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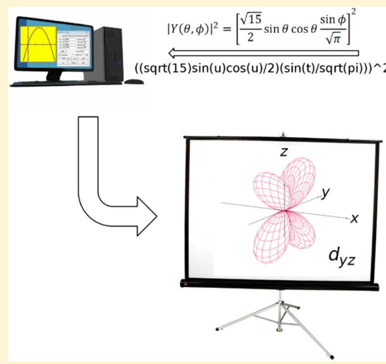
Three-Dimensional Atomic Orbital Plots in the Classroom Using Winplot

Wilfredo Credo Chung*

Department of Chemistry, De La Salle University—Manila, 2401 Taft Avenue, Manila, 1004 Philippines

Ⓢ *Supporting Information*

ABSTRACT: The Winplot software makes the relationship between an atomic orbital and the wave function of a hydrogen-like atom easy to understand. This relationship can be quickly demonstrated in the classroom.



KEYWORDS: *Upper-Division Undergraduate, Physical Chemistry, Computer-Based Learning, Quantum Chemistry*

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Physical chemistry teachers often have difficulty demonstrating to their students that the well-known atomic orbitals of varying sizes and shapes, depending on the quantum numbers assigned to them, are plots of the wave function of a hydrogen-like atom, that is, an atom with only one electron in it: the simplest quantum chemical system. Before computers were available in the classroom, teachers used prepared slides or transparencies showing the orbital plots alongside the equations that define them. When the overhead or slide projector was not yet a regular classroom fixture, teachers would simply draw orbital shapes on the chalkboard. In some cases, the equations are no longer shown and emphasis is given on the implication of the orbital shapes on the chemistry of systems.

Computer-assisted instruction (CAI) has been shown to improve understanding of students compared to traditional methods.[1−3] The availability of computers in the classroom gave teachers a chance to show to their students—in real time, right before their eyes—that the orbitals originate from the wave function of a hydrogenic atom, the simplest electron-bearing atom that can be considered. Several approaches have been described in this *Journal* ranging from using the now-obsolete software BASIC[4−6] to expensive mathematics softwares like Mathcad[7−9] and Mathematica.[10,11] At present, Gnuplot[12] is a popular choice among scientific plotting softwares due to its availability, versatility, and portability. However, as explained below, the use of Gnuplot offers some inconveniences when speed is essential and a spherical polar plot, such as that needed to plot atomic orbitals, is desired.

■ ABOUT WINPLOT

Winplot[13] is a versatile plotting software developed by Richard Parris of Phillips Exeter Academy at New Hampshire. Its installer is freely downloadable from the World Wide Web and runs on virtually any PC running Windows 95, 98, ME, 2000, XP, Vista, or 7. Linux and Mac versions of Winplot are not available at present. It is a small program consisting of a single 1.86 MB executable file and can even be launched from a USB flash drive, a convenience when administrator rights are required to install a program on a computer shared by many users. "Installing" Winplot is as easy as copying a single file into a drive. The current version of Winplot was compiled on 13 September 2012. Winplot is popular with those who teach mathematics but is virtually unknown to chemistry teachers.

■ DERIVING THE MATHEMATICAL EXPRESSION TO PLOT

The concept of quantum numbers is introduced to the students. Then, the teacher explains that, for a system as trivial as a hydrogen-like atom, an exact solution to the time-independent Schrödinger equation can be obtained when the wave function Ψ, expressed here in spherical polar coordinates rather than Cartesian coordinates, is assumed to be separable into radial, $R(r)$, and angular, $\Theta(\theta)\ \Phi(\phi)$, parts, that is,

$$\Psi(r, \theta, \phi) = R(r)\ \Theta(\theta)\ \Phi(\phi) \tag{1}$$

Separation of the variables results in three differential equations whose solutions are readily obtained. One may refer to any standard physical chemistry or quantum chemistry textbook for the solutions, but only the angular parts of the solution are needed to establish a connection with the concept of orbitals. The plot of the probability density of the spherical harmonics

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$Y(\theta,\phi) = \Theta(\theta)\ \Phi(\phi)$ would reveal the shape of the orbital. The radial part $R(r)$ would only influence the size of the orbital but not its overall shape.

The spherical harmonics corresponding to an atomic orbital having a set of quantum numbers l and m_l is then obtained by taking the product of the appropriate solution to the Θ and Φ equations (see Table 1 of the Supporting Information). The probability density is the square of the absolute value of the spherical harmonics. For example, for the d_{yz} orbital ($l = 2$, $m_l = \pm1$),

$$\Theta_{2,\pm1}(\theta) = \frac{\sqrt{15}}{2}\sin\theta\cos\theta \text{ and } \Phi_{\pm1}(\phi) = \frac{\sin\phi}{\sqrt{\pi}} \quad (2)$$

Thus,

$$|Y(\theta,\phi)|^2 = |\Theta_{2,\pm1}(\theta)\ \Phi_{\pm1}(\phi)|^2 = \left[\frac{\sqrt{15}}{2}\sin\theta\cos\theta\ \frac{\sin\phi}{\sqrt{\pi}}\right]^2 \quad (3)$$

The challenge is to demonstrate that plotting $|Y(\theta,\phi)|^2$ on spherical polar coordinate space reveals the well-known orbital shapes.[14]

■ USING WINPLOT[15]

Winplot is launched, and a window is revealed. One clicks on the "Window" pull-down menu and chooses "3-dim" to launch a new window designed for plotting three-dimensional functions. From the pull-down menu of the new window, the teacher clicks on "Equa" (which stands for "equation"; as the analytical form of the equation to be plotted is known) and chooses "Spherical" to launch yet another window (Figure 1) designed for input of the analytical form of the expression to be plotted and written in terms of spherical polar coordinates. Alternatively, the F3 and F5 keys are pressed in succession to launch the window shown in Figure 1.

