Visualizing the Hydrogen Atomic Orbitals: A Tool for Undergraduate Physical Chemistry

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Abstract

Despite the prominence of orbitals throughout the curriculum of undergraduate chemistry, high-quality visualization of the atomic orbitals is out of reach for most scientists. Rigorously visualizing the atomic orbitals even for simple hydrogen-like atoms and ions is rather challenging due to the complex 3-D structure and geometric variability of the orbitals across three distinct quantum numbers. In this article, a graphical user interface (GUI)-based tool for visualizing 3-D volumetric density plots of hydrogen atomic orbitals is introduced. This tool is written in Python, and a Jupyter notebook version with explanatory blocks interspersed in the code is included for pedagogical purposes. The user can manipulate a large number of features using the GUI, which allows customization of the orbital illustrations. Because this visualizer is capable of visualizing orbitals with any quantum numbers and showing their nodal surfaces, it can serve as a supplement to students' lecture and textbook education on this topic.

Keywords

First-Year Undergraduate, Upper-Division Undergraduate, Atomic Structure, Quantum Chemistry, Computer-Based Learning

Introduction

In undergraduate chemistry courses, especially first-year general and upper-level physical chemistry courses, students are introduced to the atomic orbitals for the hydrogen atom in varying levels of detail.[1–16] In first-year courses, students are told about the quantum numbers n, l, and m (often called m_l) used to label the wavefunctions and energy states of the hydrogen atom.[3–10] Students are then taught to associate distinct sets of the quantum numbers with specific shapes of the electron orbitals.[17] Students often, and even professional chemists occasionally, struggle to understand what is meant by an orbital due to the inherent connection between the strange wave-particle duality of the electrons and the electron orbital geometry.[17,18] This wave-particle duality manifests in the electrons spreading throughout space in a wide array of different orbital geometries. Perfecting the mental images students associate with the orbitals is thus of critical pedagogical importance. To this end, students are shown basic illustrations of the orbitals, typically represented as "shells" of the wavefunction generated using iso-probability surfaces (sometimes called boundary surfaces).[3–10] Many articles in this Journal have suggested a range of methods for representing orbital iso-probability surfaces, contour plots, and occasionally density diagrams.[19–26] Notably, more modern articles typically include more useful 3-D representations using random points or density plots, but most still rely on the construction of surfaces rather than showing the density of the orbital in space.[17,24–26]

The shortcomings of basic orbital pictures become clearer as the value of n is increased for a given l and m. For instance, consider the series of p_z orbitals with $n = 2, 3, 4$ shown in Figure 1. It is immediately clear that if the 3-D features of the orbitals are not adequately captured, students may miss crucial aspects of the orbitals' structure, such as the presence of radial nodes and the diffuse spread of the electrons throughout space. The latter is especially important, since isoprobability surfaces are incapable of expressing how the orbital amplitude is lower in regions far from the nucleus and how the corresponding probability density is higher. This structure is important when students begin their study of molecular orbital theory since the orbital overlap is related to bonding strength.[11] Moreover, the typical 2-D representations of orbitals do not help students reason about the orbitals' spatial alignment. While some textbooks do effectively show the radial nodes and orbital alignment using isoprobability surfaces,[1–10] several erroneously illustrate the orbitals with corresponding l and m quantum numbers and increasing principal quantum number n as simply larger versions of the previous orbitals.[27–29] It is also noteworthy that many textbooks that include some 3-D depiction of the wavefunctions have only one figure illustrating the 3-D radial structure of the wavefunction, and only for s orbitals.[3–10] While this is not an indictment of the quality of any of these texts, it does suggest that the use of interactive simulation tools capable of plotting as many distinct orbitals as students need can help students significantly enhance their understanding and intuition. This is further supported by the popularity of online resources like the Orbitron, which contains several solid cutaway versions of the hydrogen atomic orbitals wavefunctions.[30]

While general chemistry students are exposed to the shapes of the orbitals, they are less commonly exposed to the relationships between the quantum numbers and the radial and angular nodes of the wavefunction at the general chemistry level. This is unfortunate, since reasoning about the spatial orientations and geometric structure of orbitals is critical to even a qualitative treatment of molecular orbital theory in upper-division courses. The lack of both rigorously correct visualizations of the atomic orbitals and the lack of association of the quantum numbers with nodal structure and geometry of the orbitals likely contributes to students' well-documented difficulties with molecular orbital theory.[31] This work aims to somewhat alleviate this problem by presenting an open-source graphical user interface

(GUI)-based tool developed using undergraduate physical chemistry concepts. The program allows students to easily modify 3-D representations of the orbitals and their nodal surfaces to discover and understand the relationships between quantum numbers and geometry. This tool can easily be integrated into a general chemistry course to aid in visualization of orbitals during units on introductory quantum mechanics. But to assist students with effective orbital visualizations, the nature of the orbitals being plotted must be addressed.

