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Discussing fundamental topics of quantum physics using visualizations of bound states

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Abstract. Many authors outlined the students' difficulties in the conceptual understanding of quantum physics. One of the major problems is that students find the mathematical language used to describe these systems (that cannot be seen) generally too obscure. A lot of research has been done to use computer visualizations of quantum mechanical topics and it proved to be a powerful and flexible tool, allowing to see through the mathematics.
In this work it is shown how the use of different visualizations regarding bound states (and in particular the hydrogen atom) may be useful to foster a deeper understanding of topics of very general interest for the study of quantum physics.

1. Introduction

There are many reasons why quantum physics is such a difficult subject both to understand and teach. It is a very abstract subject, and the mathematics used by scientists to describe quantum systems is quite advanced and certainly not accessible at high school level or by a general public's audience (Bao & Redish 2002). The principles and possible interpretations of quantum physics also often oppose the common perception of the world, based on abstractions such as locality and causality. As a matter of fact, it is impossible for students (as for any human) to have any direct experience of the quantum world, and it is difficult – and not without complications – even to refer to pictures, videos or experiments to fill this gap.

Computer visualizations proved to be a flexible and powerful cognitive tool for teaching quantum physics (Catalohlu & Robinett 2002, Dwyer 1972, Gilbert 2005, McCormick *et al.* 1987, Robinett, 2000), as it directly translates complex mathematical equations describing systems that cannot be seen into interactive, visual representations. Teachers may then focus on discussing the physics and the general principles underlying those systems using intuitive and fascinating images to help both developing and memorizing mental models about the discussed topics (Johnston *et al.* 1998, Karplus 1977).

It is very important to be able to develop educational approaches to quantum physics that are based on hands-on activities rather than on a more traditional kind of lecture in which students are simply sitting and passively listening (McKagan *et al*. 2008, Zollman *et al.* 2002), so interactivity play a major role in the design of educational visualizations and simulations. User interfaces and visual representations of the physics need to be research based (McKagan *et al*. 2008) to increase the effectiveness of the activities and, most of all, to avoid misinterpretations and misconceptions that may arise from a bad design. Education research and direct teaching experience help understanding the students' main difficulties and misconceptions, so that they can be the targeted by computer based activities (Kohnle 2012, Kohnle *et al.* 2014). Research based on the sum over paths approach and Geo Gebra simulations has also been made (Malgeri *et al.* 2014).

In this work we focus on ways of presenting topics of very general interest about quantum physics based on visualizations of bound states, and especially on the hydrogen atom (Rosi & Oss 2015). In

fact, the hydrogen atom is a very interesting system to focus on. First of all, it is a very important system for historical reasons and it is mentioned at any level of QM didactics. Most importantly, it is a real system for which simple low-cost experiments may be done (Onorato *et al.* 2015) (differently from square wells or the harmonic oscillator).

2. Fundamental topics that can be discussed

What is a wavefunction? Where is the electron?

First of all, the concept of wavefunction is one of the most important and fundamental ones, as it is a crucial ingredient in connecting theory and experiments, to be able to discuss about measurements, probability, uncertainty and so on (Bao & Redish 2002, Chhabra & Das 2016, Singh 2001). Visualizing a wave function may be a good way to start discussing what it represents: there is no need of using formal mathematical tools and it is possible to focus on the meaning of a probability density.

1D infinite and finite wells are generally discussed and many visualizations regarding them are available (even for the 2D case) (Thaller; Falstad; "PhET"; "QuVis"; "Physlet Quantum Physics"). For example, "Quantum Bound States" by "PhET" allow users to "explore the properties of quantum 'particles' bound in potential wells" letting you see "how the wave functions and probability densities that describe them evolve (or don't evolve) over time".

A very interesting system, the one that we prefer and that we suggest to start with, is the hydrogen atom (Rosi & Oss 2015, Thaller, Falstad, "Hydrogen!", "Atom in a Box"). Students probably already have a mental representation of it – an electron orbiting around a proton – so teachers need to focus on the difference between orbits and orbitals. To help teachers with this, the hydrogen atom orbitals may be seen in classroom, and students can interactively choose which one to see and look at them from different perspectives. Some simple features of the hydrogen atom may easily be seen: for example, it can be noticed simply by changing the quantum numbers that the size of orbitals gets larger as the corresponding energy gets larger too, as shown in Fig. 1.

