

Atomic orbitals and their representation: Can 3-D computer graphics help conceptual understanding? (Orbitais atômicas e a sua representação: Podem gráficos computacionais 3-D ajudar na compreensão conceptual?)

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Quantum mechanics is a non-intuitive subject. For example, the concept of orbital seems too difficult to be mastered by students who are starting to study it. Various investigations have been done on student's difficulties in understanding basic quantum mechanics. Nevertheless, there are few attempts at probing how student's understanding is influenced by appropriate visualization techniques, which are known to help conceptual understanding. "Virtual Water" is a 3-D virtual environment we have designed and built to support the learning of Physics and Chemistry at final high school and first-year university levels. It focuses on the microscopic structure of water and explores, among others, atomic and molecular orbitals. Having asked a group of first-year students of Sciences and Engineering courses at the University of Coimbra, Portugal, to describe how they conceive electrons in atoms we found some common misconceptions. We have tried, with partial success, to overcome them by making students explore our virtual environment. The most relevant characteristics of the virtual environment which contributed to student's conceptual understanding were 3-D perception and navigation.

Keywords: quantum mechanics, atomic orbitals, virtual reality, virtual environment, visualization, conceptual understanding.

A mecânica quântica é uma teoria que escapa à intuição. O conceito de orbital é um bom exemplo disso, sendo normalmente muito difícil de ser dominado pelos alunos que o abordam pela primeira vez. Foram já realizados vários estudos que incidem nas dificuldades que os alunos têm na compreensão da mecânica quântica ao nível introdutório. Contudo, poucos trabalhos trataram a influência de técnicas avançadas de visualização, geralmente reconhecidas como bastante úteis, na compreensão conceptual dos alunos. "Água Virtual" é um ambiente virtual 3-D que foi desenvolvemos com o propósito de apoiar o ensino e a aprendizagem de conceitos de Física e de Química a alunos dos anos terminais do ensino secundário e do primeiro ano da universidade. O programa centra-se na estrutura microscópica da água e explora conceitos relacionados com orbitais atômicas e moleculares. Utilizando aquele programa com uma amostra de alunos do primeiro ano dos cursos de Ciências e de Engenharia da Universidade de Coimbra, em Portugal, detectámos algumas concepções erróneas dos alunos sobre os electrões nos átomos. Com a ajuda do programa "Água Virtual" foi possível, com algum sucesso, ultrapassar algumas das dificuldades encontradas. As características mais relevantes do ambiente virtual que contribuíram para tal foram a percepção 3-D e a navegação pelo ambiente.

Palavras-chave: mecânica quântica, orbital atômica, realidade virtual, ambiente virtual, visualização, compreensão conceptual.

1. Introduction

The idea of atoms goes back to the Greek philosopher Demokritos who lived in the 5th century BC. However, as late as in the second half of the 19th century, atoms were seen as useful concepts and not real objects. At that time some scientists and philosophers still considered atomic theory a metaphysical idea.

One of the great advances in human knowledge of the 20th century was the emergence of quantum mechanics. The development of quantum mechanics has firmly established atomic theory. It has led not only to a general theoretical framework explaining a plethora of phenomena but also to artifacts which are of common use today, including the transistors that make up computers and other electronic equipment.

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An essential concept for understanding atoms, molecules and solids is that of orbital. According to quantum mechanics and in the independent particle approximation, an electron may exist in various states, called wavefunctions or orbitals. An orbital is a complex function (a function with a real and an imaginary part) in 3-D space.

Students learning quantum mechanics have to use probabilistic notions which are very different from the deterministic ones they are accustomed to. An electron, in a given state, may be detected in different points of space with different probabilities given by the square modulus of the wavefunction. However, traditional instruction of quantum mechanics assumes that students master the notion of probability. In fact, the notion of probabilistic occupation of space seems too difficult to be appreciated by beginning students of quantum mechanics. It is therefore not strange that many teachers and textbooks do not manage to awake student's interest and that misconceptions are common among students. There have been recently many investigations focusing on those problems and their consequences. Much of the early work came from groups in Frankfurt, Bremen, and Berlin, in Germany [1-4]. Further research has been carried out in Australia by Johnston, Crawford, and Fletcher [5], and in the United States by Styer [6], Bao, Redish, and Steinberg [7], and Ireson [8].

In spite of the number the studies on student's conceptions of specific topics in quantum mechanics, there are few attempts at probing how student's understanding is influenced by appropriate visualization techniques, which are known to be useful to accomplish conceptual understanding. In fact, the shapes, the nodes and the symmetry proprieties of atomic orbitals can be taught and studied more effectively if students could view adequate spatial representations.

