi(\theta, \phi) \cdot \overline{\Psi(\theta, \phi)}) \cdot \sin(\theta) \cdot \sin(\phi) \]

\[ Z(\theta, \phi) := \Psi(\theta, \phi) \cdot \overline{\Psi(\theta, \phi)} \cdot \cos(\theta) \]

Now display the angular wavefunction. First, click on Insert, Graph, then Surface Plot (Alternatively, hit Ctrl 2). There should be a black rectangle at the bottom left-hand corner of the graph. Type (X, Y, Z) in this rectangle (include the parentheses!).

Graph 5: Display of the Angular Portion of the 2Po orbital

(X, Y, Z)
Question 7:

a. Display the probability distribution for a 1s orbital above. Go back to expression 2 and evaluate the appropriate associated Legendre polynomial for a 1s orbital \((l = 0, m = 0)\). (Be careful! Mathcad won’t calculate a zeroth derivative! However, the “zeroth derivative” of any function is simply the function itself!) Define this polynomial as \(P(x)\) in yellow above. Do you get the familiar result?

b. Display the probability distribution for the 3d\(_{z^2}\) orbital above. Go back to expression 2 and evaluate the appropriate associated Legendre polynomial for a 3d\(_{z^2}\) orbital \((l = 2, m = 0)\). Define this polynomial as \(P(x)\) in yellow above. Do you get the familiar result?

c. Display the probability distribution for the \(2p_{+1}\) and \(2p_{-1}\) orbitals above. Go back to expression 2 and evaluate the appropriate associated Legendre polynomial for a \(2p_{+1}\) and \(2p_{-1}\) orbitals \((l = 1, m = 1 \text{ or } -1)\). Define this polynomial as \(P(x)\) in yellow above. Do you get the familiar result?

You probably noted in part c of question 4 that the probability distributions of the \(2p_{+1}\) and \(2p_{-1}\) are not those normally displayed in text books. Customarily, linear combinations of eigenfunctions of the \(\Phi(\phi)\) portion of the angular electronic wavefunction of the H-atom are used in the construction of the probability distributions when \(m \neq 0\). This is done for two reasons.

First, when \(m \neq 0\), the angular electronic wavefunction not only depends upon both \(\theta\) and \(\phi\), but also contains an imaginary component in the \(\phi\) dependence. Second, the probability distributions for the \(m = 1\) and \(m = -1\) (or any other combination of \(m = \) plus or minus \(x\)) wavefunctions are identical. But chemists are very interested in the directional character of each orbital, as this offers clues into how atoms interact in bonding. So how are these "textbook" probability distributions graphed? Linear combinations of eigenfunctions of the \(\Phi(\phi)\) portions are constructed. The \(\phi\)-dependent wavefunctions, \(\Phi(\phi)_{2px}\) and \(\Phi(\phi)_{2py}\), are eigenfunctions of the Schrodinger equation for the \(\phi\)-dependent portion of the H-atom electron. Because quantum operators are linear operators, linear combinations of these eigenfunctions must also be eigenfunctions. By taking linear combinations of the \(\Phi(\phi)_{2p_{+1}}\) and \(\Phi(\phi)_{2p_{-1}}\) wavefunctions and multiplying these linear combinations (different ones for each case) with \(N_{l,m}\) and \(P_{l}^{m}(\cos \theta)\), we can construct the "textbook" \(2p_{+1}\) and \(2p_{-1}\) wave functions and probability distributions.

To display the \(\Phi\) portion of the \(2p\) \((l = 1, m = -1, 0, 1)\) angular orbital wavefunctions, we define:

\[
\Phi_{-1}(\phi) := e^{-i(1)(\phi)} \quad \text{for } m = -1
\]

\[
\Phi_{0}(\phi) := e^{-i(0)(\phi)} \quad \text{for } m = 0
\]

\[
\Phi_{+1}(\phi) := e^{-i(1)(\phi)} \quad \text{for } m = +1
\]
Clearly, \( \Phi_m(\phi) \), \( \Phi_{p2}(\phi) \) and higher are evaluated by simply substituting in the appropriate value for \( m \):

\[
\Phi_{\text{minus2}}(\phi) := e^{-i(-2)\cdot \phi} \quad \text{for } m = -2
\]

\[
\Phi_{\text{plus}}(\phi) := e^{-i(2)\cdot \phi} \quad \text{for } m = +2
\]