Quantum Theory and the Hydrogen Atom

Once students learn how to solve the time-independent Schrödinger equation in physical chemistry, they are exposed to some of the mathematical details of the wavefunctions for the hydrogen atom.[11–15] Students are then taught that what they have called atomic orbitals throughout their chemistry careers are nothing more than the wavefunction solutions to the time-independent Schrödinger equation for the hydrogen atom. The probability of finding an electron at some location in space is then related to the square modulus of the wavefunction.[11,12] It should be emphasized to students that the wavefunction is not observable, but its square modulus that describes the spatial electron density is observable.[11] What students recognize as orbitals in multi-electron atoms and molecules is an "orbital approximation" to the wavefunction for that system.[17] Written in abstract form in spherical coordinates, the time-independent Schrödinger equation and its solutions for the hydrogen atom have the form,[11]

$$\hat{H}\psi_{n,l,m}(r,\theta,\phi) = E_n\psi_{n,l,m}(r,\theta,\phi) \tag{1}$$

$$E_n = -\frac{R_H}{n^2} \tag{2}$$

$$\psi_{n,l,m}(r,\theta,\phi) = R_{n,l}(r)Y_l^m(\theta,\phi) \tag{3}$$

In equations (1)-(3), $\hat{H}$ is the Hamiltonian (total energy) operator with energy eigenvalues E_n, $\psi_{n,l,m}$ is one of the hydrogen wavefunctions, R_H is the Rydberg constant, $R_{n,l}(r)$ is

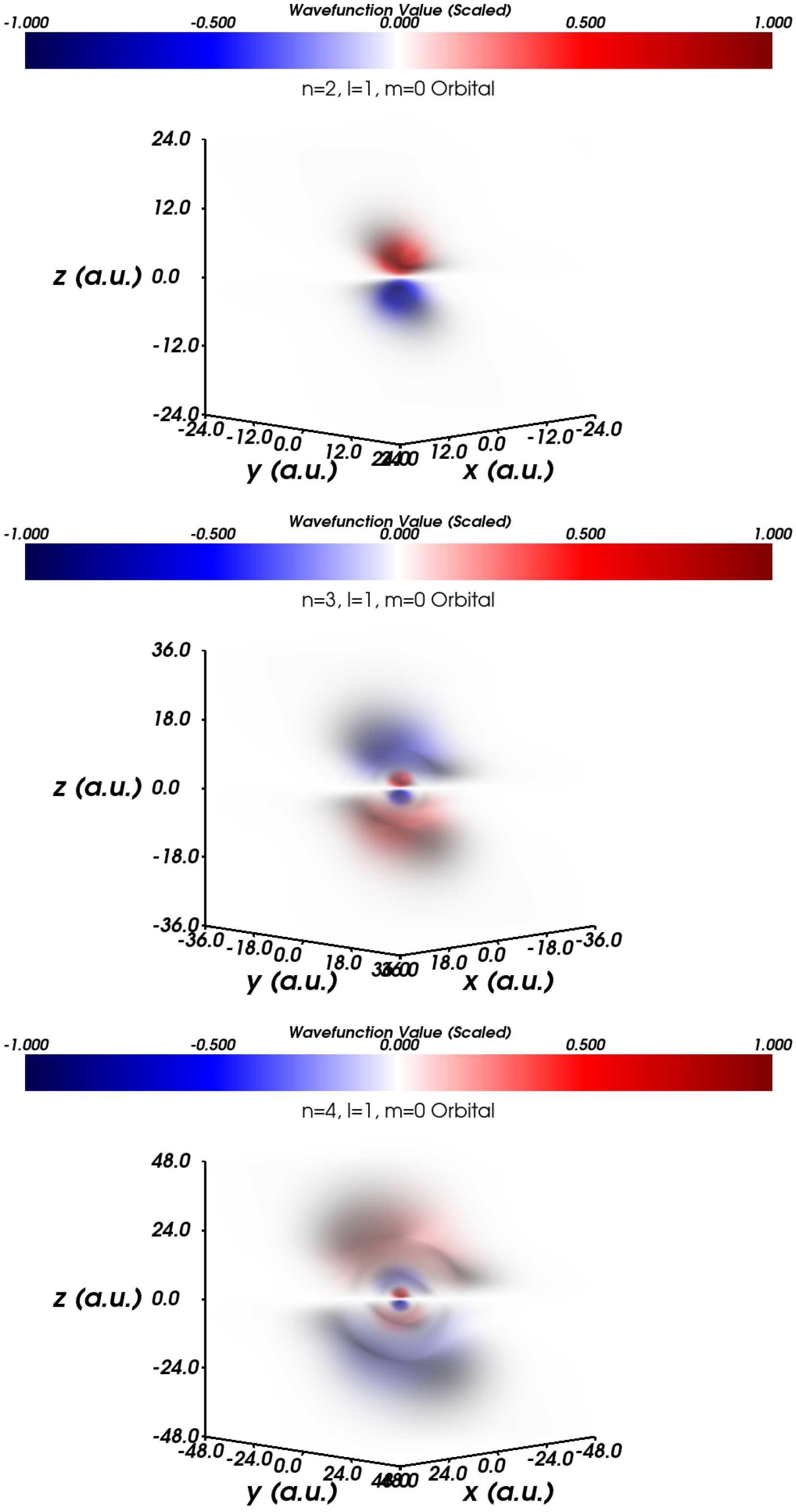


Figure 1: Illustration of $\phi_{n,1,0}$, also known as p_z orbitals, for $n = 2, 3, 4$. This demonstrates how the number of radial nodes varies with the quantum number n.