Various authors [9-12] have defended the use of computer simulation and visualization tools in Physics and Chemistry teaching. They had argued that students should be given an active role in using these kinds of tools [13]. In particular, German researchers at the University of Munich [14] presented a new introductory course on quantum mechanics in which conceptual issues are taught with abundant graphical resources. Emphasis is placed on qualitative reasoning and, using virtual laboratories, students become acquainted with phenomena which deviate appreciatively from our classical experience. Another recent work has been carried out by Cataloglu and Robinett [15], who have developed an assessment instrument designed to test conceptual and visual understanding of quantum theory. According to these authors, visualization can shift the focus away from abstract mathematical methods.

One of the most promising means to support science education is virtual reality. This is a computer interface characterized by a high degree of immersion and interaction, which may even make the user believe that

he is actually inside the virtual environment. A pedagogical advantage of virtual reality is the ability to visualize microscopic processes at a macroscopic scale (*e.g.*, the behaviour of water molecules in its different phases) or to make more realistic some abstracts concepts (*e.g.*, atomic or molecular orbitals). 3-D representations, with the bonus of interactivity and navigation, have a great potential to increase student's understanding.

In order to analyze the utility of virtual environments in Physics and Chemistry learning we have designed and built a 3-D virtual environment called "Virtual Water" (the program is available from us upon request). The minimal hardware requirements are a Pentium III processor, 128 MB of RAM, 150 MB of free hard disc, graphics board accelerator, and Microsoft Windows NT 4.0 or higher.

"Virtual Water" is intended to describe the microscopic structure of water. Besides the study of phases and phase transitions, it allows to explore atomic and molecular orbitals. We have shown [16] that "Virtual Water" helps students with high spatial aptitude to acquire better conceptual understanding of solid, liquid and gaseous phases, including the transitions between them.

To further study the pedagogical utility of that software we present and discuss some of the student's answers to an inquiry on atomic orbitals done two moments: before and after using our virtual environment.

Our study involved 20 first-year students attending Physics, Chemistry, Industrial Chemistry, Physics Engineering and Civil Engineering courses at the University of Coimbra, Portugal, the same sample as in [16]. Atomic orbitals belong to the "General Chemistry" syllabus and had been taught to our subjects at an introductory level (the standard textbook is [17]).

Before presenting our findings on orbitals, we want to highlight some general ideas about them and the utility of computational means in their representation.

2. What is an orbital and how it can be represented

2.1. A brief history of atomic orbitals

The idea of energy quantization was introduced in Atomic Physics in 1913 with the first explanation of the hydrogen electronic structure by the Dane Niels Bohr. Inspired by Planck's theory of black-body radiation, Bohr admitted that the electrons in hydrogen atom can only exist in stationary states with a well-defined energy. Transitions between these states occur by absorption or emission of energy. Bohr defended that electrons in such states follow classical circular orbits around the nucleus. The idea of orbitals as probability functions was still to come.

Influenced by the interpretation of the Compton

effect, the Frenchman Louis de Broglie suggested, in 1924, that the accepted wave-particle duality for photons could be extended to any moving particle which would then have a wavelength associated with it. The somewhat mysterious wave of de Broglie was the predecessor of the wavefunction. The wavefunction contains all of the important properties of the electron: knowing it we can calculate the value of any measurable quantity.

The probabilistic interpretation of the wavefunction was proposed, also in 1924, by the German Max Born. The wavefunction is simply related to the position of the electron in space. The square module of the wavefunction,

$$|\psi(x, y, z)|^2 = \psi^*(x, y, z) \cdot \psi(x, y, z)$$

is the probability density for finding the particle at the (x, y, z) position. The sum of all probabilities in full space is unity since the particle should be anywhere.

Helped by that interpretation, from 1925 to 1927, a pool of young physicists developed the complete theoretical machinery for getting the wavefunction and obtaining information from wavefunctions. An important step was given in 1925, when the Austrian Erwin Schrödinger, inspired by the de Broglie theory, proposed a wave approach to quantum mechanics. For the simplest case of a free particle the Schrödinger equation is a differential equation involving a second-order spatial derivative of the wavefunction, ψ and the unknown energy E (a real number),

$$\hat{H}\psi = E\psi$$

with

$$\hat{H} = -\frac{\hbar^2}{2m} \left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} \right)$$

an operator describing the kinetic energy which acts on the wavefunction (\hbar is Planck's constant and m the particle mass). If the particle is confined to a limited region of space (box) the solution of the wave equation leads to a discrete set of energy values. Energy quantization appears, therefore, associated to the localization of the wavefunction. For a particle under a potential, the operator \hat{H} has to include a potential term.