Presenting hydrogen orbitals may also come in handy when discussing spectroscopy, as it will be seen later.
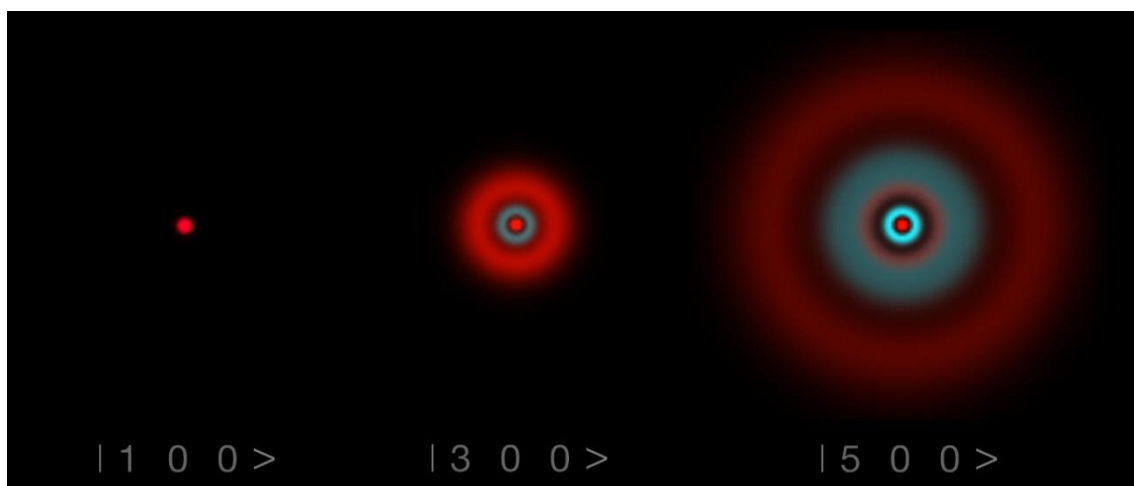

Fig. 1. Examples of hydrogen orbitals (Rosi & Oss, 2015; "Hydrogen!")

The correspondence principle

It is very important to be able to connect the quantum world to the classical results students have being studying all along.

Other authors spent much efforts to show how under the right conditions quantum objects will behave as their classical counterparts e.g. using the sum over paths method: applying this method in the

GeoGebra environment students are able to get results of classical mechanics and geometrical optics working with quantum objects (Malgeri *et al*., 2014).

It is possible to refer to visualizations of the hydrogen atom again to build a bridge between classic and quantum physics, meaning to get an intuitive idea of the Correspondence Principle: in fact, it can be seen that a hydrogen orbital with large quantum numbers resembles a classical orbit (Rosi & Oss 2015, "Hydrogen!", Falstad, "Atom in a Box"), as shown in Fig. 2. Of course it is fundamental to specify the differences between the two models, as in the quantum mechanical orbital the electron is still delocalized over it, a highly non-classical behaviour.
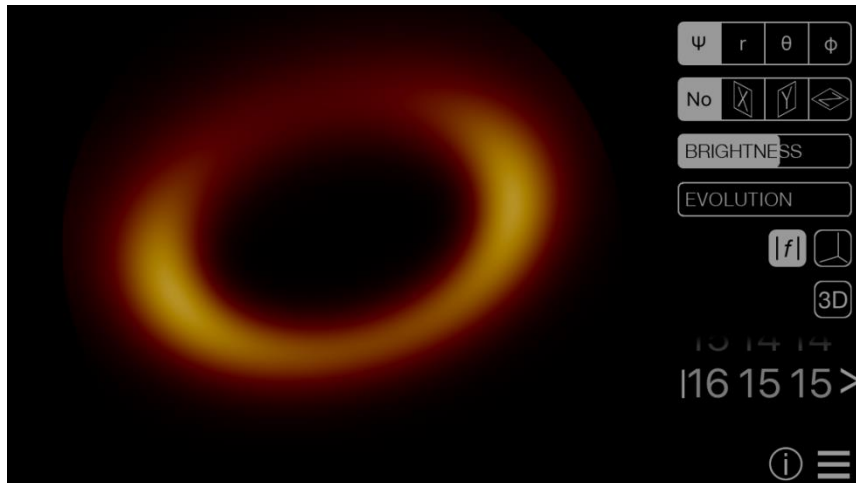

Fig. 2. For large quantum numbers a hydrogen orbital resembles a classical orbit. It is here shown the modulus of the $n = 16, l = 15, m = 15$ orbital (Rosi & Oss 2015, "Hydrogen!")

