Simulation programs for teaching quantum mechanics

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Abstract

Fundamentals of quantum mechanics are part of most physics curricula for engineering students. For the teacher this is a quite nontrivial didactical task, since the mathematical tools necessary for a deeper understanding are much too advanced and the phenomena themselves are mind-boggling. Simulation programs can be useful here by illustrating the behaviour of quantum mechanical systems and allowing a hands-on approach. Several example applets will be presented that solve the two-dimensional Schrödinger equation to help understand notions like uncertainty, the tunnel effect and energy eigenstates.

Quantum mechanics for engineering students

Fundamentals of quantum mechanics are a standard part of the physics education for engineering students. Since the mathematical tools necessary for the description of quantum systems are too advanced, teachers have to resort to some basic ideas and presentation of results without derivations. Furthermore due to the often perplexing quantum phenomena students have problems to create any intuitive pictures or to make contact to their knowledge about "classical" systems.

To remedy this situation several authors have produced tools to simulate and visualise quantum systems, among them two very comprehensive packages: Physlet Quantum Physics (Belloni (2006)) and the Visual Quantum Mechanics project (Thaller (2000)). The first provides a large number of simulation programs ready for interactive use in the form of applets embedded in web pages, the second consists of an overwhelming set of animations describing mostly two-dimensional systems on a high level.

Especially the two-dimensional examples are very helpful since they can be compared to standard wave tank simulations. Studying a properly chosen set of examples the students can understand, where classical pictures still work, and where they have to be modified by new ideas, most importantly the uncertainty relation. Unfortunately most of the Physlets present one-dimensional systems – the few exceptions relying on analytical solutions – , whereas the animations from Thaller (2000) are not interactive. This restriction is due to the large amount of computations necessary for a numerical solution of the Schroedinger equation.

But with better algorithms and the always growing performance of standard PCs the situation has changed. As part of the PhysBeans project (Junglas (2008)) programs have been developed that compute the solution of the 2d Schroedinger equation in "real-time", i.e. as fluently running animations with variable parameters. The example applets presented in the following will show how they allow a hands-on approach to several standard topics of a quantum mechanics course.

Simulating the Schrödinger equation

The Schroedinger equation describes the time evolution of the wave function ψ(x,t) of a particle in $\mathbf{R}^n$ in a potential V(x). In properly chosen units it reads

$$H \psi(x,t) = i \frac{\partial}{\partial t} \psi(x,t)$$

with the Hamilton operator

$$H = \frac{1}{2}\left(\frac{\partial^2}{\partial x_1^2} + \ldots + \frac{\partial^2}{\partial x_n^2} \right) + V(x)$$

One is mainly interested in solutions $\psi \in \boldsymbol{L_2}(\boldsymbol{R^n})$ with an $\mathbf{L}_2$-norm of one. The square of the absolute value |ψ(x,t)|² can then be interpreted as the probability distribution of the particle.

The algorithm for the numerical solution of the Schroedinger equation used in the applets is based on the method given in DeRaedt (1994). To get rid of reflections at the boundary it has been augmented by a PML boundary layer (Antoine (2008)). More details about the implementation are given in Junglas (2009). The visualisation of complex wave functions is a non-trivial task, which is discussed extensively in Thaller (2000). Its author favours a clever combination of amplitude and phase representation. The interactivity of the programs presented here allows for a more straight-forward approach: The user can switch between several representations (real/imaginary part, absolute value, square of the absolute value, phase) to get the most information from the wave function.

Example Applets

The following programs are all built up from the same elements:
- a display showing the two-dimensional wave function for immediate qualitative understanding of the phenomena,
- a graph of the wave function along a line in the x-y plane, allowing to make accurate "measurements", or alternatively values of some observables as functions of time.
- a set of input elements for changing physical or visualisation parameters and control of the simulation.

The free particle

The first example shows the behaviour of a Gaussian wave packet with given initial position, velocity and width. This is as close to the intuitive picture of a slightly "smeared" particle as one can get. The time evolution shows mainly the classical behaviour: The packet moves along a straight line with the given velocity. Quantum mechanics shows up in the spreading of the wave function which is due to the range of velocities that are inherent in the Gaussian.The spreading gets faster with smaller initial

width. In a hands-on session the students are asked to quantify this behaviour, which leads to a first glimpse at the Heisenberg uncertainty relation.

The uncertainty relation for a free particle

After the notions of position and momentum uncertainty have been introduced, the next program displays their explicit values as functions of time for the Gaussian wave packet. Here the students can experiment with the packet to find the minimal "combined" uncertainty $\Delta x \cdot \Delta p$ and thereby reproduce the Heisenberg relation. One could use additional programs with different initial functions to show the distinctive minimisation properties of the Gaussian wave packet.

Another point to notice here is the behaviour of the displayed values when the wave function leaves the simulated area: The uncertainties drop to much too small values, which violate the uncertainty relation. This is an artefact of the numeric algorithm, which can only use the part of the wave function still inside the computed area.