At any rate, real representations of the \( \phi \)-dependent portion of \( p_{+1}, p_{-1} \) and \( p_0 \) orbitals are then constructed by the following linear combinations:

\[
\Phi_x(\phi) := \frac{\Phi_{\text{plus1}}(\phi) + \Phi_{\text{minus1}}(\phi)}{\sqrt{2}}
\]

\[
\Phi_y(\phi) := \frac{-i(\Phi_{\text{plus1}}(\phi) - \Phi_{\text{minus1}}(\phi))}{\sqrt{2}}
\]

\[
\Phi_z(\phi) := e^{-i(0)\cdot \phi}
\]

We view these linear combinations to verify that they are indeed real:

**Graph 6a**

- \( \Phi_x(\phi) \)

**Graph 6b**

- \( \Phi_y(\phi) \)
Viewing the real representations of the $2p_{+1}$ and $2p_{-1}$ orbitals is now easy! For $p_{+1}$, $l = 1$ and $m = 1$. We therefore define $l$, $m$ and determine the normalization constant:

$$N = \left[ \frac{(2l + 1) \cdot (1 - |m|)!}{4\pi \cdot (l + |m|)!} \right]^{\frac{1}{2}}$$

Now we use Expression 2 to find and define the appropriate Legendre polynomial:

$$P(x) := -\left(1 - x^2\right)^{\frac{1}{2}}$$

We redefine $\Psi(\Theta, \phi)$ to include the real representation of the $\phi$-dependent portion ($\Phi_x(\phi)$) for the $2p_x$ orbital:

$$\Psi(\theta, \phi) := N \cdot P(\cos(\theta)) \cdot \Phi_x(\phi)$$
Since we want the probability distribution, we multiply each function above by its complex conjugate, take each product and transform into Cartesian coordinates:

\[ X(\theta, \phi) := (\Psi(\theta, \phi) \cdot \overline{\Psi(\theta, \phi)}) \cdot \sin(\theta) \cdot \cos(\phi) \]

\[ Y(\theta, \phi) := (\Psi(\theta, \phi) \cdot \overline{\Psi(\theta, \phi)}) \cdot \sin(\theta) \cdot \sin(\phi) \]

\[ Z(\theta, \phi) := \Psi(\theta, \phi) \cdot \overline{\Psi(\theta, \phi)} \cdot \cos(\theta) \]

Finally, we display the orbital:

**Question 8:**

a. Does the orbital in graph 7 represent the “textbook” version of a \(p_x\) orbital?

b. How does the orientation of the orbital in graph 5 compare to the orientation of the orbital in graph 7, with respect to the x, y and z-axes?
**Question 9:**

a. Display the probability distribution of the "textbook version" the 2p_y (l = 1, m = -1) orbital in Cartesian coordinates.

b. The "textbook" representations of the 3d orbitals are constructed by using the following linear combinations in the φ-dependent portions of the angular electronic wavefunction of the H-atom:

\[
d_{z^2} = \phi_0(\phi) \quad (l = 2, m = 0)
\]

\[
dx_z = \frac{[\phi_{+1}(\phi) + \phi_{-1}(\phi)]}{\sqrt{2}} \quad (l = 2, m = 1)
\]

\[
d_{yz} = -\frac{[\phi_{+1}(\phi) - \phi_{-1}(\phi)]}{\sqrt{2}} \quad (l = 2, m = -1)
\]

\[
d_{x^2-y^2} = \frac{[\phi_{+2}(\phi) + \phi_{-2}(\phi)]}{\sqrt{2}} \quad (l = 2, m = 2)
\]

\[
d_{xy} = -\frac{[\phi_{+2}(\phi) - \phi_{-2}(\phi)]}{\sqrt{2}} \quad (l = 2, m = -2)
\]

Define equations for, and display in spherical coordinates the:

a. d_{z^2} orbital

b. two other 3d orbitals

**Mastery Exercise:**

Display the "textbook" wavefunctions and probability distributions for a few of the 7 f orbitals. You may need to do a bit of literature or internet searching to find the appropriate linear combinations of eigenfunctions to use in the construction of these probability distribution plots.