

Learning Quantum Mechanics

Visualization of Hydrogen Atom States

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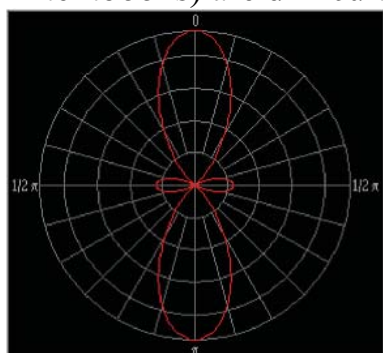
Abstract

In an introductory university course on quantum physics we found that students often misinterpret polar graphs and hydrogen eigenstate probability density plots. This paper describes our project designed to improve this and the project outcomes. The students solve different tasks from their workbook using small special designed programs which enable them interactive work with graphs and to build their understanding of the plots. The tasks were designed according to experiential learning approach. Described activity was part of the standard introductory course on quantum mechanics for future physics teachers. Students found the project useful and interesting.

Motivation: Why have we done this?

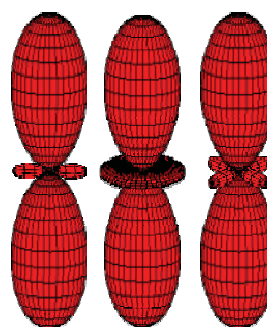
According to research (Buddle et al., 2002a) and our experience, learning a quantum atomic model raises many difficulties. Many students imagine the atom like the Bohr's model – electrons like planets moving around the nucleus. Although some of them realize that this is not correct, Bohr's concept seems to be very persistent. (Müller & Wiesner, 2002) Detailed survey of various students' preconceptions and teaching difficulties can be found in Buddle et al., 2002a. There are new approaches how to deal with students' problems and lead them to better understanding (Buddle et al. 2002b, Niedderer & Deylitz 1999, Müller & Wiesner, 2002). They all call for using appropriate images and pictures.

Besides these conceptual problems our experience shows that for students it is very difficult to imagine the spatial probability density of hydrogen atom eigenstates. Especially the polar and spherical plots (most common in textbooks) are difficult for students to understand.



And your views?

Let's make a test



1. Is this statement true?: “On the left picture we can see shape of some orbital. An electron can be observed only inside the red bubbles and cannot be observed outside.”¹⁵
2. No matter how you answered the previous question, try to choose the correct spatial shape for the previous planar cut from the three images on the right-hand side.¹⁶

We were looking for a tool which would help students to understand *step-by-step* how the angular and radial part of hydrogen eigenstate functions determine the orbital shape. We can easily find many images of atom orbitals in textbooks, various pictures and applets can be also found in the internet (e.g. Falstad 2005, Manthey 2004) or in other publications (e.g. Brant et al. 2003). However, all of them show only spherical harmonics (in polar graphs) and some of them also plot the probability density. Because we were unsuccessful in our search for a suitable interactive tool, we made it ourselves.

Realization: What did we do?

We designed a set of **interactive tools** that visualize the radial and angular part of wave functions and probability density plots of hydrogen atom eigenstates in variety types of graphs. Computer tools allow very good visualization of functions, better than common printed images. Computer generated graphs are accurate, not only hand-drawn shapes as in some textbooks. Moreover, good images and interactivity (e.g.: zoom and rotation of 3D graphs) can increase students' interest.

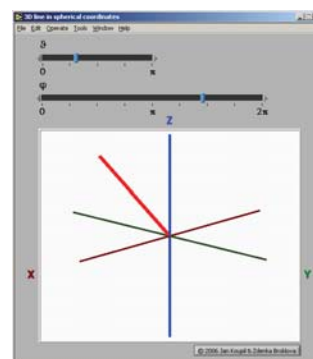


Fig. 1: Program 3D_line

The programs were accompanied by a **workbook** containing tasks, results and explanations (and some small hints how to use the programs as well). The workbook was designed to lead students to active working and thinking. They should construct the entire wave function step-by-step from its parts. After each step they can check if they interpret pictures correctly. For designing the tasks it was crucial that students could correct their answers themselves, using only the computer tools, and learn from their own mistakes.

The project was designed for and tested out on the 2nd-year university students. But before we present outcomes of the project, we describe computer tools and workbook in more details.

