"Using Maple to Visualize Atomic Orbitals"

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Abstract

Introducing a rudimentary treatment of quantum mechanics leading to the advent of atomic orbitals in chemistry curriculum has been a challenging task. While this challenge may partly be due to less coverage based on the mathematical details of the topic, there are also varying degrees of difficulties seen in the orbital contours reproduced in the chemistry texts. To alleviate the difficulties, a procedure was developed in which solutions of Schrödinger's equation for Hydrogen atom are used to generate special graphs called density plots in Maple platform. Several misconceptions clouding the minds of the students are addressed and removed when students create these plots themselves. As it is extremely difficult to plot the entire wavefunction, 2-d density plots are made for different slices of the orbitals, from which a 3-d image may be constructed. Suggestions are made to use this method as a pedagogical tool to illustrate the complex quantum mechanical idea in a graphical representation in the undergraduate chemistry curriculum. Details pertaining to the procedure to map 2-d density plots in Maple, and the results will be presented for s, p, and d orbitals.

Keywords: Orbitals, Functions, Chemistry Curriculum, Computational skills

1. Introduction

Education research in chemistry indicates that in general, undergraduate students complete General Chemistry courses without fully grasping the mathematical ideas that form the basis of some concepts.[1,2] This trend is more prevalent and the problem is acute when students learn the basics of quantum mechanics in an attempt to draw the shape of different atomic orbitals which are usually taught almost towards the end of a semester long General Chemistry course. Although undergraduate students are taught that Bohr's model of atomic structure is invalid for elements other than hydrogen, it is by no means an easy task to quickly introduce the basic axioms or postulates of quantum mechanics that eventually lead to understanding the shapes of the atomic orbitals, which are the solutions of the Schrödinger's wave equation.[3-7] Of course, once the shapes of the atomic orbitals are dealt with, automatically a quantum leap takes place leading to concept of *aufbau* principle to produce the electronic configuration of multi-electron systems. We strongly feel that there is a pedagogical inadequacy in this approach. Even the fundamental point that the electrons in an atomic system are described by a probability density is difficult to comprehend without knowing the mathematical reasoning for it. By way of offering a partial solution to this problem, as a prototype example, we employed Maple software to map out different functions that represent the atomic orbitals.

  Maple, a powerful software package that offers excellent graphics options and numerical integration possibilities, can be used to help teach introductory science courses. It is now recognized that there is increasing evidence that undergraduate curriculum must include computations, and developing computational skills can be achieved by several means – one of them is learning Maple, writing codes for simple situations, and generating useful plots to visualize the concepts.[8] Using Maple in such a manner can help students to gain a more in-depth understanding of the atomic orbitals, which can furthermore provide a sound foundation for them as they proceed to more rigorous classes concerning quantum mechanics/computations. We present in this manuscript the method used to generate

the atomic orbital using Maple software package and suggest the use of this as an undergraduate exercise in General Chemistry. This approach, we believe, will force students to learn that different orbital shapes are nothing more than mathematical functions that are solutions to a differential equation, the Schrödinger's equation.

2. Misconceptions

Even after learning about electron cloud, students still visualize an atom as electrons orbiting a nucleus in concentric circles. This is probably due to the connection that the Bohr model makes with their experience. It is not easy to give up nice planetary systems that they have encountered from an early age for the world of orbitals, electron cloud, and probability density. The cursory treatment of these topics in General Chemistry is inadequate to prepare students for more advanced work. Another misconception is that labels s, p, d, and so forth are merely names for the different shapes of orbitals. Students do not correlate these names with actual functions that describe the probability density of electrons. It is worthwhile for students to work with these functions, even if they cannot derive the origin of these functions. To further the misconceptions, some textbooks offer images of these orbitals without much discussion. Students are left to wonder what are inside these shapes and whether the atom actually looks like this. Some textbooks leave out the shading that reflects the high or low probability density or do not make the connection to the probability density at all. Students do not realize that the probability density is actually over all space, but is negligible outside the region of the orbital. More advanced introductory textbooks mention the quantum numbers l and m. They may mention that the names s, p, d, etc. refer to the quantum number l, but fail to mention the quantum number m in reference to the images. The fact that the $l \neq 0$ orbitals, such as p and d, are linear combinations of different m values is glossed over. Why are these linear combinations formed? Why are images not produced for different m values as they are for different l values?