the radial wavefunction, and $Y_l^m(\theta, \phi)$ is a spherical harmonic function, the angular part of the wavefunction.[32] Depending on the emphasis of the course, students are often shown how to find these solutions with differential equations techniques or ladder operators.[11,33] It is $Y_l^m(\theta, \phi)$ that gives rise to the "shapes" (sphere, dumbbell, clover, etc.) of the atomic orbitals. The quantum numbers n, l, and m are the usual principal, angular momentum, and magnetic quantum numbers for the hydrogen atom orbitals with the same limits taught to general chemistry students,[1–16]

$$n \in \mathbb{N} \qquad (n = 1, 2, 3, \ldots) \tag{4}$$

$$l \in [0, n-1] \subset \mathbb{Z} \qquad (l = 0, 1, 2, \ldots, n-1) \tag{5}$$

$$m \in [-l, l] \subset \mathbb{Z} \qquad (m = -l, -l+1, \ldots, 0, \ldots, l-1, l) \tag{6}$$

where $\in$ denotes set inclusion, $\subset$ denotes a subset, $\mathbb{N}$ is the set of natural numbers, and $\mathbb{Z}$ is the set of integers.[32] The radial and angular wavefunctions can be expressed using orthogonal polynomials,[11,32,34]

$$R_{n,l}(r) = C_{n,l} e^{-\frac{r}{na_0}} \left(\frac{2r}{na_0}\right)^l L_{n-l-1}^{(2l+1)}\left(\frac{2r}{na_0}\right) \tag{7}$$

$$Y_l^m(\theta, \phi) = N_{l,m} P_l^m(\cos(\theta)) e^{im\phi} \tag{8}$$

In equations (7) and (8), a_0 is the Bohr radius, $L_{n-l-1}^{(2l+1)}$ is an associated Laguerre polynomial, and P_l^m is an associated Legendre polynomial. These polynomials are defined via recursion relationships or the Rodrigues formulas,[32,34]

$$P_n(x) = \frac{1}{2^n n!} \frac{d^n}{dx^n} (x^2 - 1)^n \tag{9}$$

$$P_l^m(x) = (-1)^m (1 - x^2)^{\frac{m}{2}} \frac{d^m}{dx^m} P_l(x) \tag{10}$$

$$L_n^{(\alpha)}(x) = \frac{x^{-\alpha} e^x}{n!} \frac{d^n}{dx^n} (e^{-x} x^{n+\alpha}) \tag{11}$$

The normalization constants $C_{n,l}$ and $N_{l,m}$ are given by,[11]

$$C_{n,l} = \sqrt{\left(\frac{2}{na_0}\right)^3 \frac{(n-l-1)!}{2n(n+l)!}} \tag{12}$$

$$N_{l,m} = \sqrt{\frac{(2l+1)(l-m)!}{4\pi(l+m)!}} \tag{13}$$

With the mathematical form of the wavefunctions in hand, a connection between the mathematics of quantum mechanics and general chemistry intuition finally seems to be in reach. For curious students that consider the mathematical form of the wavefunctions, however, a somewhat surprising issue arises. For orbitals with $m \neq 0$, the wavefunction is intrinsically complex due to the term $e^{im\phi}$. Thus, rationalizing a picture of the orbitals becomes more complicated. If students do plot the 3-D form of the real and imaginary parts of a wavefunction with $m \neq 0$, they discover that the real and imaginary parts of an individual $2p$ orbital with $m = \pm 1$ take on the expected form for both the p_x and p_y orbitals. Even more confusingly, instead of the traditional “dumbbell” shape, the magnitude of the wavefunction for a $2p$ orbital with $m = \pm 1$ is rather like a “doughnut,” or more properly a torus. The real or imaginary parts are what have the expected appearance of a dumbbell. This is shown in Figure 2. The corresponding real and imaginary parts of the orbital $\psi_{2,1,-1}$ simply have the real and imaginary orientations swapped and the same shapes as the components of the orbital $\psi_{2,1,1}$. Since the wavefunctions $\psi_{n,l,m}$ do not entirely look like students expect based upon their general chemistry intuition, a connection between the solutions to the Schrödinger equation and the orbital pictures drawn in introductory chemistry courses must be made. Otherwise, it is unclear what exactly it is that textbooks are plotting and calling the orbitals.