¹⁵ No. On the picture is shown only the angular part of the probability density of the chosen eigenstate. The length of the “bubble” means only that it is more probable to find an electron in this direction. To obtain the probability of electron observation, we have to combine this angular part with radial part. As well as electron observation “prefers” some directions, it prefers some distances from the nucleus.

¹⁶ The 2nd image is correct.

1. Computer Tools

This part could be difficult to follow without the computer tools.

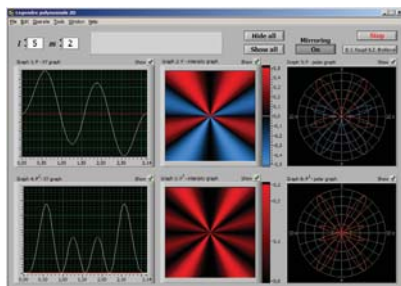


Fig 2: Program Legendre_2D

The computer tools were made to let students see and compare different methods (in different types of graphs) of spherical functions visualization. However, the aim is not only to visualize functions. We enriched the tools by special properties that enabled us to prepare tasks for the workbook. All programs used in our activities were made in the LabVIEW environment. The programs were compiled to run without having LabVIEW completely installed. At least the

LabVIEW Runtime Engine is required. The Runtime Engine and all tools can be downloaded for free from our website.

The first tool (program), *3d_line* (Fig. 1), is very simple. It draws a line for given angles θ , and ϕ , in spherical coordinates. While using this program, students should remember spherical coordinates and familiarize with them. If you want to use polar graphs, it is necessary to understand spherical coordinates very well.

The second program, *Legendre_2D* (Fig. 2) offers three different views of Legendre polynomial of the argument $\cos \vartheta$. The function is selected by entering the quantum numbers l and m . The first row of graphs contains the function itself; in the second row is the square of it (angular part of density of probability as we will see later). Figures on the left are “classical” XY graphs, the middle ones show the density of probability by intensity of color, and the figures on the right are polar graphs (most used). All of the figures may be switched on or off independently. This feature is used during the students’ tasks.

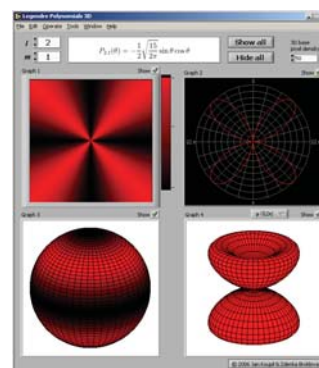


Fig 3: Program Legendre_3D

In the next step we add the third dimension and deal with the angular part of probability density. In the program *Legendre_3D* (Fig. 3) students enter the l and m quantum numbers and the program shows the angular part of the probability density (square of the appropriate spherical harmonic). Two figures in top line are identical to the graphs in the previous program: the color intensity graph and the polar graph. The bottom line contains a spherical cut through space (left one) – the intensity of color agrees with function value – and a standard 3D polar graph (right one).

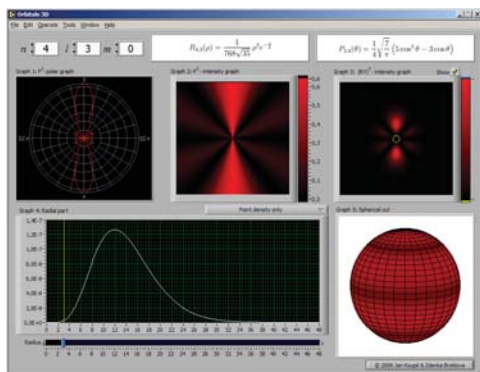


Fig 4: Program 3D_orbitals

The last program, 3D_orbitals (Fig. 4), contains both angular and radial parts of probability density of hydrogen atom eigenstates. Besides the graphs of the radial part of the function (bottom left) and angular part (top left and top middle), the program also shows their product in the form of planar cut (top right, the cutting plane contains z axis) and spherical cut (bottom right). The radius of the spherical cut may be

changed. The actual value of the radius is shown in the graph of the radial part and in the planar cut in the form of a yellow line / circle.

Because the maxima of the radial part of the wave function are not of similar height, the graph of the probability density for finding an electron has a “brightness zoom” (see fig. 5). The entire graph can be brightened by moving the blue pointer on the color scale. Places with a value higher than the slider position are marked by white color. These figures show the proper shapes of orbitals, i.e. areas where the probability of finding electron is significant.