Some more attention to details is necessary to prepare students for future work and to build computational skills. Some exercises using Maple that focus on these misconceptions may be useful. It will at least give students experience with these important ideas, which may make it easier for them to grasp advanced ideas, such as molecular orbitals.

3. Procedure/Method of Creating Orbitals:

We used the wavefunctions to generate the density plots in respective Cartesian coordinates. Table 1 lists representative examples of a few normalized wavefunctions that denote different orbitals taken from the literature.[9]

Table 1: A list of wavefunctions with both the radial and angular parts, where a_0 is the Bohr radius. The corresponding quantum numbers are also listed.

n	l	m_l		$\psi_{nlm_l}(r,\theta,\varphi)$
1	0	0	1s	$\dfrac{1}{\sqrt{\pi}a_0{}^{3/2}}e^{\frac{-r}{a_0}}$
2	1	± 1	2p	$\dfrac{1}{8\sqrt{\pi}a_0{}^{3/2}}\dfrac{r}{a_0}e^{\frac{-r}{2a_0}}\sin\theta\,e^{\pm i\varphi}$
3	2	± 2	3d	$\dfrac{1}{162\sqrt{\pi}a_0{}^{3/2}}\dfrac{r^2}{a_0{}^2}e^{\frac{-r}{3a_0}}\sin^2\theta\,e^{\pm i2\varphi}$

Using the Cartesian coordinates enabled us to see a more standard image in comparison to plots generated using polar coordinates which Maple software is also capable of producing. By exploring many possible options for plotting in Maple, it was found that an excellent way to plot the electron density of an atom is by using a 2-d density plot. Since the wavefunctions are three-dimensional, different slices are plotted. A slice of the wavefunction in the

yz-plane is obtained by putting $x = 0$. Similarly, putting $y = 0$ and $z = 0$ yield slices in the *xz*-plane and *xy*-plane, respectively. Note that the modulus squared of the wavefunction is plotted to represent the electron probability density. However, for $l \neq 0$, this does not give distinct functions. For instance, $|\psi_{211}|^2 = |\psi_{21-1}|^2$. To get as many wavefunctions as there are values of *m* (3 for p orbitals and 5 for d orbitals), a linear combination is used. For example, the $3d_{x^2-y^2}$ orbital is produced by

$$3d_{x^2-y^2} = \frac{1}{\sqrt{2}}\psi_{322} + \frac{1}{\sqrt{2}}\psi_{32-2}$$

$$= \frac{1}{\sqrt{2}}\frac{1}{162\sqrt{\pi}a_0^{3/2}}\frac{r^2}{a_0^2}e^{-\frac{r}{3a_0}}\sin^2\theta\,(e^{i2\varphi} + e^{-i2\varphi})$$

$$= \frac{1}{\sqrt{2}}\frac{1}{162\sqrt{\pi}a_0^{3/2}}\frac{r^2}{a_0^2}e^{-\frac{r}{3a_0}}\sin^2\theta\,(2\cos 2\varphi)$$

$$= \frac{2}{\sqrt{2}}\frac{1}{162\sqrt{\pi}a_0^{3/2}}\frac{1}{a_0^2}e^{-\frac{r}{3a_0}}(r^2\sin^2\theta\cos^2\varphi - r^2\sin^2\theta\sin^2\varphi)\,,$$

where $\cos 2\varphi = \cos^2\varphi - \sin^2\varphi$ has been used in the last step. The expression in the parenthesis is $(x^2 - y^2)$, hence the name $3d_{x^2-y^2}$. In the equation, we describe the linear combinations used for p orbitals.

3.1 Equation

The linear combination that is talked about in this paper is done when the modulus squared of the wavefunction are not distinct for all the *m* values. In order to get distinct functions, Euler's identity must be used:

$$\cos\phi = \frac{1}{2}\left(e^{i\phi} + e^{-i\phi}\right) \tag{1}$$
$$\sin\phi = \frac{1}{2i}\left(e^{i\phi} - e^{-i\phi}\right) \tag{2}$$