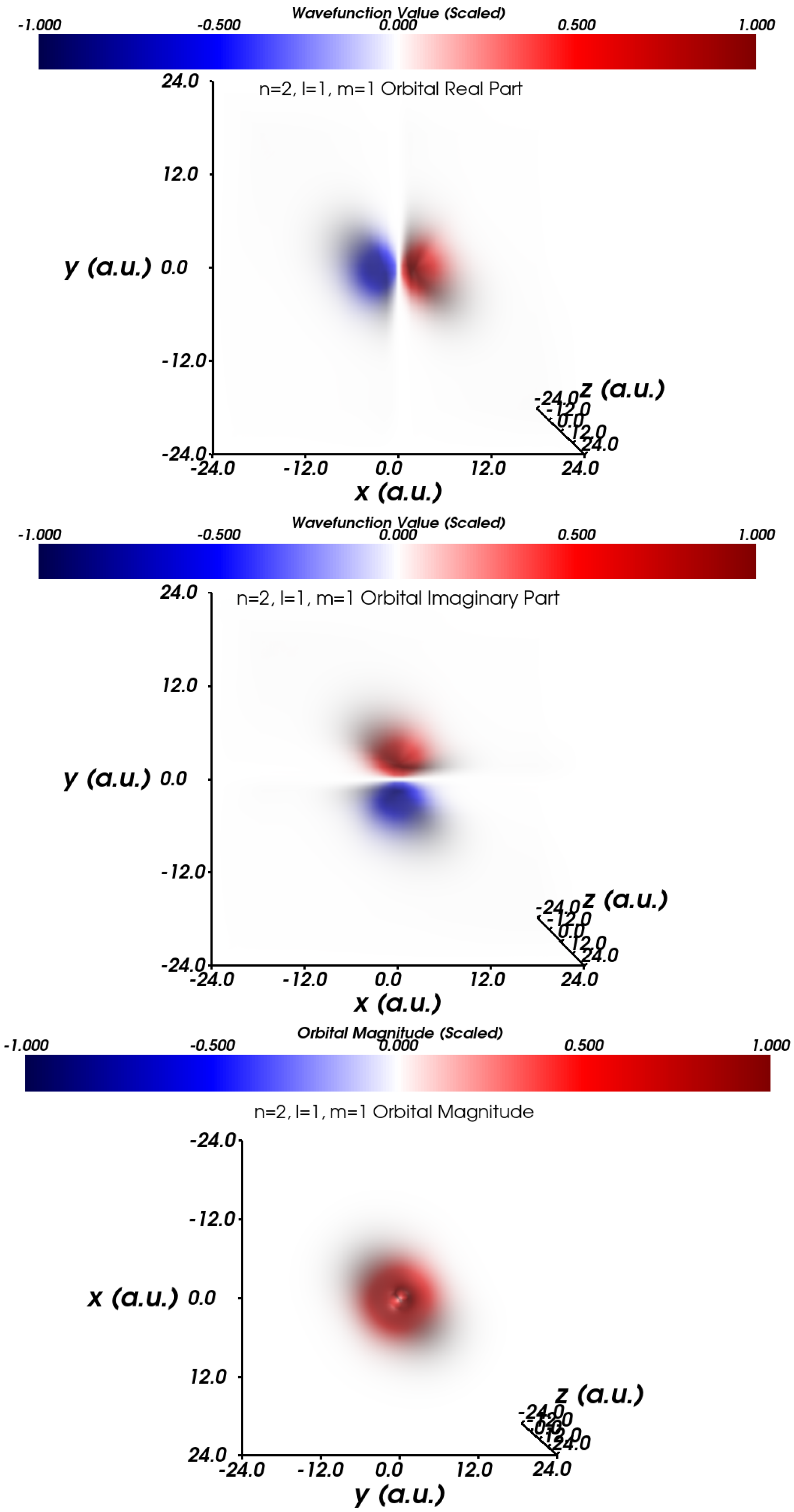


Figure 2: Illustration of the real and imaginary parts of the orbital $\psi_{2,1,1}$, one of the $2p$ orbitals, and the orbital's absolute magnitude. Note that the magnitude of the complete orbital is shaped like a doughnut (torus) rather than the traditional dumbbell.

A Modified Hydrogen Orbital Basis

The connection between the mathematical wavefunctions and general chemistry intuition can be shown using some clever mathematical manipulations of the Legendre polynomials in the angular wavefunction. A different, though in some ways more convenient, form of the hydrogen atom orbitals that retains all of the necessary properties (degeneracies, orthonormality) can be constructed. This new set of orbitals will be entirely real, and so the imaginary wavefunction component $e^{im\phi}$ is what must be dealt with. An identity that follows from manipulation of the Rodrigues formula for the associated Legendre polynomials is,[32,35]

$$\begin{aligned} P_l^{-m}(\cos(\theta)) &= \frac{(l-m)!}{(l+m)!}P_l^m(\cos(\theta)) \qquad (14) \\ \implies P_l^{-m}(\cos(\theta)) &\propto P_l^m(\cos(\theta)) \end{aligned}$$

Note that some authors will include a factor of $(-1)^m$, called the Condon-Shortley phase, in equation (14).[32] This factor is omitted in this paper to simplify the algebraic presentation. The identity in equation (14) suggests that various angular functions can be combined in a useful way. Using the normalization constant $N_{l,m}$ from equation (13) gives,

$$\begin{aligned} N_{l,m}P_l^m(\cos(\theta)) &= \sqrt{\frac{(2l+1)(l-m)!}{4\pi(l+m)!}}P_l^m(\cos(\theta)) \\ N_{l,-m}P_l^{-m}(\cos(\theta)) &= \frac{(l-m)!}{(l+m)!}\sqrt{\frac{(2l+1)(l+m)!}{4\pi(l-m)!}}P_l^m(\cos(\theta)) \\ &= \sqrt{\frac{(2l+1)(l-m)!}{4\pi(l+m)!}}P_l^m(\cos(\theta)) \\ &= N_{l,m}P_l^m(\cos(\theta)) \qquad (15) \end{aligned}$$

Equation (15) says that the θ part of the angular wavefunction corresponding to $-m$ is the same as for m when including the normalization constant. Finally, the Euler formula for

$\cos(\phi)$ in equation (16) can be used to address the ϕ part of the wavefunction,

$$\cos(\phi) = \frac{e^{i\phi} + e^{-i\phi}}{2} \tag{16}$$

$$\begin{aligned} Y_l^m(\theta,\phi) + Y_l^{-m}(\theta,\phi) &= N_{l,m}P_l^m(\cos(\theta))e^{im\phi} + N_{l,-m}P_l^{-m}(\cos(\theta))e^{-im\phi} \\ &= N_{l,m}P_l^m(\cos(\theta))\left[e^{im\phi} + e^{-im\phi}\right] \\ &= 2N_{l,m}P_l^m(\cos(\theta))\cos(m\phi) \\ &= 2\mathrm{Re}\Big(Y_l^m(\theta,\phi)\Big) \qquad (17) \end{aligned}$$

