

Visualisation of Hydrogen Atom States

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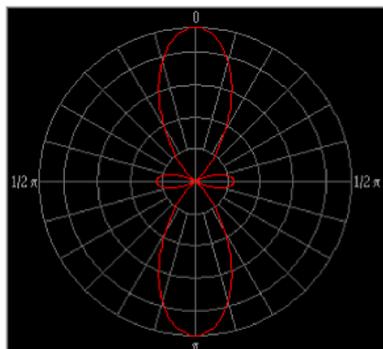
Abstract

We found out that students very often misinterpret polar graphs and hydrogen eigenstate probability density plots which are studied in an introductory course of quantum physics. 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. This activity was part of the standard introductory course of Quantum Mechanics for future physics teachers.

Motivation: Why have we done this?

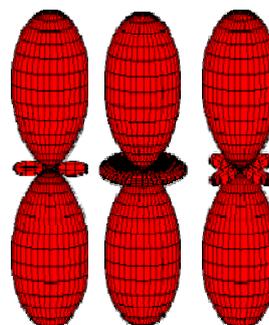
According to research (Buddle et al., 2002a) and our experience, learning quantum atomic model raises many difficulties. Many students imagine the atom like the Bohr's model – electrons like planets moving around the nucleus. Although some of them realize that it's not correct, this concept seems to be very resistant. (Müller & Wiesner, 2002) Detailed survey of various students' preconceptions and teaching difficulties can be found at Buddle et al., 2002a. There are new approaches how to deal with these problems and lead students 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 and especially the polar and spherical plots (most common in textbooks) are difficult for students to be understood correctly.



And your views?

Let's make a test



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

¹ 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.

² The 2nd image is correct.

We can easily find many images of atom orbits in textbooks. Lots of 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). All of them show spherical harmonics (in polar graphs of course) and some of them also plot the probability density plots. But we were looking for a tool which would help students to understand the effects of the angular and radial part of hydrogen eigenstate functions at the orbit shape *step-by-step by their active work*. Because we were unsuccessful in our search for a suitable tool we made it ourselves.

Realization: What did we do?

We designed a set of **interactive tools** that visualize the parts of wave functions and probability density plots of hydrogen atom eigenstates in variety types of graphs. Computer tools allow very good visualisation of functions, better than common printed images. 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.

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 leads students to active working and thinking. They compound 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.

1. Computer Tools

The computer tools were made in order to let students see and compare different methods (in different types of graphs) how to visualize spherical functions. However, the aim is not only to visualise functions. We enriched the tools by special properties that enabled us to prepare tasks to the workbook. All programs used in our activities were made in the LabVIEW environment. The programs were compiled to be run without having entire LabVIEW installed, but at least presence of the LabVIEW Runtime Engine is required. The Runtime Engine and all programs can be downloaded for free from our website.

The first program, 3d_line (Fig. 1), is very simple. It draws a line from given angles - 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.

Fig. 1: Program 3D_line

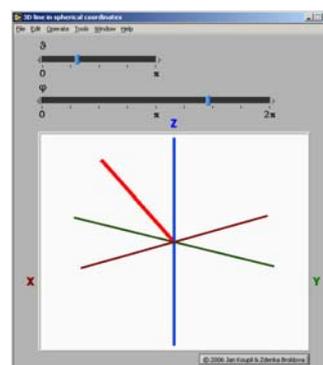
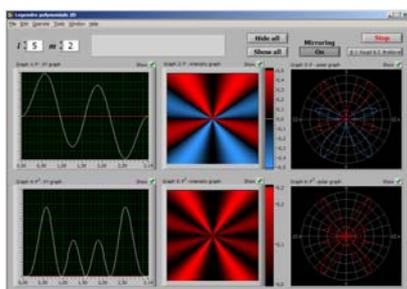


Fig 2: Program Legendre_2D



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 colour, 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.