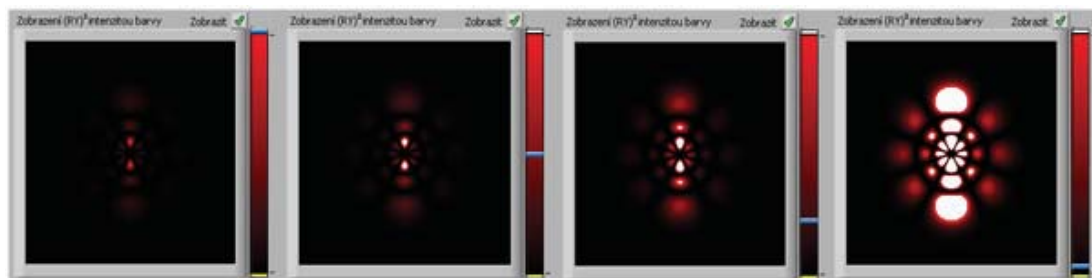


Fig 5: Brightness zoom

2. Workbook

The computer tools are accompanied by a workbook. It has 14 pages with approximately 25 various tasks. We assumed that it would take students about 2 hours to fill it in.

The topic (solving the Schrödinger equation for the Coulomb potential in an x -representation) was lectured previously. The workbook supposes such previous knowledge, but crucial parts are remembered and summarized there. According to our experience, students' understanding of this topic after only following the lecture is not very deep and they are not able to imagine the function correctly. We assumed that after solving the tasks, students would build up their own spatial image of the orbitals. The tasks were based on students' active work. Besides the more common questions we used so-called “redrawing” tasks for which the computer tools were equipped by the independent graph switching.

Follow fig. 6: At first the students switch off all graphs, adjust quantum numbers and switch on only one of the graphs (left part). Then they try to redraw it into the other types of graphs in their workbook. In the middle you can see one of students' solutions. Finally they switch on all graphs again and correct their work themselves. Then students repeat "redrawing" with modified initial settings – different quantum numbers and different type of graph switched on at the beginning. We found this type of activity to be very suitable for the chosen approach – experiential learning.

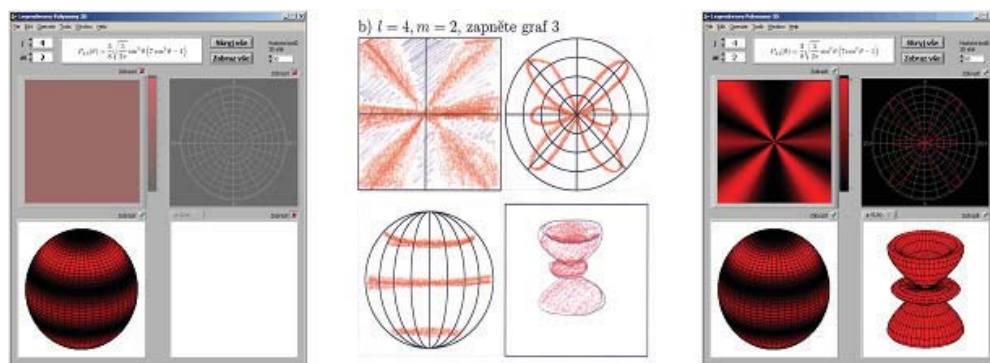


Fig 6: Redrawing task

The workbook consists of nine sections:

1. *Before we start* – installation guide, instructions on how to work with programs, to suppress fear of making mistakes we stressed the aim of the project – to improve understanding, not to evaluate students' knowledge
2. *Spherical coordinates* – we suppose basic knowledge of spherical coordinates but ask students to solve some simple tasks to familiarize with them further (supported by `3d_line` tool)
3. *Wave functions of hydrogen atom eigenstates* – theoretical section – remembering of coordinates' separation in the wave function and the role of quantum numbers
4. *Legendre polynomials* – through using program `Legendre_2D`, students should understand and get used to different types of graphs in which the functions of coordinate ϑ can be drawn
5. *Spherical harmonics* – in this section students build up their spatial image of the Legendre polynomials' square (using program `Legendre_3D`)
6. *Radial part* – students combine angular and radial parts together and draw probability density graphs (using `3D_orbitals` tool), at the end of this section is an explanation of difference between radial probability density and radial part of the probability density
7. *Orbitals* – firstly students describe their view of orbital, then the explanation and warning about common textbook mistakes follows
8. *Solutions*
9. *Questionnaire* – we asked students about their opinion on the whole project

Another example of student's solution is on the fig. 7. The student drew each bottom plot (combination of angular and radial part of probability density) according to the above ones (angular and radial part displayed separately) that were displayed by computer.

