UTILIZANDO PLOTAGEM DE EQUAÇÃO BASEADA EM ANDROID COMO FERRAMENTAS PARA O ENSINO E APRENDIZAGEM DE ORBITAIS ATÔMICOS

USING ANDROID-BASED EQUATION PLOTTERS AS SUPPORTING TOOLS FOR TEACHING AND LEARNING ATOMIC ORBITALS

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RESUMO

Os estudantes de graduação em Química são obrigados a dominar a teoria da mecânica quântica como o requisito básico para estudar as propriedades da partícula submicroscópica. No entanto, muitos estudos mostraram as dificuldades dos alunos em trazer o conceito de mecânica quântica para o mundo macroscópico e vice-versa. O uso da ferramenta de visualização computacional será muito útil para ensinar e aprender o conceito quântico, especialmente o elétron e seus orbitais atômicos relacionados. Este artigo demonstra algumas das aplicações baseadas no Android como, por exemplo, a calculadora *FuncXY, TriPlot 3D Graphing* e *Graphing* para converter, de forma eficaz, rápida e precisa, as funções de onda em várias visualizações orbitais atômicas de hidrogênio. Ao selecionar a coordenada esférica e inserir a equação de onda, esses dispositivos gráficos do smartphone visualizam orbitais atômicos tridimensionais. Os usuários também são fáceis de girar, aplicar zoom e manipular o objeto. Finalmente, estes plotters de fácil utilização são muito recomendados para auxiliar os educadores de química no ensino da mecânica quântica.

Palavras-chave: *Aprendizado baseado em computador, Química quântica, Visualização orbital atômica*

ABSTRACT

Chemistry undergraduate students are required to master the theory of quantum mechanics as the basic requirement to study the properties of the submicroscopic particle. However, many studies showed the students' difficulties to bring the quantum mechanical concept to the macroscopic world and vise-versa. The use of computer visualization tool will very useful for teaching and learning the quantum concept, especially electron and its related atomic orbitals. This technological report paper demonstrates some of the Android-based applications i.e *FuncXY*, *TriPlot 3D Graphing*, and *Graphing calculator* to effectively, quickly, and accurately convert wave functions into various hydrogen atomic orbital visualizations. By selecting spherical coordinate and entering wave equation, these smartphone graphical devices visualize three-dimensional atomic orbitals. Users are also easy to rotate, zoom and manipulate the object. Finally, these user-friendly plotters are very recommended to assist chemistry educators in teaching quantum mechanics.

Keywords: *Computer-Based Learning, Quantum Chemistry, Atomic Orbital Visualization*

INTRODUCTION

The theory of quantum mechanics (QM) is a necessary topic in the chemistry curriculum at the University level. Generally, this topic provides the theoretical basis to study of electrons behaviors in atoms and molecules. Students are introduced to postulates, Schrödinger equations, quantum states, orbitals, symmetry, etc. (Atkins & Paula, 2010; Mortimer, 2008; McQuarrie, 1983). Eventually, the QM concept can be applied to explain various phenomena and core concepts in chemistry.

The problem is that learning this topic brings students to the dilemma of the mode of thinking and reasoning from macroscopic world to QM context and vise-versa (Kalkanis, Hadzidaki, & Stavrou, 2003). As also revealed by Singh, sources of major difficulties in learning QM are the abstractness, paradigms, and complex mathematical intuitions, as well as a far-reaching gap to our everyday life (Singh, 2005). Furthermore, guiding students to understand the physical meaning of equations becomes challenges for chemistry teachers. They are required to use various learning strategies and innovations that conform to the characteristics of subject matter.

Teaching QM using traditional methods lead to inconsistent learning and generally fail to configure a comprehensive understanding to the students (Hadzidaki, 2008). In particular, it has been proved that teachers' inappropriate ways of introducing subatomic phenomena lead to the mixing of concepts between classical physics and quantum mechanics (Millar, 1999). Consequently, instructors should avoid traditional method in teaching QM (Ozcan & Gercek, 2015; Müller & Wiesner, 2002). To improve students' understanding and overcome misconceptions associated with QM, Singh suggested that instructors combine computer-based visualization with research-based pedagogical strategies (Singh, Belloni, & Christian, 2006). Graphical visualization softwares can be very effective tools in bridging the theoretical aspects of QM and physical phenomena. They can be applied in the classroom as supplements to lectures or outside the class as homework or as self-study tool by students (Saputra et al., 2015; Singh, 2005).