The linear combination of angular functions in equation (17) is entirely real, and thus much easier to deal with. An exactly analogous result for the difference linear combination is obtained using the Euler formula for $\sin(\phi)$ in equation (18),

$$\sin(\phi) = \frac{e^{i\phi} - e^{-i\phi}}{2i} \tag{18}$$

$$\begin{aligned} Y_l^m(\theta,\phi) - Y_l^{-m}(\theta,\phi) &= N_{l,m}P_l^m(\cos(\theta))e^{im\phi} - N_{l,-m}P_l^{-m}(\cos(\theta))e^{-im\phi} \\ &= N_{l,m}P_l^m(\cos(\theta))\left(e^{im\phi} - e^{-im\phi}\right) \\ &= 2iN_{l,m}P_l^m(\cos(\theta))\sin(m\phi) \\ &= 2i\mathrm{Im}\Big(Y_l^m(\theta,\phi)\Big) \qquad (19) \end{aligned}$$

The linear combination in equation (19) is entirely imaginary, so multiplying by i gives an entirely real function. Utilizing these results, a purely real new set of orbital wavefunctions called $\phi_{n,l,m}$ is defined such that,

$$\begin{aligned} \phi_{n,l,\pm m}(r,\theta,\phi) &\equiv \begin{cases} \psi_{n,l,m}(r,\theta,\phi) & m = 0 \\ \pm\frac{i^{0.5\mp 0.5}}{\sqrt{2}}\left[\psi_{n,l,m}(r,\theta,\phi) \pm \psi_{n,l,-m}(r,\theta,\phi)\right] & m \neq 0 \end{cases} \qquad (20) \\ &= \begin{cases} \psi_{n,l,m}(r,\theta,\phi) & m = 0 \\ \pm\frac{i^{0.5\mp 0.5}}{\sqrt{2}}R_{n,l}(r)\left[Y_l^m(\theta,\phi) \pm Y_l^{-m}(\theta,\phi)\right] & m \neq 0 \end{cases} \end{aligned}$$

where the factor of $i^{0.5\mp 0.5}$ gives a result of 1 when using the positive linear combination from equation (17) and i when using the negative linear combination in equation (19). This ensures that the resultant orbitals are strictly real. Using equation (3) for the hydrogen wavefunctions $\psi_{n,l,m}$, the fact that the radial wavefunction is completely real, and equations (17) and (19), the orbitals $\phi_{n,l,m}$ can be neatly written,

$$\phi_{n,l,m}(r,\theta,\phi) = \begin{cases} \psi_{n,l,m}(r,\theta,\phi) & m = 0 \\ \frac{2}{\sqrt{2}}\mathrm{Re}\Big(\psi_{n,l,m}(r,\theta,\phi)\Big) & m > 0 \\ \frac{2}{\sqrt{2}}\mathrm{Im}\Big(\psi_{n,l,-m}(r,\theta,\phi)\Big) & m < 0 \end{cases} \tag{21}$$

where the extra factor of 2 comes from equations (17) and (19) and the requirement of normalization. This set of orbital wavefunctions $\phi_{n,l,m}$ is completely real for every set of quantum numbers. Note that while McQuarrie does explain this construction of the "real representation" of the hydrogen orbitals in the context of the p and d orbitals, this construction is entirely general and too frequently left unexplained.[11]

The new set of functions $\{\phi_{n,l,m}\}$ is a complete spanning set of orthonormal functions that is a legitimate replacement for the hydrogen atom wavefunctions. The original hydrogen atom wavefunctions $\psi_{n,l,m}$ obey the orthonormality relationship expressed in Dirac's bra-ket notation,[11,33]

$$\langle \psi_{n,l,m} | \psi_{n',l',m'} \rangle = \int_{\mathbb{R}^3} \psi^*_{n,l,m}(r,\theta,\phi)\psi_{n',l',m'}(r,\theta,\phi)d\tau = \delta_{n,n'}\delta_{l,l'}\delta_{m,m'} \tag{22}$$

where δ_{jk} is the Kronecker delta (1 if $j = k$ and 0 otherwise), $\mathbb{R}^3$ is all of 3-D space and $d\tau$ is the volume element ($d\tau = dxdydz$ in Cartesian coordinates, $d\tau = r^2\sin(\theta)drd\theta d\phi$ in spherical coordinates).[32,34] The same relationship is obeyed by the new functions $\phi_{n,l,m}$,

$$\langle \phi_{n,l,m} | \phi_{n',l',m'} \rangle = \int_{\mathbb{R}^3} \phi^*_{n,l,m}(r,\theta,\phi)\phi_{n',l',m'}(r,\theta,\phi)d\tau = \delta_{n,n'}\delta_{l,l'}\delta_{m,m'} \tag{23}$$

which can be verified case-by-case using equations (20) and (22).