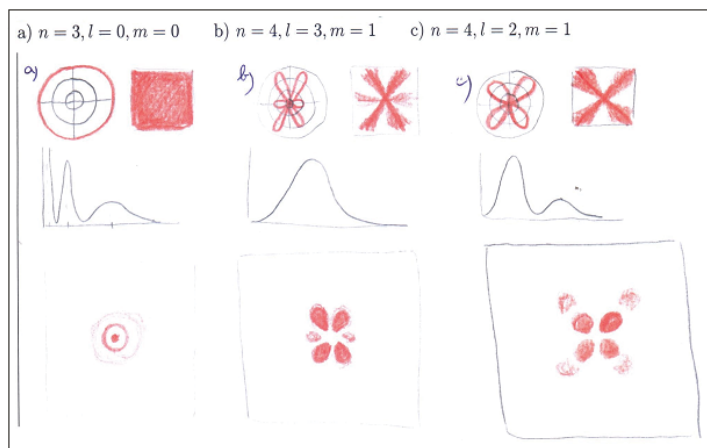


Fig 7: Combination of angular and radial part (part of student's workbook)

The tasks were designed according to the principles of experiential learning (to be specific, according to the *Kolb's learning cycle*) (Luckner & Nadler 1997). Each section of the workbook follows the same pattern described below. Kolb's stages are indicated in the brackets.

- Firstly, students are asked to play with each program and build up their own hypotheses (on the basis of previous knowledge) of what the programs draw. (*Concrete experience*) This part also deals with their tendency to play and enjoy the nice pictures before they start serious work.
- As the second step the students confront their hypotheses with explanation offered in their worksheet. (*Reflective observation*)
- Then they are asked to “prepare a plan” how to redraw one type of graph to other types or how to build 3D plot from planar cut. (*Abstract conceptualization*)
- In the final step they use their “plan” and solve “redrawing” tasks, or other tasks. (*Active experimentation with new concrete experience*) They check their answers immediately. This enables them to correct the tasks as well as their solving methods. (*Reflective observation*)
- In the end of each section they should write down the pros and cons of the different ways in which the functions can be illustrated. (*Reflective observation*)

3. Project design

The whole project was designed for *university students* (the 2nd year, future physics teachers) as a part of their compulsory introductory quantum mechanic course. Each student received a copy of the workbook that contains everything necessary (as installation instructions, tasks,

results, explanations ...). Software was available on the internet or on a CD. They solved the tasks as homework (or they could work it up in school computer laboratory). After that we collected the filled-in workbooks, made notes to their answers, gave them back to students and discussed their answers (in small groups outside the regular class) as well as their opinions about project.

We decided to do this as homework, not during a lesson (in fact the homework substituted a lesson which was cancelled) because of the following reasons:

- Students can work at their own pace (it is crucial in the experimentation phase) and return to previous parts if they needed.
- Working without a teacher needs a very precise and detailed workbook, but minimizes fear of making mistakes. Students could of course ask a tutor (personally or via email) for help in case of any problem during the project.
- It would have been difficult to find enough computers for all students working at one time and not disturbing others.

Outcomes: Students' opinions

After collecting the workbooks we summarized outcomes from the piloting of this project (summer term 2006). We received 10 completely filled-in workbooks in total.

1. Comparison of different visualization methods

We asked the students to compare different types of graphs which were used in the tools. Here we summarize their answers in the following two tables.

Because different students mentioned various pros and cons of all used types of graphs, we concluded that it was useful to show the same function in different types of graphs. Different aspects are better visible in different graphs and students can build their view according to all of the graphs.