Like the energy, any measurable physical quantity, or observable, has associated with it an operator, which acts on the wavefunction to yield the wavefunction multiplied by a real number, the value of the observable which should be measured.

In 1927, the German Werner Heisenberg identified incompatible observables meaning that we could not measure with arbitrary precision on pair of observables. That is the case of (linear) momentum and position. This so-called uncertainty principle expresses therefore the impossibility of preparing a state for which both position and momentum can be determined with arbitrarily small uncertainties.

Still in 1927, with the first observations of electron diffraction by Clinton Davisson and Lester Germer, in the United States, and by George Thompson, in Great Britain, the fundamental aspects de Broglie's theory were confirmed. Further observations confirmed the validity of Bohr's interpretation, the Schrödinger equation and Heisenberg's uncertainty principle. Until now, none of the predictions of quantum mechanics have been contradicted by experiment.

2.2. On drawing orbitals

When dealing with atomic systems and going beyond old quantum theory, the classical notion of particle trajectory has to be abandoned, since, in contrast to Newtonian Mechanics, a well-defined position and momentum are no longer possible at a given time. We can only describe the probability for the particle to be at a certain position, or the probability for it to have a certain momentum. Trajectories are replaced by diffuse spatial distributions. These distributions can be represented by surfaces on which all points have the same value of probability density ψ^2 , the so-called isodensity surfaces.

Electrons surrounding atoms are concentrated in regions of space described by atomic orbitals. The boundaries of an atomic orbital are conventionally drawn by the surface of 90% probability, but they extend to infinity.

From the Schrödinger equation we can calculate the wavefunction of the hydrogen atom and therefore the probability for the position the electron can take [18]. For hydrogen the energy depends on the principal quantum number n , which is an integer ($n = 1, 2, \dots$).

Angular momentum is also an observable. It is found that the angular momentum is quantized according to:

$$\hat{L}^2\psi = \ell(\ell + 1)\hbar^2\psi,$$

with ℓ the angular momentum quantum number ($\ell = 0, \dots, n - 1$). The z-component of the angular momentum is given by

$$\hat{L}_z\psi = m_\ell\hbar\psi,$$

where m_ℓ is the magnetic quantum number ($m_\ell = -\ell, \dots, +\ell$).

In the lowest-energy state (ground-state) of the hydrogen atom the electron has a spherical distribution in space since the wavefunction has spherical symmetry. At higher energy the orbitals may take other shapes.

The use of computational means

The major challenge in representing atomic orbital functions arises from the fact that each location in 3-D space has an associated value of ψ^2 .

Physical interpretations of the apparent shapes change with the method of representation may be erroneously interpreted (namely, they are sometimes thought to represent different instants of classical electron motion). Traditional representations of orbital shapes are based on attempts to reduce the dimensionality of the ψ^2 functions.

For instance, the plot of radial distribution *vs.* distance from the nucleus describes how the electron density changes with the distance. It is a 1-D representation of a 3-D function which represents the probability to find the electron at a certain distance. In the case of the 1s orbital, Fig. 1 shows that the electron is never found at the nucleus and that the electron is unlikely to be found far from the nucleus (since the wavefunction is vanishing small far away from the nucleus). The electron is to be found around a_o (0.0529 nm) where $r^2 R_{nl}(r)$ is large, with a_o the Bohr radius (this is the most likely distance). Thus the electron in the hydrogen 1s orbital is normally found at 0.026 to 0.1 nm from the nucleus.

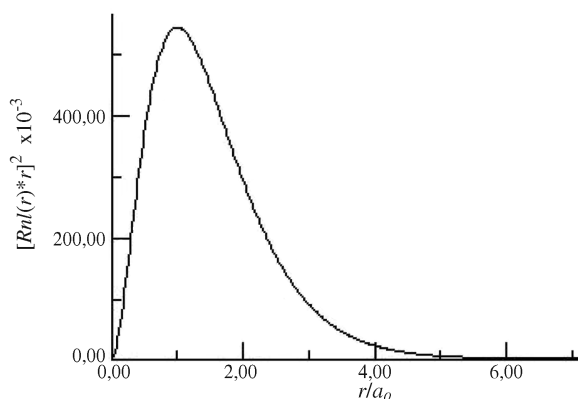


Figure 1 - Plot of radial distribution *vs.* distance from the nucleus for the 1s orbital of hydrogen [19].