Superposition and interference
Superposition and interference play major roles in quantum physics. They are the key concepts underneath the double slit experiment which is probably the most cited experiment in introductory quantum mechanics courses. These concepts may as well be discussed using interactive visualizations that allow teachers and students to create superpositions of wave functions and see how they interfere with each other, meaning to visualize the "complex" nature of quantum wave functions. This allows to focus on the difference between classical and quantum probability, analogously to what is done presenting the double slit experiment.

It is possible to create superpositions of states using many different applets (see for example "Superposition states in an infinite square well" from "QuVis" or "Quantum Bound States" from "PhET").

Again, this interference of states may also be seen in the hydrogen atom (Rosi & Oss 2015, "Hydrogen!", Falstad). See for example Fig. 3: here the sum of two orbitals, namely the $n = 3$, $l = 2$, $m = -2$ and the $n = 3$, $l = 2$, $m = 2$ is shown on their right. Interestingly, in some regions the summed orbitals cancel out and the result goes to zero (destructive interference) while in others the result is larger than the starting orbitals (constructive interference). A more advanced subject may also be the representation of a particle in a harmonic potential using superpositions of the 2D harmonic oscillator eigenfunctions (Falstad).
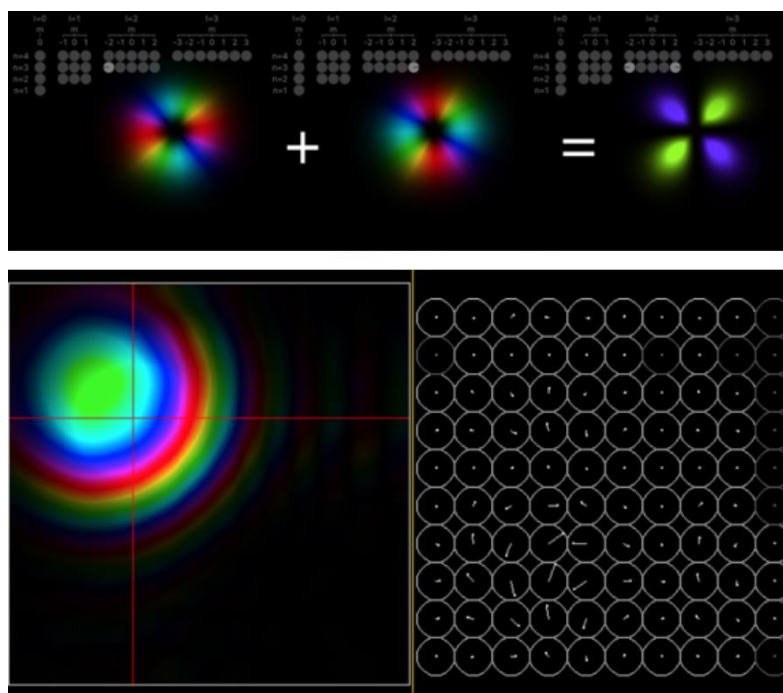
Fig. 3. Examples of visualisations of superpositions. (Top) Interference between two hydrogen orbitals (Rosi & Oss 2015, "Hydrogen!"). (Bottom) Simulation of a particle in a two dimensional rectangular square well (Falstad)

Stationarity and non-stationarity

The time evolution of such superpositions (and their moduli) may be a challenge to imagine, but they certainly may be visualized. Choosing appropriate superpositions it is straightforward to visualize the conceptual meaning of the difference between a stationary and a non-stationary state. For example, in Fig. 4 it is shown the time evolution of the modulus of a linear combination of three hydrogen orbitals with different energies: since the linear combination results in a non-stationary state (the rate of the rotation of the phase of the orbitals is proportional to their energy), its shape changes in time. The shape of a stationary state (for example of a single orbital) instead, never changes in time.
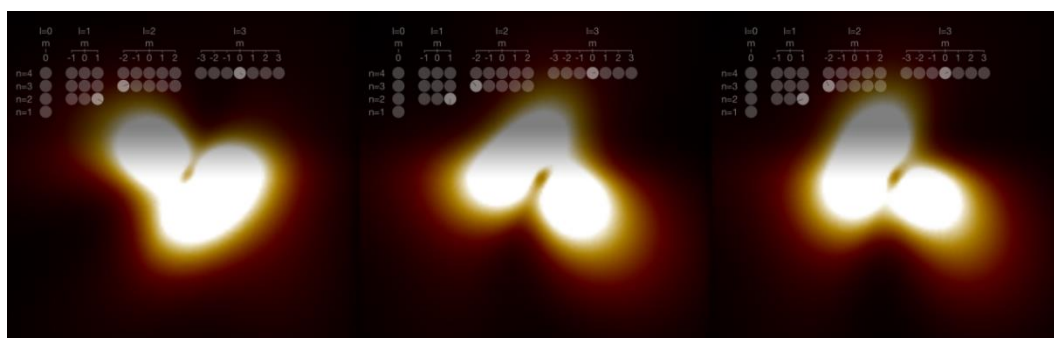

Fig. 4. The modulus of a superposition of states with different energies may be visualised to see the evolution of a non-stationary state (Rosi & Oss 2015, "Hydrogen!")

