

VISUALIZATION OF THE HYDROGEN ATOM WAVE FUNCTIONS

James R. Kirk

Department of Physics and Technology
Edinboro University of Pennsylvania

Abstract

The probability of electron location in three dimensions is displayed in a graphical user interface (GUI) using the three-dimensional plotting features of MATLAB[®]. There are three displays: the probability of electron location as a function of the inclination angle and radial distance from the proton, the angular distribution determined by the spherical harmonic portion of the wave function, and radial probability density. The latter is a two dimensional plot that can be used to calculate the probability of the electron between two user selected radial distances. Electron states are chosen from a menu that includes a selection of principle quantum numbers ranging from one to nine.

Introduction

In modern physics and quantum mechanics courses around the world, solving the Schrödinger equation for the hydrogen atom is standard practice. Many useful techniques in solving partial differential equations are illustrated, and the fundamentals of quantum theory demonstrated. The outcome of such a solution yields somewhat complex functions of three variables in spherical coordinates r , θ , and ϕ , where r is the electron's radial distance from the proton, θ is the inclination angle (from the z -axis in the xyz Cartesian coordinate system), and ϕ is the azimuthal angle measured from the x -axis. The angles may be defined differently in different textbooks [1]. Modern physics and quantum mechanics textbooks typically display the solutions graphically for one or several of the wave functions in a variety of ways mostly in two-dimensions [2-4]. The wave functions are complex in their mathematical structure and

thus the displays found in textbooks are usually limited to only a few. An exception to this is Anderson [2] where 20 wave functions are displayed in two-dimensional plots.

The advent of computer visualization in three-dimensions allows for an expansion of the visualization plots in Anderson [2] and other textbooks and websites. In this paper, a GUI written in MATLAB[®] that allows the user to display a choice of three different plots for a menu selected wave function is described. One option is to display the angular probability distribution of the wave function in three-dimensions. This kind of plot is seen in textbooks [3]. A second option is to plot the normalized probability distribution as a function of radial distance and inclination angle. This type of plot does not display known azimuthal symmetry. Finally, of computational interest is the probability of finding an electron between two radial distances for all angles, and displaying the expectation value of radial distance. The display of radial probability density as a function of radial distance is a two-dimensional plot. The computation to find the probability of electron location is typically done analytically by integration of the probability distribution between the radii of interest. This can be a laborious task and is probably only done for a few low energy states by students in modern physics or quantum physics courses. In the GUI, the user selects two radii, and the computation is performed within the MATLAB[®] program and displayed to the user immediately. This feature can allow rapid investigation of the radial probability.

The usefulness of the GUI is two-fold. First, an investigation of the radial probability can be undertaken by students using the radial

probability density feature. Second, the three-dimensional plots can bring the mathematical functions representing the solutions to one of the most important problems in modern physics to life. Summarized in one plot is the whole story of electron location -- a satisfying result.

The Equations

The equations for the normalized spherical harmonics are well known and can be found in mathematical handbooks or modern physics textbooks. The spherical harmonics are:

$$Y_m^l(\eta, \phi) = \frac{1}{2^l l!} \sqrt{\frac{2l+1}{4\pi}} \sqrt{\frac{(l+m)!}{(l-m)!}} e^{im\phi} \left(\frac{1}{1-\eta^2}\right)^{\frac{m}{2}} \left(\frac{d}{d\eta}\right)^{l-m} (\eta^2-1)^l, \quad (1)$$

where $\eta = \cos \theta$, l is the total angular momentum quantum number, and m is the z-component of angular momentum quantum number. For the various states of l and m this function was evaluated using Mathematica[®]. Its square was then used to calculate the angular distributions plotted in the GUI.