For example, to do the linear combination for P_y, we use $\frac{1}{\sqrt{2}}(\psi_{211} - \psi_{21-1})$. This yields

$$\frac{1}{\sqrt{2}}(\psi_{211} - \psi_{21-1}) = \frac{1}{\sqrt{2}}\frac{1}{8\sqrt{\pi}}e^{\frac{r}{2}}r\sin\theta\left(e^{i\phi} - e^{-i\phi}\right)$$
$$= \frac{1}{\sqrt{2}}\frac{1}{8\sqrt{\pi}}e^{\frac{r}{2}}r\sin\theta\,(2i\sin\phi)$$
$$= \frac{2i}{\sqrt{2}}\frac{1}{8\sqrt{\pi}}e^{\frac{r}{2}}y \tag{3}$$

The name P_y orbital is given to this combination because of the presence of the factor y in eq(3). Similarly, the P_x orbital is found by the linear combination $\frac{1}{\sqrt{2}}(\psi_{211} + \psi_{21-1})$. The modulus squared of P_x and P_y are distinct in comparison to the modulus squared of ψ_{211} and ψ_{21-1}. In order to reproduce the standard textbook images, one should use the Cartesian coordinates when plotting these functions with Maple.

The necessary commands/codes to graph the density plots for the Hydrogen atom in Maple is given below for $a_0 = 1$ and $x = 0$ for the 1s and $3d_{x^2-y^2}$ orbitals, where the modulus squared of the wavefunction is plotted to represent the probability or charge density:

<div style="border:1px solid">

Maple Code:

with(plots):

$$\text{densityplot}\left(\left(\frac{e^{-\sqrt{y^2+z^2}}}{\sqrt{\pi}}\right)^2, y = -3..3, z = -3..3, \text{brightness} = \quad 0.4, \text{contrast} = 1, \text{title} = \right.$$

$$\left. \text{"1s where x = 0"}\right)$$

$$\text{densityplot}\left(2*\left(\frac{e^{-\sqrt{(x^2+y^2)}/3}}{162\sqrt{\pi}}*(x^2-y^2)*(x^2+y^2)\right)^2, x = -3..3, y = -3..3, \text{brightness} = \right.$$

$$\left. 0.4, \text{contrast} = 1, \text{title} = \text{"3d[x^2 - y^2] when z = 0"}\right)$$

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By inputting these codes into the Maple program, a 2-d plot is generated that represents a slice of an orbital. To get a slice from each plane, the sequence should be ran three times by setting x, y, or z equal to zero in a successive manner.

This procedure described above yields two dimensional density plots showing the probability density of the electrons. For plotting orbitals using the 1s through the 3d wavefunctions, this method can be used. The brightness indicates the probability density of the electrons and it can be inferred from the plots shown that it decreases radially. Some representative slices obtained using Maple software[8] for 1s and $3d_{x^2-y^2}$ orbitals are shown in Figures 1 and 2 respectively. By using Maple in this manner, students in introductory chemistry courses will be more likely to gain a better understanding of the orbitals and wavefunctions by creating the plots themselves.