Permitted transitions and spectroscopy

Energy quantization and energy level diagrams can be confusing for students, and it is often counter-intuitive for them to accept that energies of photons coming from a lamp depend on the energy differ-

ence between two levels (Zollman *et al*. 2002). It can be really rewarding to do some spectroscopy experiments and then use software visualizations to help them understand how energy levels models can correctly explain their observations ("VQM"; "Hydrogen!"; "PhET"; "Physlet Quantum Physics", "Atom in a Box"). For example, the "Emission Spectroscopy" applet from "VMQ" (shown in Fig. 5, on the left) allows students to look at spectra of different gas lamps and to interactively adjust energy levels to try to get the correct transitions by trial and error. On the right of the same figure, instead, the "Dipole Transitions" mode of "Hydrogen!" is shown, in which for a chosen starting orbital all transitions allowed by selection rules are displayed. With this mode it is possible to see, for example, that the 2s state cannot have any orbital with lower energy for which a dipole transition exists: this is why it is a so-called "metastable state", meaning that it has a longer lifetime than the other excited orbitals.
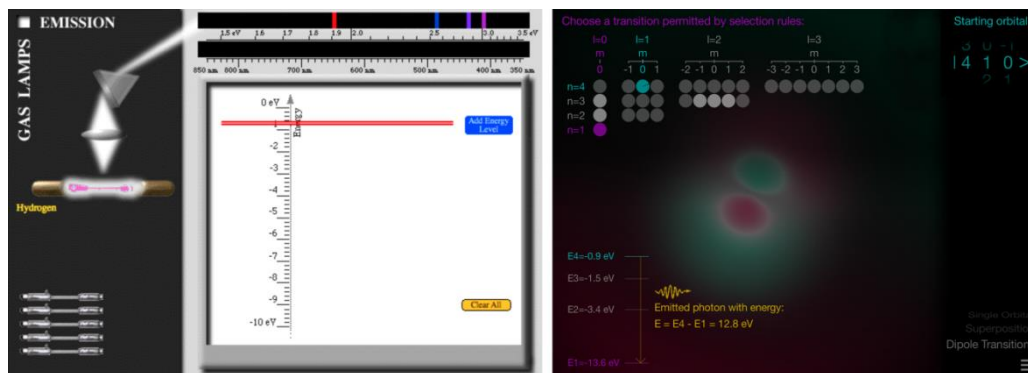

Fig. 5. Visualisations may be useful to understand theoretical models based on energy levels, especially when used after some spectroscopy in the laboratory has been done. (Left) "Emission Spectroscopy" applet from "VMQ" (Zollman *et al*. 2002). (Right) "Dipole Transitions" mode of "Hydrogen!" (Rosi & Oss 2015, "Hydrogen!")

3. Conclusions

We showed how the use of visualisations regarding bound states may be useful to discuss many topics of very general interest for the study of quantum physics. Particular attention was paid for visualisations of the hydrogen atom, a very important system of which some simple, low-cost experiments may be done in classroom.

First of all, visualisations are helpful in introducing the concept of wave functions, helping to focus on their link with probability density. For example, using the hydrogen atom, the teacher may focus on the difference between classical orbits and orbitals, and thus the importance of reasoning in terms of probability when dealing with quantum objects.

The capability of interactively creating superpositions of states is really helpful as students may see the influence of interference on such superpositions, analogously to what happens in the double slit experiment. Visualizing the time evolution of superpositions also allow to get an intuitive idea of the difference between a stationary and a non-stationary state.

An intuitive idea of the Correspondence Principle may also be given looking at a single hydrogen orbital with large quantum numbers, as it becomes more and more similar to a classic circular orbit as its corresponding quantum numbers get larger and larger (even though particular care must be put in emphasising the differences between the two models that still exist).

As a last example, the so-called "permitted transitions" of the hydrogen atom may be displayed, allowing to take a further step in the exploration of the discrete–dominated world of bound states. It was also pointed out that as this subject is discussed, it can be very rewarding to also do some spectroscopy in the laboratory, so that a bridge between experimental observations and theoretical models can be built, as such bridges can play a very important role in the learning process.

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