The orbitals $\phi_{n,l,m}$ have identical energies to the unmodified hydrogen orbitals $\psi_{n,l,m}$ since $\hat{H}\phi_{n,l,m} = E_n\phi_{n,l,m}$. This set of orbitals will span all $2l+1$ possible values of m for any particular choice of n and l since we have defined a set of orbitals $\{\phi_{n,l,m}\}$ that are unique and orthonormal for every value of m. Mathematically, this means that the definition of $\phi_{n,l,m}$ can be interpreted as a change of basis for the hydrogen atomic orbitals $\psi_{n,l,m}$. The $\phi_{n,l,m}$ orbitals are also strictly real, and can thus be plotted using a single picture for each distinct orbital. Plotting the orbitals corresponding to $\phi_{n,l,m}$ and $\phi_{n,l,-m}$ for $2p$ orbitals in the same fashion as before gives the familiar looking pictures corresponding to $2p_x$ and $2p_y$ orbitals shown in Figure 3. It turns out that when chemists are trained to visualize the atomic orbitals for hydrogen, they are typically introduced, at least implicitly, to this modified basis set $\{\phi_{n,l,m}\}$ rather than the direct solutions to the Schrödinger equation $\{\psi_{n,l,m}\}$. This is due to the simplification of only needing one plot of the orbital in its "real representation," as McQuarrie describes it.[11] This is a detail often missed by even veteran chemistry instructors. An explanation of how these 3-D visualizations of the orbitals were generated and the tool that students may use to explore the orbitals is now in order.

Implementation of the the Hydrogen Orbital Visualizer

The method used in this paper to capture the 3-D structure of the orbitals exploits a fairly unique suite of visualization tools available in packages of the Python coding language.[36] The orbitals are drawn using the scalar field visualization tool within the Mayavi package, where the colormaps are derived from the sign and magnitude of the wavefunction at various points in space.[37] The magnitude of the wavefunction is also used to determine the opacity of the regions of the scalar field. This feature is not particularly common in other plotting software, including Python's matplotlib suite, which motivated the use of Python's Mayavi package to produce the orbital illustrations.[38] The 3-D plots can be easily manipulated with

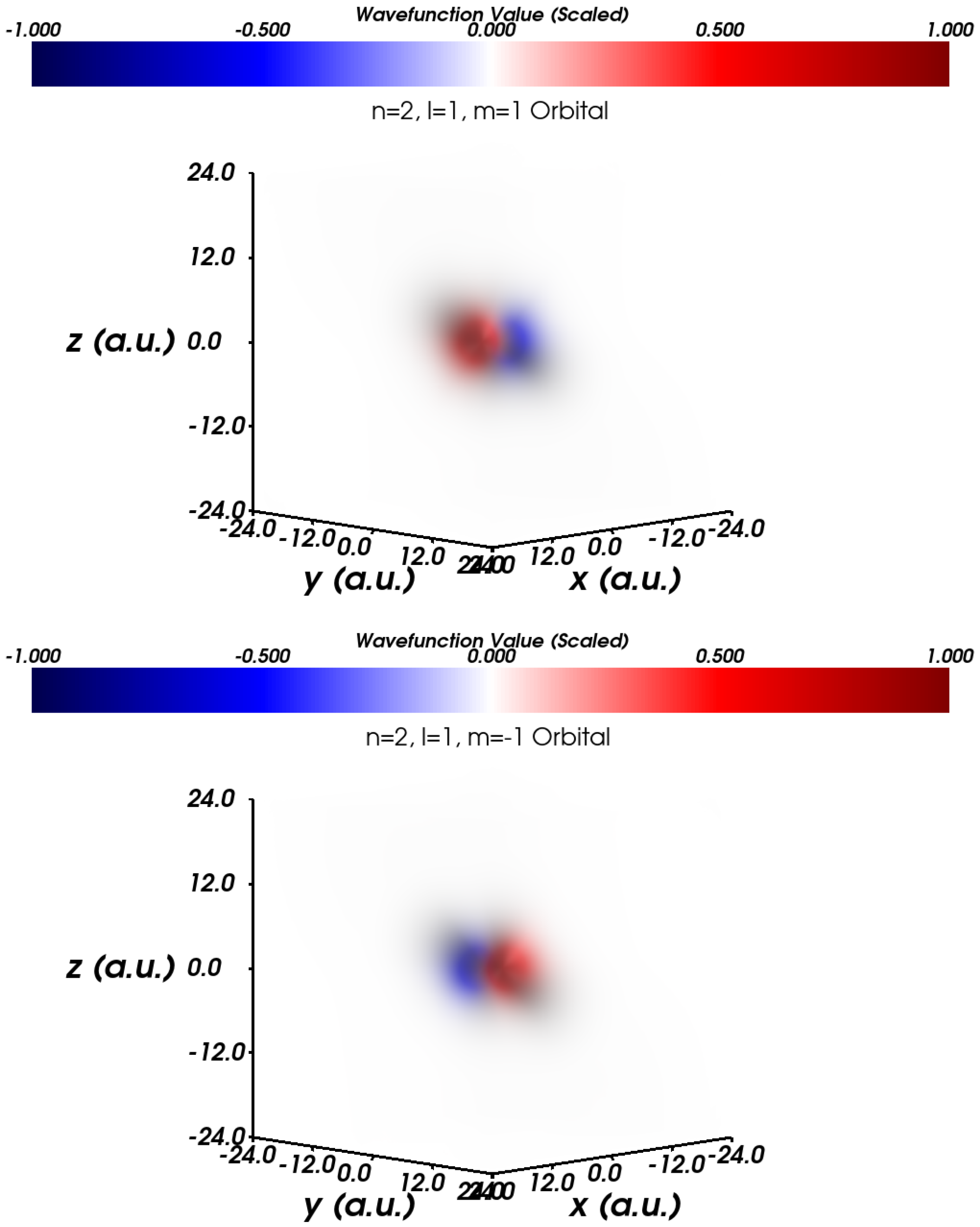
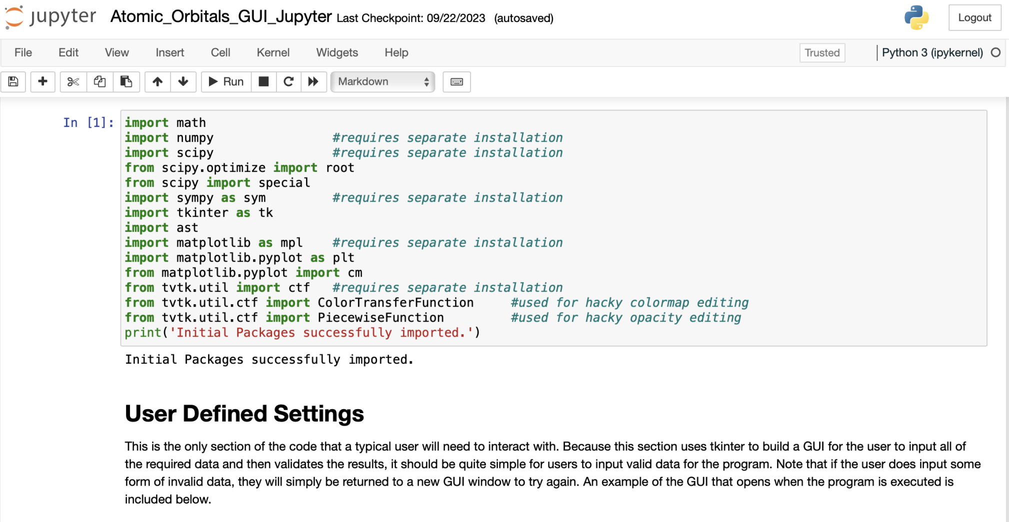