This observation can be a good starting point to discuss intrinsic limitations of simulation programs. On the other hand it can be too demanding for students who already struggle with the peculiarities of quantum mechanics. For that reason it might be a good idea to introduce a stop time and to constrain the parameters of the program accordingly. Due to the modular structure of the programs and the availability of the source code this can be done easily (Junglas (2008)).

The double-slit

The famous double-slit experiment is especially bewildering when done with single photons. This applet shows what happens with a single electron – modelled as usual by a Gaussian wave function – that is going through a double-slit (cf. Fig. 1).

The resulting simulation shows a wealth of features: First one notices an interference pattern in front of the slits that is due to reflections. The students are already familiar with this behaviour from a previous example. Next one sees two "bubbles" coming up immediately behind the slit, which is more or less what one would expect. But after a while a third bubble appears in the middle, which together with the other two develops into the well-known interference pattern at the screen.

To better understand where this central part comes from, one can study the example again, this time looking at the real part of the wave function instead of the absolute value. The emerging pattern should be familiar from classical wave theory, it resembles the diffraction pattern stemming from Huygens principle and shows how the central maximum is produced by "bending around the corner".

Many more interesting features can be studied by varying the parameters. Most important probably is the increase of the number of maxima with rising particle velocity, which is best seen in the backwards scattering. Classically this comes as a surprise, but a moments (quantum-mechanical) thought reveals the cause: With rising velocity – and therefore momentum – the Compton wavelength of the electron

decreases, which leads to smaller scattering angles, just as in classical wave theory. Again, this can be seen directly in the real part image.
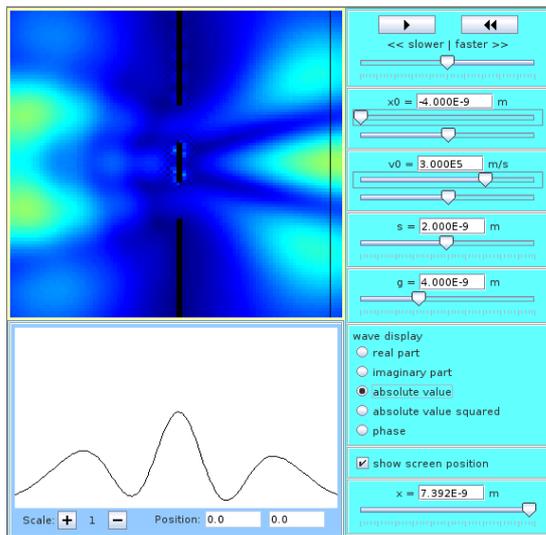
Figure 1: Double slit
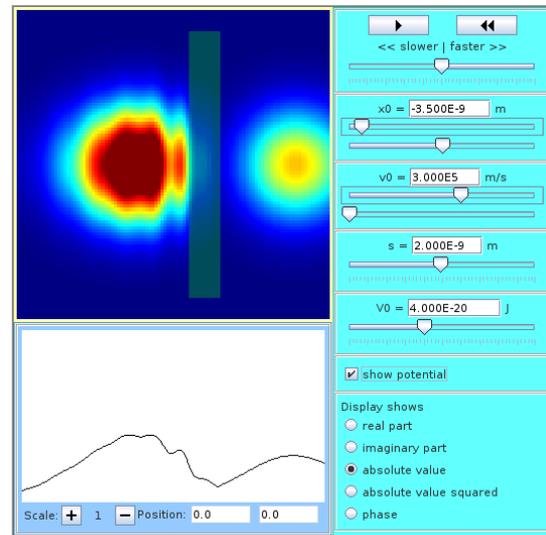
Figure 2: Potential barrier

Particle running against a potential barrier

The next example deals with a particle running against a potential barrier (cf. Fig. 2). The simulation shows the splitting of the wave function into a transmitted and a reflected part. Thinking of EPR and entangled states it might be tempting to expand here on the interpretation of a "bilocalised" state, but this is probably too advanced and causes more confusion than it provides deeper understanding. Therefore the situation is interpreted only in a statistical way.

In exercises students try to "measure" the transmission coefficient as function of the incoming velocity or the potential. The results are compared to the classical situation, which leads to the discovery of quantum tunneling.

Eigenfunctions of the 2d Coulomb Hamiltonian

Understanding the eigenstates of the hydrogen atom provides the basis of the modern understanding of atoms, including the whole of chemistry and material sciences. Therefore it is one of the major goals of an exposition to quantum mechanics. Unfortunately it is not so easy with its complicated scheme of quantum numbers and complex spherical harmonics.

Here, the two-dimensional Coulomb potential comes in handy: Its eigenfunctions are much simpler and easier to visualise, but share many features with its famous 3d-cousin. The energy level is given by a "main quantum number" n, the quantisation of the angular momentum L_z leads only to one additional quantum number m with simple eigenfunctions and $m < n$.