An example of the 2-D diagrams is a contour plot representing some of concentric isodensity surfaces. Figure 2 shows the 3s orbital of hydrogen. With 2-D pictures the viewer may have difficulties to visualize the 3-D electron cloud, especially how diffuse or concentrated it actually is in different regions.

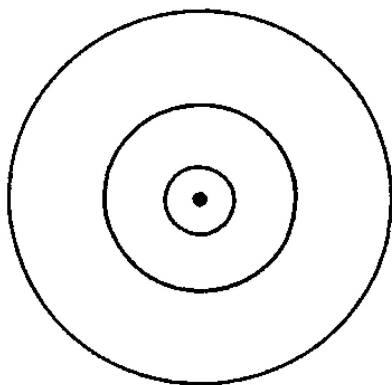


Figure 2 - Contour plots of 3s orbital of hydrogen [19].

Since students are now much more routinely exposed at early stages to computer-generated materials, more sophisticated graphical representations are necessary in schools.

At the beginning of the 70s, Bordass and Linnett [20], Olcott [21], and Streitweiser and Ownens [22] were among the first to use computer-generated 3-D contour diagrams to represent atomic and molecular orbitals. Presentations of quantum mechanics materials have changed a lot over the years. The most recent examples of course materials, including textbooks, software, and hardware, allow students to visualize and experiment orbitals in 3-D. Some examples of these modern means are:

“Atom in a box”, by Dager Research (<http://dager.com/orbitals>, retrieved on July 2003). It is a Macintosh application that nicely displays electron orbital as a cloud. The cloud’s density is determined by the probability density.

“Visual Quantum Mechanics”, by the Physics Education Research Group of the Kansas State University Department of Physics (<http://phys.educ.ksu.edu/info/summaryOfVqm.html>, retrieved on July 2003). This program involves instructional units that introduce quantum mechanics to high school and college students who do not have a background in modern Physics and advanced Mathematics. To reach these students, the instructional units include, in an activity-based environment, interactive computer programs, multimedia and text documents.

“Haptic representation of the atom”, by Harvey and Gingold, from Fairmont State College, West Virginia, USA. They used 3-D haptic interface for perceiving the 1s and 2s orbital significance. According to the authors, “the sensible technology’s Phantom allows the user to move a pen, connected to a mechanical arm, within a 3-D workspace on the user’s desk. The software directly maps the 3-space of the atom into the 3-space of the Phantom’s workspace. The electron probability density function drives the force exerted on the user. The force is proportional to the probability density function for the electron at any point, given by the square of the wave-function describing a particular atomic orbital. The gradient of the probability function governs the direction in which the pen is pushed. The user, by moving the Phantom’s pen around the workspace, probes different points in the atomic orbital. The Phantom responds by continuously updating the forces acting on the user with the output from the ψ^2 function, creating a tangible electron probability density field. On the computer screen, a 2-D projection of a three-dimensional electron density isosurface provides the user with an additional point of reference for understanding the location of the probe in relation to the nucleus” [23].

3. “Virtual Water” and understanding of atomic orbitals

The following are some examples of common student’s misconceptions:

- Bohr’s atomic model (circular orbit). Students often conceive electrons flying around the nucleus, with high speed, in prescribed classical orbits [14].
- Incorrect understanding of charge. Many students have wrong conceptions on the repulsion and attraction between charges [1].
- Conception of a fixed shell. Students think that electrons are fixed or move in a shell [1].

According to Styer [6] a very effective strategy to overcome these difficulties is to assign a traditional quantitative/analytical problem which renders the misconception concrete.

With “Virtual Water” we studied the effect of 3-D interactive simulations on student’s visualization and comprehension of atomic orbitals of hydrogen. We used

3-D isodensity surfaces for better conceptual understanding of shapes, nodes and symmetry proprieties. Indeed, the most complete and accurate representations of atomic orbitals involve the use of dot frequency. The average electron density in small volume elements is calculated and then represented by a number of dots. This type of representation is most effective when the image can be rotated. The major drawback is that internal details about electron density are obscured by the outer parts of the image. A navigable three dimensional representation is needed, one which would allow the viewer to fly through the orbital.