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

Fig 3: Program Legendre_3D

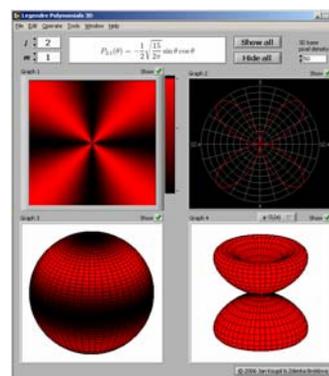
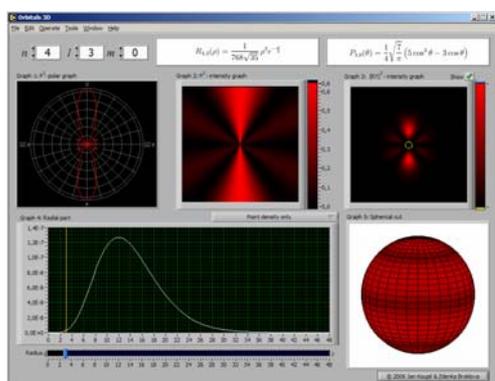


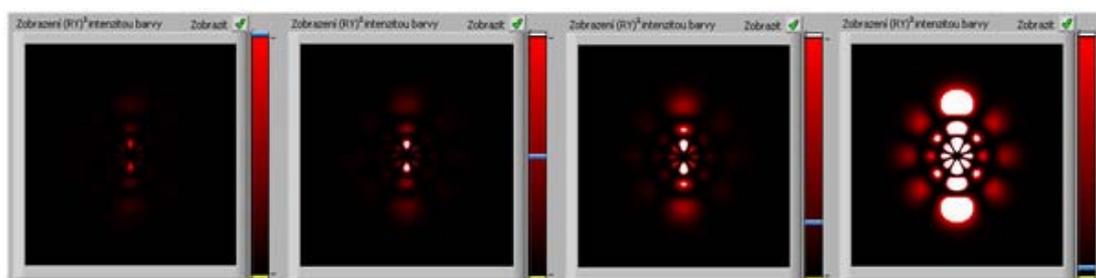
Fig 4: Program 3D_orbits



The last program, 3D_orbits (Fig. 4), contains both angular and radial parts of probability density of hydrogen atom eigenstates. Besides the graphs of separated radial part of the function (bottom left) and angular part (top left and top middle) the graphs offer 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 radius is shown in the graph of radial part and in the planar cut in the form of yellow line / circle.

Because the maxima of radial part of the wave function are not of similar height, the graph of probability density of finding electron has a “brightness zoom” (see fig. 5). Entire graph can be brightened by moving the blue pointer on the colour scale. Places of value higher than the slider position are marked by white colour. These figures show the proper shape of orbits = 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 about 2 hours to fill it in.

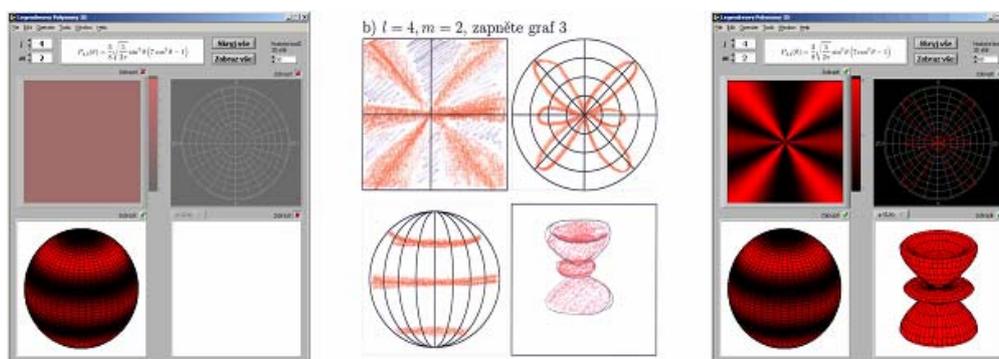
The topic (solving Schrödinger equation for Coloumb potential in x -representation) was lectured previously. The workbook supposes such previous knowledge but crucial parts are

remembered and summarized there. According to our experience, students' understanding of this topic after passing only the lecture is not very deep and they are not able to imagine the function correctly. We assumed that after solving the tasks, students built up their own spatial image of the orbits.