Teaching QM in chemistry cannot be separated from visual representations of various forms of orbital as an interpretation of the Schrödinger wave equation. An orbital itself is the square of a wave function that provides information about the probability finding of electrons in an atom. It will be hard to grasp the physical meaning of wave function without knowledge of the visual form of the orbital. However, physical chemistry teachers often have some difficulties in demonstrating the forms of hydrogen atomic orbitals from its corresponding wave function. Most teachers prefer to display only the implication of the orbital shapes on the chemical systems than the wave function and its relation to the orbitals character (Chung, 2013).

Based on the aforementioned theoretical background, this paper informs some Android-based graphical visualization softwares i.e *FuncXY* (Ammeraal, 2017), *TriPlot 3D Graphing* (Seriocon, 2017), and *Graphing Calculator* (Stephens, 2017), as learning aids concerning to the 3D plotting of orbitals from its corresponding wave equation. Supported by the widespread use of Android smartphones among students, authors believe the use of these tools will support student learning performance inside and outside the classroom.

EXPERIMENTAL

Wave Equation

The complete wave function, in spherical polar coordinates, is composed of radial, R(r), and angular, Y(θ,φ), parts. The radial part determines the size of the orbital, whereas the angular part determines the shape and orientation of orbitals. Then, the square of the combination of each part represents the orbitals image correctly. However, using the complete wave equation is discouraged for educational purposes because a fairly complicated radial part will make it hard for students to plot orbital. Therefore, it would be easier for students to use only the angular equations without a significant difference to the resulted orbital image. Hence, the use of Android-based plotter in this paper focuses on the angular part by explaining some limitations on the image. The forms of wave functions for hydrogen atomic orbitals is not presented here and it can be found in many quantum chemistry books (Atkins & Paula, 2010; Mortimer, 2008; McQuarrie, 1983).

FuncXY

FuncXY is launched and a window with four coordinate options appeared. Select spherical, checklist on show axes option, and click ok to launch a new window for entering equations. Set the angle range $0 \leq \theta \leq 2\pi$ and $0 \leq \varphi \leq \pi$, then write the desired equation (see Supplementary Material). In some plotters, the range of θ and φ angle could be different depending on assumptions applied for this angle. The same angle range is found in FuncXY and TriPlot 3D Graphing, but not for Graphing calculator that used $0 \leq \theta \leq \pi$ and $0 \leq \varphi \leq 2\pi$. Finally, by a simple click on a green checklist icon, an orbital image appeared. Visualization of the d_{z^2} orbital is shown in Figure 1(a).

TriPlot 3D Graphing

In the TriPlot 3D Graphing main window, click on the Function Type icon and choose polar coordinate. Fill the equation in TriPlot 3D Graphing code (See Supplementary Material), set the grid points to 200, and one click on the plot graph to visualize the orbital. Plotting d_{xz} orbital using TriPlot 3D Graphing is shown in Figure 1(b).

Graphing Calculator

Activate Graphing calculator and click on 3D Graph to work on three-dimensional visualization. Select the spherical according to the desired coordinates and fill the equations using Graphing Calculator code. Click ok and the program will spontaneously display the 3D image of the d_{yz} orbital as shown in Figure 1(c).

LIMITATION

Many researchers have shown the weaknesses of visualization software in presenting the orbital isosurface (Ogryzlo & Porter, 1963; Ramachandran & Kong, 1995; Rhile, 2015). Isosurfaces are the standard shape used for orbitals visualization that is surface of the wave function with a constant value of ψ or ψ2 (or ψ*ψ) (Rhile, 2015). Detailed description and visualization of accurate orbital isosurface have shown by Rhile (2015). Despite its drawbacks, these softwares provide many advantages to support the students' learning activities in the classroom such as: free distributed, user-friendly and real-time plotting. Therefore, these Android-based equation plotters facilitate teachers and students especially those who do not have specific skills in coding or scripting to keep visualizing the orbital from its wave function.

CONCLUSION

This paper informed some plotters integrated with Android Smartphone, named FuncXY, TriPlot 3D Graphing, Graphing calculator, that applicable for quick and real-time visualization of hydrogen atomic orbital. All the softwares is user-friendly to perform in teaching and learning orbital in the classroom.

SUPPLEMENTARY MATERIAL

Material with detailed description of the square of the angular wave function, $|Y_{(\theta,\phi)}|^2$, for hydrogen atomic orbitals (s, p_x, p_y, p_z, d_{xy}, d_{xz}, d_{yz}, $d_{x^2-y^2}$, d_{z^2}) are available in a form ready for input to FuncXY, TriPlot 3D Graphing, and Graphing calculator.

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Figure 1. Visualization of orbital (a) d_{z}^{2} in FuncXY, (b) d_{xz} in TriPlot 3D Graphing, dan (c) d_{yz} in Graphing calculator