Figure 3: Illustration of the modified orbitals $\phi_{n,l,m}$ and $\phi_{n,l,-m}$ for the $2p$ orbitals. Note that these match the traditional $2p_x$ and $2p_y$ orbitals taught to general chemistry students as well as the real and imaginary parts of the orbital $\psi_{2,1,1}$.

point and click controls, allowing students and instructors the freedom to display important 3-D features of the orbitals from multiple viewing angles.

Because of the mathematical definitions of the orbitals, Python's robust scientific and mathematical packages like Numpy and Scipy were used to calculate the values of the orthogonal polynomials on a coordinate grid.[39,40] This makes the process of generating any orbital fully algorithmic. The only necessary inputs to the program for each different orbital are the values of the quantum numbers n, l, and m. Many other customized options are also available to users, including choices of plotting the modified orbitals $\phi_{n,l,m}$, their probability densities $\phi^2_{n,l,m}$, or the real and imaginary parts and magnitudes for the original orbital basis $\psi_{n,l,m}$, various colormaps, opacity scaling, background and foreground color schemes, wavefunction magnitude cutoffs, grid spatial extensions, and grid point densities. Default values of these parameters are chosen that work well for most low-lying orbitals. Note, however, that because of Mayavi's lighting system there will be shadows present in the image that may be mistaken by students for data with a higher amplitude than intended. This potential pitfall should be preempted by instructors. A full explanation of the program's features is included in the Supporting Information. When plotting $m = 0$ orbitals, a quadrant can also be carved out facing the default viewing angle so that the internal radial structure can be more easily visualized. This is particularly helpful for visualizing s orbitals that contain several radial nodes.

All of the options for this program are input through a graphical user interface (GUI) built using Python's Tkinter library.[41] In addition, the individual components of the wavefunction including the radial wavefunction $R_{n,l}(r)$ and radial probability function $(r^2 \left|R_{n,l}(r)\right|^2)$, θ angular wavefunction $N_{l,m}P_l^m(\cos(\theta))$, and ϕ angular wavefunction $e^{im\phi}$ for the orbital requested are also plotted to help with interpretation of the displayed figures, though this feature is made optional in the pure Python version of the code via inclusion of an additional GUI option. Finally, a plot of the components of the RGBA (red, green, blue, and alpha, which denotes opacity) tuple used to illustrate the orbitals are also given. Examples of the result of modifying many of the various parameters and settings are given in the Supporting Information. One version of the program is embedded within a Jupyter notebook to take advantage of the pedagogical nature of the Jupyter environment.[42] Namely, the Python code is embedded within explanatory code blocks and example images that allow interested users to more thoroughly understand what is being done, if desired. Comments are used generously throughout the code blocks to maximize readability, though experience with Python will be necessary to fully understand the code structure. An example of the Jupyter environment is shown in Figure 4. The code can, however, be run using the command line outside of the Jupyter environment, if desired.



```
import math
import numpy                #requires separate installation
import scipy                #requires separate installation
from scipy.optimize import root
from scipy import special
import sympy as sym         #requires separate installation
import tkinter as tk
import ast
import matplotlib as mpl    #requires separate installation
import matplotlib.pyplot as plt
from matplotlib.pyplot import cm
from tvtk.util import ctf   #requires separate installation
from tvtk.util.ctf import ColorTransferFunction      #used for hacky colormap editing
from tvtk.util.ctf import PiecewiseFunction          #used for hacky opacity editing
print('Initial Packages successfully imported.')
```

```
Initial Packages successfully imported.
```

User Defined Settings

This is the only section of the code that a typical user will need to interact with. Because this section uses tkinter to build a GUI for the user to input all of the required data and then validates the results, it should be quite simple for users to input valid data for the program. Note that if the user does input some form of invalid data, they will simply be returned to a new GUI window to try again. An example of the GUI that opens when the program is executed is included below.