The radial portion of the solution is:

$$R_{nl}(r) = -2 \left(\frac{1}{na_0}\right)^{3/2} \sqrt{\frac{(n-l-1)!}{n!(n+l)!}} \left(\frac{2r}{na_0}\right)^l e^{-r/na_0} L_{n+l}^{2l+1}\left(\frac{2r}{na_0}\right), \quad (2)$$

where L_{n+l}^{2l+1} are the associated Laguerre polynomials, n is the principle quantum number, and a_0 is the Bohr radius. The associated Laguerre polynomials are:

$$L_{n+l}^{2l+1}(\rho) = \left(\frac{d}{d\rho}\right)^{2l+1} \left[e^\rho \left(\frac{d}{d\rho}\right)^{n+l} (\rho^{n+l} e^{-\rho}) \right], \quad (3)$$

with $\rho = (2/na_0)r$.

Once again Mathematica[®] was used to compute the Laguerre polynomials and the radial solution. The total wave function is:

$$\Psi = R_{nl} Y_m^l, \quad (4)$$

and the probability per unit volume in 3-d space is $\Psi^* \Psi$. To find the radial probability density one must compute $r^2 R_{nl}^2$. This quantity represents the probability per unit radial distance for the wave function. It is obtained by integrating the total wave function over all angles. Multiplication by Δr will yield the probability of finding an electron in the range r and $r + \Delta r$.

The GUI

Figure 1 shows the GUI as it first appears when run from the MATLAB[®] command window. There is a menu bar, three buttons, and two sliders. There are text display fields that pop up when a radial probability calculation is called. The default plot is a MATLAB[®] standard 3-d plot of a function in MATLAB[®] called "Peaks."

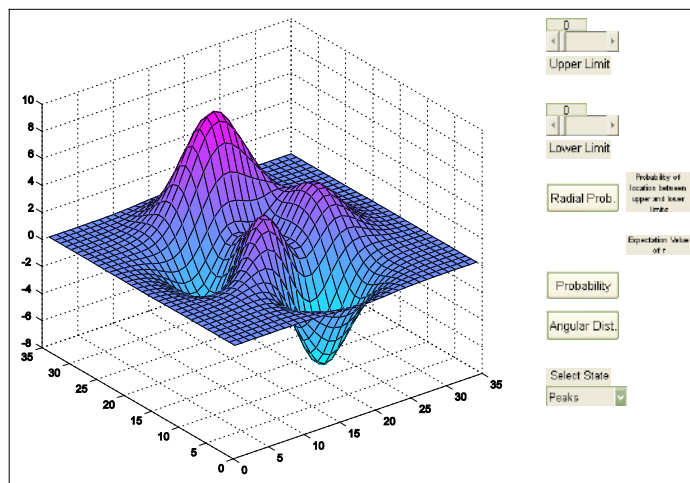


Figure 1. The hydrogen atom wave function GUI as it first appears when first run out of the MATLAB[®] command window.

Menu Bar

The menu bar titled SELECT STATE allows selection of the hydrogen atom wave function that is to be displayed. The first number

indicates the principle quantum number n . This is followed by a letter indicating the total angular momentum quantum number l using the standard S, P, D, F, G, H, I ... for $l=0, 1, 2, 3, 4, 5, 6, 7 \dots$. The final number is the m quantum number for the z -component of the angular momentum. Thus, 3D0 is the $n = 3, l = 2$, and $m = 0$ state of the hydrogen atom. Users select the state they want to explore and then click on the buttons to display a plot of interest. Selected states from $n = 1$ to $n = 9$ are included.

Angular Distribution

The ANGULAR DIST. button is used to plot the 3-d angular portion of the probability distribution. The radial distance from the origin of the coordinate system is proportional to the probability of finding the electron at a particular inclination angle. The actual value of such a radial distance is only a relative measure of probability compared to other angles. The axes for the plot are set to range from -1 to 1, and the default orientation of the coordinate system is with the z -axis upward. Azimuthal symmetry is evident in each plot, and a cut-away section is provided so users can see inside the 3-d plot. Figure 2 shows the 5F1 angular distribution.