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 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.

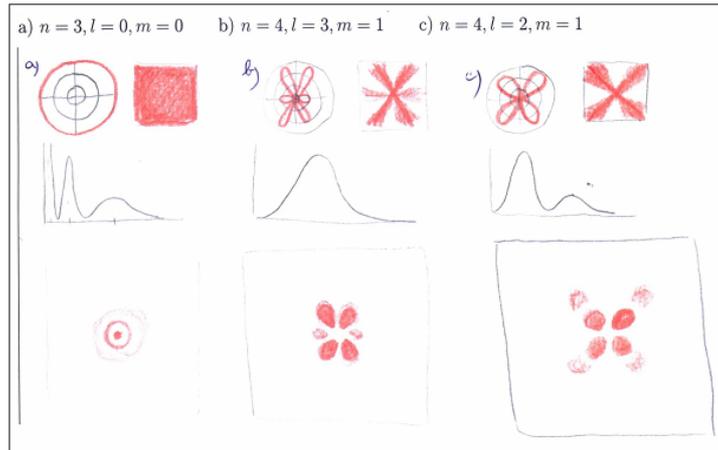
Fig 6: Redrawing task



The used 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. *Orbits* - 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

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



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.

The tasks were designed according to the principles of experiential learning (to be specific, according to the *Kolb's learning cycle*) (Luckner & Nadler 1997). Let's go through the scheme of each part of the workbook. Kolb's stages are indicated in the brackets.

- Firstly, students are asked to play with each program arbitrarily and build up their own hypotheses (on the basis of previous knowledge) on what do the programs draw. (*Concrete experience*) This part should also fulfil their need to play and enjoy the nice pictures before they started 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 others or how to build 3D plot from planar cut. (*Abstract conceptualisation*)
- In the final step they use their "plan" and solve "redrawing" 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 name the pros and cons of different ways of how 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 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) due to the following reasons:

- Students can work on their own pace (it is crucial in the experimentation phase) and come back to previous parts if they needed.

- Working without teacher needs very precise and detailed workbook but minimizes fear of making mistakes. Of course, students could ask tutor (personally or via mail) for help in case of any problem during the whole project.
- It would have been difficult to find enough computers for all students working at one time and not disturbing others.

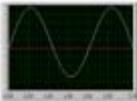
Outcomes: Students' opinions

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 visualisation methods

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

Graphs of angular density of probability



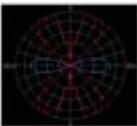
XY Graph

- + **well known** to students
- not connected to spatial distribution of probability density



Intensity Graph

- + a good visualization of spatial dependence
- + the illusive limitation by radius doesn't occur as in the polar graphs
- + it's clear that the **radius can be extended** and the value would be the same
- difficult to read function values



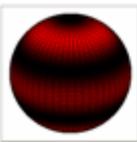
Polar Graph

- + 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!)



3D Polar Graph

- + nicer than 2D, more attractive
- it is difficult to read function values



Sphere

- + gives better view than flat graphs
- impossible to read function values

Graphs of probability density



Planar Cut

- + 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



Spherical Cut

- + 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)

On the base of students' answers 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 all of them.

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 amusing detective story if 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 ("... as late as I had to draw pictures I realized that I didn't understand the explanation well and needed to read it again", "before working with these tools I wasn't able to image what does it mean: 'orbit like sphere inside another sphere'"). Generally they appreciated remembering the spherical coordinates at the beginning and good sequence of sections.

The only negative factor they mentioned was long time they spent with solving the tasks (approx. 4-5 hours, 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 offer the materials available for teachers willing to use this tools and methods. To make them more easy-to-use, we are dividing whole 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 middle school curricula and middle school students (and even teachers) often lack the imagination of orbits. So we are transforming some tasks to this level and preparing 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 orbits

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

Conclusion

It is quite easy to find on the internet various tools for visualizing different parts of the atomic wave functions, probability densities etc. However, most of these sites contain tools that can be used only for visualization. Even after a long search we didn't 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.

If you are interested, you can find all materials on the following address:

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

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