Figure 4: Example of the Jupyter window showing both a code block (with comments) and an explanatory text block. Both are used throughout the visualizer program to give interested users more insight into the code and its design.

Student Learning Outcomes and Assessments

One of the major learning outcomes for students using this tool is understanding the relationship between the quantum numbers associated with an orbital and the 3-D structure of that orbital. The nature of the radial and angular nodal structure of the wavefunctions is made clearer when students are able to both plot and manipulate 3-D representations of the orbitals with and without the nodes drawn. Better yet, students can be challenged to discover the patterns between the number of very particular types of nodes and the various quantum numbers. The patterns they will discover for the orbitals $\phi_{n,l,m}$ are,

1. The total number of nodes is given by $n - 1$.
2. The total number of angular nodes is given by l.
3. The number of radial nodes is given by $n - l - 1$.
4. The number of angular nodes perpendicular to the $x - y$ plane is given by $|m|$.
5. The number of angular nodes along θ cutting through the z axis is given by $l - |m|$.

Students should be encouraged to explore many different wavefunctions, including wavefunctions describing orbitals that are not even used on the periodic table like g or h orbitals with $l = 4, 5$, respectively. Once students have a firm grasp on the patterns connecting the nodal structure and the quantum numbers, they should even be able to predict the structure of unfamiliar wavefunctions *a priori*. It is this solid foundation that will prepare them well for future courses in physical and inorganic chemistry wherein intuition about the geometry of the wavefunctions is required for a robust understanding of molecular orbital theory.

To assess the effectiveness of this learning tool, students were given an assessment both before and after the lecture and laboratory periods pertaining to the atomic orbitals where the orbital visualization tool was used. The assessment focuses on the identification of wavefunction structures and nodes in relation to the quantum numbers, the relationship between quantum numbers and energy, and predicting wavefunction shapes based on quantum numbers. One assessment item testing student knowledge of orbital degeneracies was used as a control. This assessment was given at Le Moyne College, an undergraduate-focused institution, in the Spring 2024 Physical Chemistry II lecture course. Students were in the middle of the course when the pretest was given and had not yet discussed the hydrogen atom.

The posttest was given two weeks later, after the students had derived the solutions of the Schrödinger equation and the Rydberg energy formula.

The data obtained are summarized in Table 1. The student scores were obtained by adding up students' scores (binary 0 or 1) on all items within each question and the dividing by the total number of items. No partial credit was given on solutions. While the degeneracies of orbitals is relevant to the topic at hand, no explicit mention of the degeneracies of the orbitals was given until after the posttest assessment. This allowed for a comparison of students' growth with and without deliberate intervention. In all cases apart from the control, students demonstrated significant growth in their ability to ascertain information about the nodes from quantum numbers, relationships between quantum numbers and energies, and even predicting how an orbital would look when projected into the 2-D plane. While this latter exercise showed less substantial growth, it also required greater understanding of the relationships between the quantum numbers and the orbital shape and orientation than the other items. This is because students had to predict the shape of an orbital from quantum numbers rather than identifying features of an orbital they could already see. Students were also not explicitly shown any examples of this task during the orbital visualizer activity, and

Table 1: Results of assessment for students at Le Moyne College ($N = 11$)

Item	Pretest Average	Posttest Average	Change
1. (Control) Identifying the orbital degeneracy from quantum numbers	54.5 %	50.9%	-3.6 %
2. Identifying the numbers and types of nodes for different wavefunctions	40.9 %	95.5 %	54.6 %
3. Recognition that Rydberg formula for orbital energy depends only on n	18.2 %	100 %	82.8 %
4. Understanding $\lvert m \rvert$ gives the number of nodal planes orthogonal to $x - y$ plane	9.1 %	72.7 %	63.6 %
5. Predicting orbital orientation and shape from quantum numbers	9.1 %	54.5 %	45.4 %

so this item essentially probed students' ability to apply their learning to novel problems. All in all, these results show that even with modest intervention, students are far stronger in their ability to grasp the geometric implications of the quantum numbers after utilizing flexible 3-D rendering tools.

One hurdle to implementing this tool and the associated exercise is that computers must be available that are capable of installing and running the relevant software. Due to the large number of dependencies, edge cases can arise where it may be difficult to implement this software on particular machines, though it has been successfully installed on over a dozen different combinations of brands, models, and operating systems. While almost all Apple and Windows PCs are capable of running Python and the relevant packages, an insufficiently powerful processor can cause the rendering and 3-D manipulation of the orbital plots to become extremely slow. This can significantly hamper the utility of this tool for students' learning. The requirements are relatively modest, but older machines or those with extremely low-end processors and graphics processing will typically struggle to render the orbitals in a reasonable amount of time. The use of smaller grid point densities is encouraged for those with low-performance computers.

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Associated Content

Supporting Information Available

The Supporting Information is available on the ACS Publications website at DOI:####

The following are included in the supporting information:

1. The Python and Jupyter code for the visualizer
2. Instructions for installing the necessary packages
3. A guide to the features of the visualizer
4. The in-class orbital activity handout
5. The pre/posttest assessments and the answer key

Additional Information Available

The most updated code and instructions can also be accessed online in a public Github repository at https://github.com/mhanson12363/Atomic-Orbitals-Visualizer/tree/main.

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