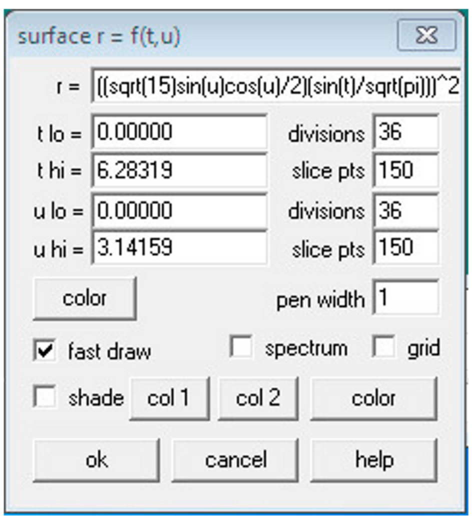

Figure 1. The Winplot window for generating 3D spherical polar coordinate plots. As an example, the mathematical expression for the d_{yz} orbital is shown. Clicking on "ok" on the window will immediately reveal the plot of the d_{yz} orbital shown in Figure 2.

As soon as a window appropriate for input of an analytical form of a spherical coordinate surface equation has been launched, the desired expression can then be input into the topmost box. (In Figure 1, the expression for the d_{yz} orbital is shown as an illustration.) Winplot uses the symbols u and t instead of θ and ϕ for the polar and azimuthal angles, respectively. The default number of divisions and slice points are generally sufficient. For convenience, the equations required to generate the orbital plots (up to the d orbitals) are enumerated in Table 1 of the Supporting Information. Shown in Figure 2 is a plot of the d_{yz} orbital generated by Winplot.

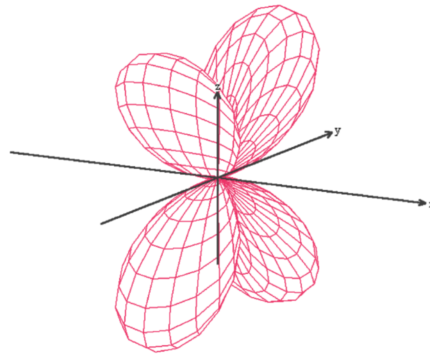

Figure 2. The d_{yz} orbital as generated by Winplot through a one-line input.

Thus, the orbital plot is generated through a simple one-line expression of the square modulus of the spherical harmonics that can be input by the teacher as an illustration or by a student as an exercise inside the classroom. The teacher may also pick a pair of students and task one to derive the analytical expression $|Y(\theta,\phi)|^2$ and task the other to input the expression derived by the partner student.

■ WHY NOT GNUPLOT?

Gnuplot is a popular plotting software. Similar to Winplot, it is also versatile, relatively small, and freely distributed. Its use for plotting orbitals has been suggested by Moore et al.[16] as early as 2000. I use it for many of my own plotting requirements. However, an elaborate script is generally required for the generation of a similar plot shown in Figure 2. (See also Figure 2 of Moore's article[16] in this *Journal*; the script used to generate the plot is found in the paragraph above Figure 2 of that article and is continued on the next page, if only to emphasize its length.) My experience is that it takes a considerable amount of time to prepare and explain the script and its function in front of the students inside the classroom. On the other hand, if the scripts are prepared before coming to class, student participation is limited and this lack of involvement may result in the failure of the students to grasp the connection between the equation and the plot. With this pedagogical consideration in mind, I prefer to use Winplot to create three-dimensional orbital plots in the classroom as it can be done without much preparation, to the extent of doing it impromptu.

It is possible to generate a plot in Gnuplot through a one-line command. For instance, if one keys in plot sin(x) into the Gnuplot command line, it generates a decent plot of the sine function. However, this is more complicated in the case of plotting in spherical polar coordinate space as Gnuplot uses a "geographic" spherical coordinate system rather than a polar one. A workaround has to be added to plot using spherical polar coordinates. This workaround somehow confuses the students and distracts them from the more important task of making a direct connection between an equation and its graph.

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Another minor drawback in Gnuplot is its insistence on the use of the asterisk symbol "*" to indicate multiplication. This is not required in Winplot (See Figure 1 above and Table 1 of the Supporting Information). As a result, Winplot equations resemble the analytical expression more closely and are easily related to the latter.

CONCLUSION

Winplot is recommended for real-time plotting of atomic orbitals from the spherical harmonics expression. It is free, small, portable, and easy to use. Winplot can even be launched from a USB flash drive. A pedagogical advantage is that generation of the orbital plot can be done through a single-line input in a matter of seconds without the use of a prepared script.

ASSOCIATED CONTENT

Supporting Information

The square modulus of the spherical harmonics, $|Y(\theta,\phi)|^2$, for the s, p, and d orbitals written in a form ready for input to Winplot. This material is available via the Internet at http://pubs.acs.org.

AUTHOR INFORMATION

Corresponding Author

*E-mail: wilfredo.chung@dlsu.edu.ph.

Notes

The authors declare no competing financial interest.

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(14) Here, we chose the solution $\Phi(\phi) = (\sin \phi)/\sqrt{\pi}$ because it is the one that would yield the d_{yz} orbital. Choosing $\Phi(\phi) = (\cos \phi)/\sqrt{\pi}$ would yield the d_{zx} orbital.

(15) The instructions given here on the use of Winplot may no longer work in future versions.

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