The chosen set of scenarios focused on the $1s$, $2s$, $2p$, $3s$, $3p$ and $3d$ orbitals (Fig. 3). In these scenarios it is possible to rotate the orbitals, choosing different perspectives of electron densities, and to experiment diverse cut plans. These orbitals models were developed and optimised with the software packages *Mathcad* and *3-D Studio Max*. The virtual scenarios were created with the software *WorldToolkit* (from Sense8).

Our dependent variable is the level of conceptual comprehension on atomic orbitals, while our independent variable was the use of 3-D interactive computer simulations.

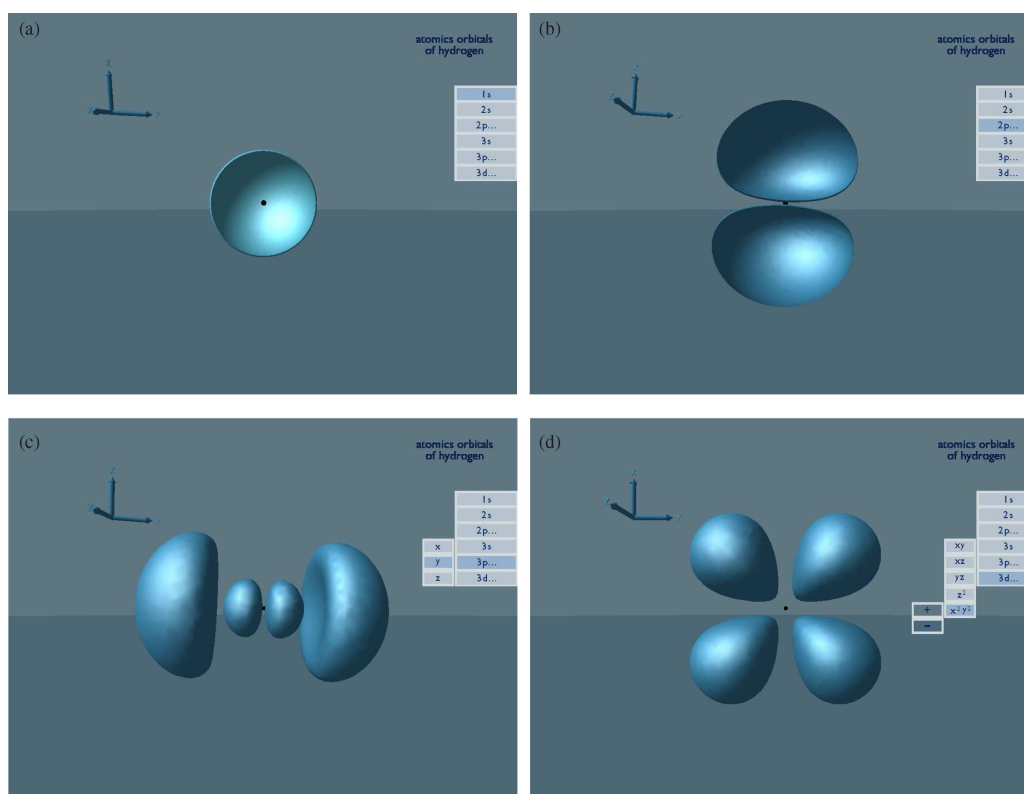


Figure 3 - Isoprobabilistic surfaces of atomic orbitals of hydrogen. The following orbitals are shown: a) $1s$; b) $2p_x$; c) $3p_y$; d) $3d_{x^2y^2}$. The dark point in the centre represents the nucleus of the hydrogen atom (proton). For each orbital the viewer may choose different aspects of electron densities. Figures a) and b) represent models that are cut along the xy plane showing the interior of the orbital.

Conceptual comprehension is the degree to which the student's understanding of a concept corresponds to the scientific explanation. According Haidar [25], the observations of student's attitudes and interviews are adequate methods in the descriptive studies like the present one. Understanding was determined by student's oral explanations in a guided interview (each interview took about 45 minutes and was tape-recorded) and by a written questionnaire.

For evaluating the utility of our program, we have compared the student's answers before and after software use. Moreover, we have tried to find correlations between conceptual comprehension and software use (namely, 3-D perception and navigation through the virtual environment).

Our research question was: "how do you conceive electrons in an atom?" Students were prompted to answer that question, before and after seeing "Virtual Water". Some examples of typical answers given by students before and after software use are the following:

Example 1:

Before software use: "Electrons are on different orbits around the nucleus and they can jump from one orbit to another".

After software use: "I do not see any electron and motion; only different shapes that change from state to state so that, we do not have exact information where the electron is".