4. Implementing the Method

Creating the aforementioned density plots using Maple software is not at all difficult. The interface for the program is very user friendly and does not demand advance knowledge of the software in order to create the plots. The commands used to plot density plots that show the orbital shapes are very fairly straightforward as shown above with only 2 or 3 lines of code. The Maple interface includes a toolbar on the side of the main window that contains helpful items that may be used in the input such as symbols or Greek letters. While typing the previously stated commands, this toolbar can be utilized so that the commands may be typed with more ease and efficiency. Once the command to open the plotting package as well as the command telling the software what equation to plot, the return key on the keyboard can be pressed resulting in the density plots.
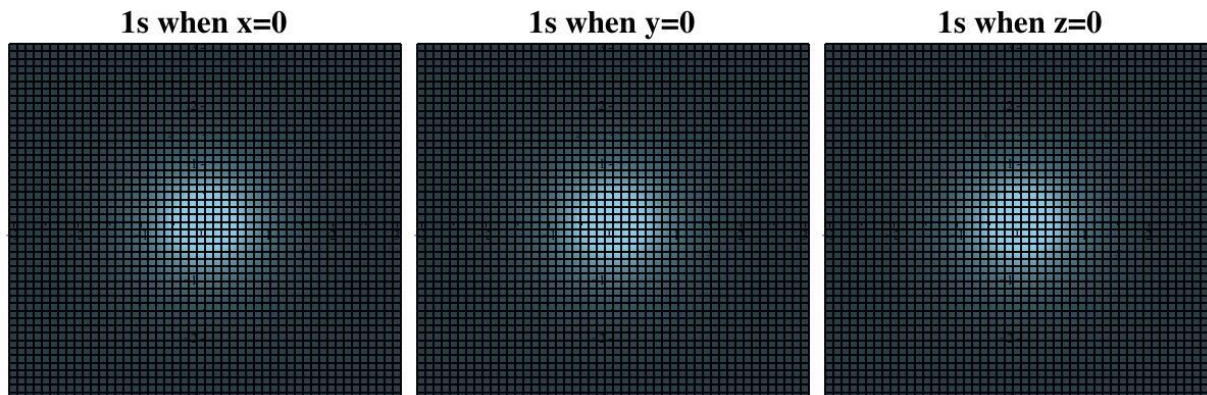
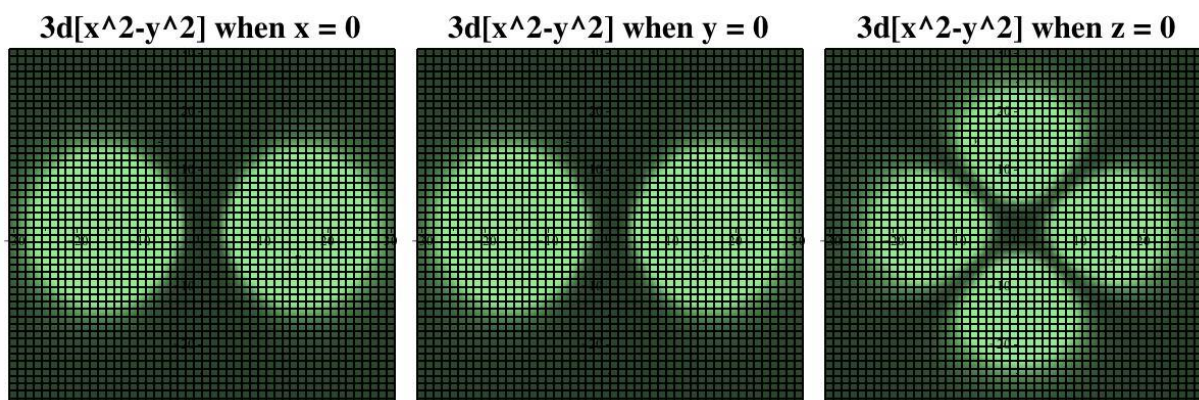Figure 1. Maple plots of the 1s orbital showing the slices from the yz, xz, and xy planes.

Figure 2. Maple plots of the $3d_{x^2-y^2}$ orbital showing different slices from the xy, yz, and xz planes.

We suggest the implementation of this method in the classroom to help students' understanding of atomic orbitals. Students can first learn of the wavefunction as well as the mathematics of linear combination through lecture. Through the practicing of normalizing wavefunctions and undertaking the process of linear combination for various wavefunctions students can start to gain a better mathematical understanding of the wavefunction. In the next class session, or as an assignment, the discussion of plotting these functions could take place. An example can be shown to the class, and the students could practice plotting the functions themselves. It is just like plotting a function in algebra such as $y = x + 3$. The program is just taking the wavefunction multiplied by its conjugate and plotting it as it would a simpler function. To make sure the material is understandable and to bring clarity to misconceptions some discussion could be done with the students either in class or as an assignment to follow up on the learning experience. Sample questions would be: Do you notice varying brightness in these plots? What do they mean? What caused them? How far do they extend? How do the labels s, p, d, and so forth relate to the atomic structure of an atom? Students can then see the mathematics of atomic structures, understand why they are shaped the way they are, and recognize the electron's probability density.

5. Conclusion

Throughout this paper we described and suggested how to use Maple to create plots that will help students in general chemistry courses. There are common misconceptions among undergraduate students in General Chemistry courses concerning atomic orbitals, and using Maple to create plots can help bring them clarity. While attempting to plot the slices of the orbitals, students will learn the about the wavefunctions, how to normalize them, and how to use linear

combination to find distinct functions of the modulus squared of the wavefunction. Lastly, by using Maple students can start to familiarize themselves with computational tools.

Since the world of computational science is growing, it is best to instill these types of skills in students sooner rather than later so that they may become more proficient in using programs such as Maple. The Maple software can be used in many general science courses to help the computational skills in students. Not only is it important to push students to obtain scientific skills, but it is also important that they achieve a thorough understanding of the general material, which will provide a solid foundation when the undergraduates move to more advanced material.

6. Acknowledgements

7. References

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