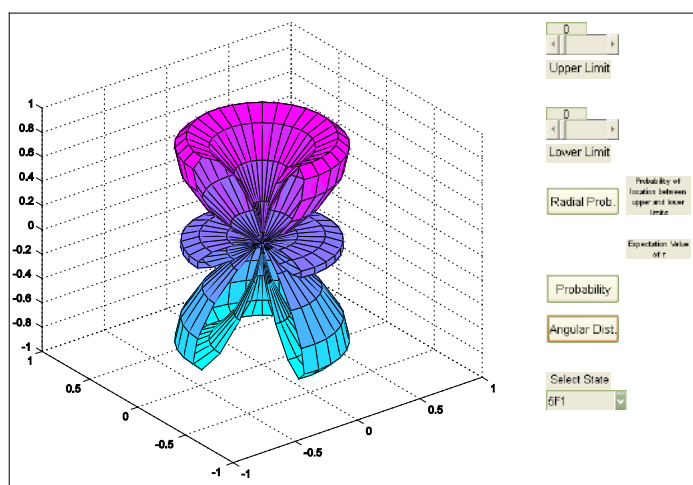


Figure 2. The angular probability distribution for the case $n=5, l=3$, and $m=1$.

Probability

The PROBABILITY button is selected if the user wishes to view the normalized probability per unit volume as a function of inclination angle and radial distance from the proton. The radial distance axis is normalized using the Bohr radius, thus the value of 1.00 along the radial axis is a radial distance equal to the Bohr radius. Figure 3 shows the 5F1 three-dimensional probability distribution.

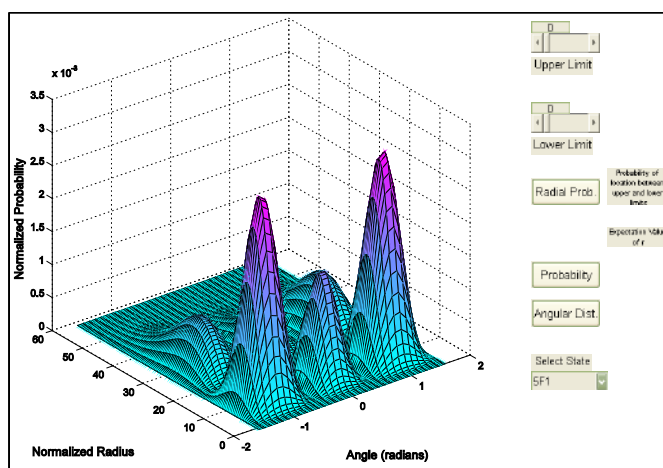


Figure 3. The normalized three-dimensional probability distribution for the 5F1 state.

Radial Probability

The RADIAL PROB. button can be used to display the two-dimensional plot of radial probability density and normalized radial distance. The two sliders range from zero to one. Selecting a value other than zero for the lower limit slider and upper limit slider allows the user to compute the probability of electron location between two radial distances. Once selected, the user clicks on the RADIAL PROB. button. The multiple of the Bohr radius is then displayed for the lower and upper limits selected by the sliders, and the value of the probability computed appears next to the RADIAL PROB. button. Also displayed is the expectation value of the radial coordinate. Figure 4 shows the radial probability function for the 5F1 state,

with the probability computed between 20.25 and 75.0 times the Bohr radius. This is the total probability of finding the electron within the radial limits of the large peak in the distribution.