The answers before software use shows that the student conceives an electron like a planetary model were electrons move around the nucleus in definite orbits. After software use, he recognized that the electron no longer moves in the classical sense.

Example 2:

Before software use: "Electrons have different positions around the nucleus but their trajectories are unknown".

After software use: "Electrons have no definite position; they are just located somewhere in a certain region".

Now, although both answers are not completely wrong, in the last one student recognize that electrons have a probabilistic localization in contrast to the answer before.

However, not all the students have improved their understanding about the concept of orbital after using the software. For example, some pupils when observing the 3-D isodensity surfaces (Fig. 4) thought that these represented the place where the electrons are located. Identical misconception has been reported by Fischler and Lichtfeldt [1], as we seen before. We think that such fact was indeed induced by the chosen type of 3-D representation.

All students' statements mentioned above were oral and qualitative. To be more precise, we have made a descriptive statistics of the student's answers. Student's

conceptions were classified on an ordinal scale. The array of variable classification ranged from 1 (dead wrong) to 5 (completely right) as done in previous studying (e.g., [25]) and according to Table 1.

Table 1 - A categorization scheme of student's conceptions.

Variable classification	Degree of understanding
1	No response ("I do not know" or "I do not understand")
2	Incorrect responses with wrong terms
3	Incorrect responses using a mixture of correct and wrong terms
4	Responses that use the correct terms but do not match the scientific conceptions
5	Responses that use the correct terms and match the scientific conception

Figure 4 shows the boxplots concerning the comprehension of orbitals before and after computer visualization. The results with software are a little better (we found more correct answers). After software use the mean score was 3.55, with a 0.94 standard deviation, in contrast with the mean score of 2.10, with a 1.25 standard deviation before software use.

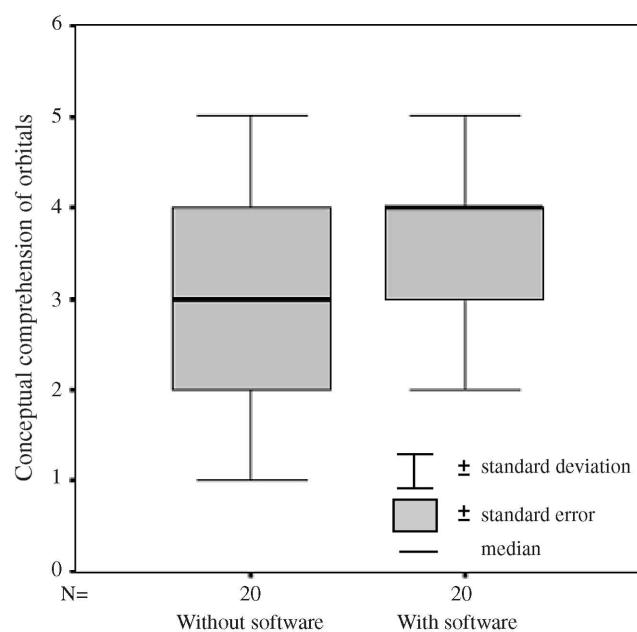


Figure 4 - Boxplots for conceptual comprehension before and after use of software concerning orbitals.

Using the Spearman test (at a confidence level of 5%) we found correlations between conceptual comprehension and some characteristics of computer visualiza-

tion, like 3-D perception (0.560, $p < 0.05$) and navigation (0.459, $p < 0.05$).

Table 2 - Correlations between computer visualization and conceptual comprehension of orbitals.

Computer visualization	
3-D perception	Navigation
0.560 ($p < 0.05$)	0.459 ($p < 0.05$)

4. Conclusions

Orbitals are a key concept in quantum mechanics. We stress that it is the electron density which can be experimentally observed and not the orbitals themselves. In fact, the observation of electron density is an exciting field in Physics [26]. We would like to stress that orbitals are only genuine wavefunctions in one-electron systems, such as the hydrogen atom. For many electrons atoms of molecules there are convenient approximations.

One of the strengths of "Virtual Water" is its ability to visualize electronic density in 3-D space. In effect, 3-D visualization tools are useful to increase student's understanding of atomic orbitals overcoming, at least partially, previous misconceptions. The most important characteristics which contribute to student's conceptual comprehension seem to be 3-D perception and navigation.

Students exposed to our computer environment were in general very enthusiastic about it. According to a student "it is easier to understand abstract things when you can visualize them".

Of course, our findings are exploratory and are non-generalisable without a method for evaluating more effectively the impact on learning, a work that goes beyond this simple descriptive study.

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