These properties can be studied with an applet, which allows to enter values for n and m and displays the corresponding eigenfunction (cf. Fig. 3) . The restriction m < n is not enforced by the design of the user interface, instead an invalid choice produces a blank screen in order to draw the student's attention to the restriction. In addition one can enter an arbitray real value for the central charge. This is a simple way to scale the image and to provide a better resolution of the central parts.

The time evolution shows the constance of $|\psi|^2$, the images of the real or imaginary part simply rotate – at least for some values of n and m. Unfortunately one easily runs into numerical problems here: If the function extends to the border, one gets boundary reflections; if it extends into the center, all kinds of artefacts show up, since the grid is too coarse to properly cope with the 1/r potential. Again, this can be turned into an advantage by making the students aware of the limitations of the simulation.
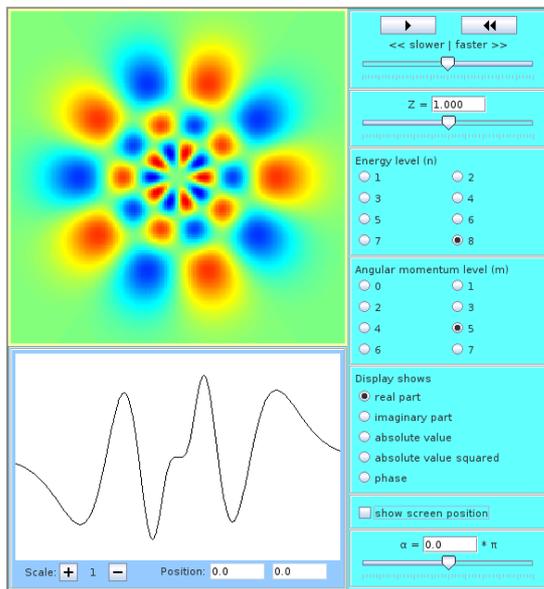
Figure 3: Coulomb eigenfunction
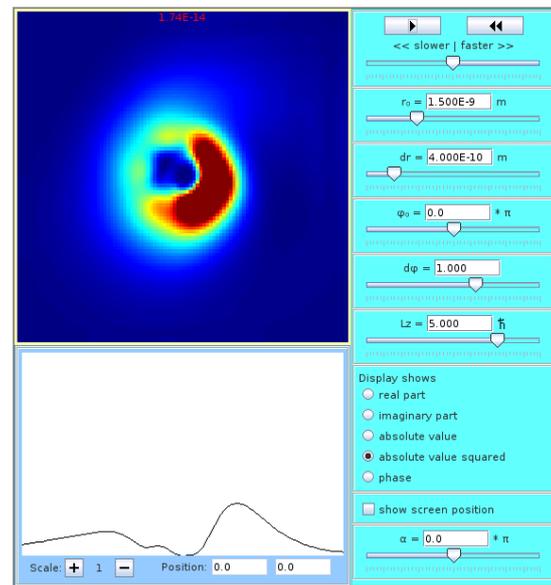
Figure 4: Coulomb "particle" state

"Particle" states in the 2d Coulomb potential

The last simulation (cf. Fig. 4) tries to transfer the notion of a "classical particle" to the Coulomb case. Preliminary experiments with a Gaussian initial state show a rather complicated behaviour, which bears very little resemblance to a classical picture. If one uses a gaussian spreading in polar coordinates instead, the results are more amenable to a quasi-classical interpretation.

The default parameters define a state that is concentrated around a given radius and spreads over a rather large angle. Furthermore it has a given mean angular momentum, which corresponds roughly to that of an eigenfunction that is concentrated in the same radial region. Starting the simulation one sees mainly a rotation around the center, combined with a spreading in angular direction, until almost a whole annulus is filled up. This could vaguely be interpreted as a classical circular motion combined with a

spreading caused by the uncertainty in L_z. The students can work this out further by measuring the orbital period and compare it with the given value of L_z.

For larger values of L_z the wave function rapidly moves outwards, like a classical particle would do. For much smaller L_z it approaches the center, where strange things happen, only partly because of the inaccurate simulation. If one tries to concentrate the particle in radial or angular direction, it blows up rapidly – the uncertainty relation takes its toll!

Conclusions

The simulation programs presented here demonstrate the general behaviour of wave packages and illustrate some basic notions of quantum mechanics. Furthermore they provide a set of examples, on which a first intuition about quantum behaviour can be based. Finally they show how previous knowledge about classical behaviour (of particles *and* waves) can be put to good use if one augments it by the uncertainty principle.

An important feature is the two-dimensionality of the examples: On the one hand the corresponding animations are more easily interpreted as the graphs of one-dimensional functions, on the other hand they allow for generic 2d-examples like the double-slit or the Coulomb problem.

The set of examples will be expanded in the near future to cover the standard situations discussed in introductory courses. Further extensions will be the simulation of the measurement process (or better: models thereof), the addition of electric and magnetic fields and of the electron spin. All programs are provided under standard open source conditions and can be downloaded from the PhysBeans homepage (Junglas (2010)).

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