Usefulness

The GUI for displaying the hydrogen atom wave functions can be used to visualize the probability distributions in a unique and exciting way. After progressing through the detailed analytical solution of one of the most intriguing

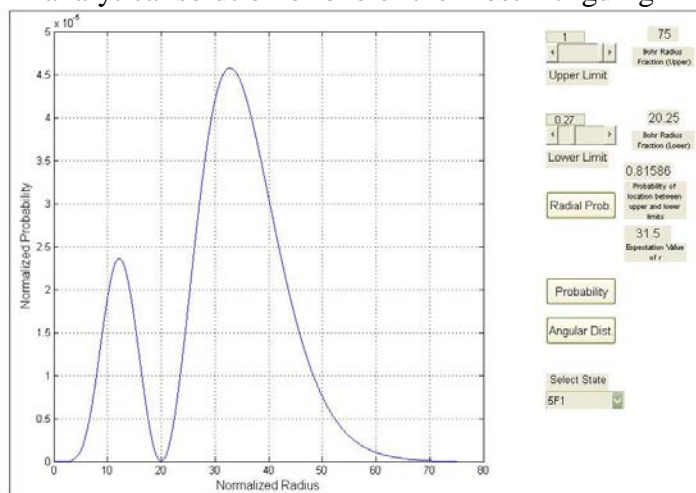


Figure 4. The radial probability density for the 5F1 state. The probability is calculated between 20.25 and 75 times the Bohr radius.

and historically exciting problem in quantum mechanics, it can be refreshing to examine the results in a colorful way. Furthermore, the MATLAB[®] figure window provides the user with several options to enhance the plots. For example, the user can zoom in or out and rotate the plots for a different view. This can be useful for examining more closely a given feature of the plots. There is also an option that can be accessed from the MATLAB[®] command window called “ginput.” With “ginput,” the user can select points of interest in the plots and display their numerical value.

The radial probability feature of the GUI can be used to examine the details of radial probability for the different states. It is quite simple to find the probability of electron

location between two radial distances. Also, the radial distance for maximum radial probability density is available for each state. This allows investigation of patterns such as the well known increase of radial distance for maximum probability with the square of the principle quantum number (for states where $l=n-1$). Many other similar explorations could be conducted.

Student Reception

The GUI for displaying a variety of features of the hydrogen atom wave functions is appropriate for use in the second semester of a two-course introductory physics sequence for all science and engineering majors. It can also be used in intermediate-level modern physics courses taken by physics and engineering majors, and advanced courses in quantum mechanics and physical chemistry. Also, the GUI has been used in recruiting and orientation settings to generate excitement. Students are enamored with the intricate computer graphics and want to know what they are examining. This opens the door for discussion and thus education. In all of these cases the GUI is run on a local computer station with a projector displaying the plots.

In the introductory courses, or in orientation and recruiting sessions, the display is used to simply raise the awareness of the probability distribution and provide a visual sense of the different possibilities. When used in this way the students are generally awestruck, but curious. For physics and engineering majors in introductory courses the GUI sparks interest in future courses because it shows them something they can look forward to studying later in full mathematical detail. This is very compelling for the students. In advanced courses the GUI provides a refreshing view of the wave functions that is unimaginable when wading through the details of complex mathematics. Thus, at the conclusion of the mathematical details, students find the GUI displays refreshing and pleasing. It has the effect of

making the students feel like all of the hard work associated with the mathematical derivations was worth the effort.

Some of the features of the GUI have only recently been added and thus it has not been used for any student projects yet. This will change during the next academic year when we make it available for student use in our bi-annual quantum mechanics course.

Conclusion

It is pleasing to examine solutions of the hydrogen atom wave functions in a variety of colorful and detailed ways. In order to run the GUI, the user would need a copy of MATLAB[®] version 7.4 or higher. MATLAB[®] is designed by the MathWorks Inc., and can be purchased directly from their website. Student and classroom use versions are available at reasonable cost. Should the readers of this paper wish to have a copy of the GUI, they can email me at kirkj@edinboro.edu, and I will email reply with an attached GUI file containing the MATLAB[®] code.

References

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Biographical Information

Dr. James R. Kirk is an associate professor of physics and technology at Edinboro University of Pennsylvania. He earned a bachelors degree in physics from Rutgers University, a masters degree in physics from the University of New Hampshire, and a PhD in Meteorology from The Pennsylvania State University. His background includes a diverse set of knowledge ranging from advanced electronics and digital signal processing to atmospheric physics.