2. Students' feeling about the project

In the last section of the workbook and in the discussion after solving it, we asked students to express their feelings about their work and opinions on the whole project. All of the students found it interesting and attractive, more like a game than study, one student wrote in the final questionnaire: “... *it was like an amusing detective story whether my ideas or pictures were correct.*”

They liked the very vivid presentation of such an abstract topic. Some of them wrote that the “redrawing” task improved their understanding (“...*when I had to draw pictures, I realized that I did not understand the explanation well and needed to read it again*”, “*before working with these tools I was not able to imagine what does it mean: ‘orbital like sphere inside another sphere’*”). Generally they appreciated recapitulation of the

spherical coordinates at the beginning and found the sequence of sections good.

The only negative factor they mentioned was the long time they spent with solving the tasks (approx. 4-5 hours, twice more than we expected). Despite it they felt that it was not waste time and appreciated the possibility to arrange time individually.

According to students' feedback it may be said that the work did amuse them. The results of their work show that their understanding of the topic has improved while working on the tasks. On the other hand, we realized some processing difficulties (timing, better after- discussion arrangement ...) which should be solved.

Future plans: What next?

The project outcomes gave us feeling that this way is suitable. So, we have continued in improving the current computer tools and tasks and developing new ones. There are some of our goals which are in progress now.

Web support

We are creating an appropriate web presentation to make the materials available to teachers willing to use these tools and methods. To make them more easy-to-use, we are dividing the project into smaller parts which can be used independently.

Widening the target group

The activities and programs were aimed at university students. However, some basic parts of quantum mechanics are part of high school curricula. Middle school students (and even teachers) often lack the imagination of orbitals. We are therefore transforming some tasks to this level and preparing a suitable way how to use these tools in the middle school.

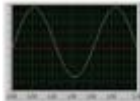




Extending the topic

We would like to continue the development of programs and activities and cover the topic further. Some of the ideas are:



- to add radial density of probability to the graphs and create an activity that would help students to understand the difference between density of probability at a given radius and the radial density
- to make a program enabling students to create and observe combinations of stationary states (real combinations, hybridization) and make a few steps towards quantum theory of chemical bond
- to show the time development of combined states and orbitals

However, these goals demand further study and maybe even the change of platform (use of Mathematica or Java instead of LabVIEW).

Graphs of angular density of probability

	<p>XY Graph</p> <ul style="list-style-type: none"> + a kind of graph well known to students – not connected to spatial distribution of probability density
	<p>Intensity Graph</p> <ul style="list-style-type: none"> + a good visualization of spatial dependence + the illusive limitation by radius doesn't occur as in the polar graphs + it is clear that the radius can be extended and the value would be the same, breaks the common misinterpretation of polar graphs of angular functions – difficult to read function values
	<p>Polar Graph</p> <ul style="list-style-type: none"> + easy to remember + it is possible to read values – more difficult to understand correctly than other graphs – leads to misinterpretation in terms of illusive limitation of probability density by radius (note: Sometimes these images are wrongly interpreted as probability density plots!)
	<p>3D Polar Graph</p> <ul style="list-style-type: none"> + nicer than 2D, more attractive – it is difficult to read function values
	<p>Sphere</p> <ul style="list-style-type: none"> + gives better view than flat graphs – impossible to read function values

Graphs of probability density

	<p>Planar Cut</p> <ul style="list-style-type: none"> + offers good view on distribution of probability density in space +/- really illustrative but one has to be aware how to create the spatial image and that this is only a cut
	<p>Spherical Cut</p> <ul style="list-style-type: none"> + good to study dependence of probability density on distance – the influence of radial part is not vivid +/- isn't of much use when alone but good in connection with other graphs (mainly the XY graph of radial part of wave function)

Conclusion

It is quite easy to find various tools for visualizing different parts of the atomic wave functions, probability densities etc. on the internet.

However, most of these sites contain tools that can only be used for visualization. Even after a long search we did not find anything more complex that would lead students to deeper understanding, accompanied by methodics or hints for teachers.

In this aspect and mostly in the emphasis on students' active work is our project innovative and, according to the response from our students, even successful. Even though students subjectively appreciated the project, the real influence on their understanding and knowledge of the hydrogen atom orbitals has not been tested yet and will be a part of further research. If you are interested, you can find all materials on the following address:

<http://kdf.mff.cuni.cz/~broklova/orbitals/>

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