Open Source and Open Access Resources for Quantum Physics Education

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Quantum mechanics is both a topic of great importance to modern science, engineering, and technology, and a topic with many inherent barriers to learning and understanding. Computational resources are vital tools for developing deep conceptual understanding of quantum systems for students new to the subject. This article outlines two projects that are taking an open source/open access approach to create and share teaching and learning resources for quantum physics. The Open Source Physics project provides program libraries, programming tools, example simulations, and pedagogical resources for instructors wishing to give a rich experience to their students. These simulations and student activities are, in turn, being integrated into a world-wide collection of teaching and learning resources available through the Quantum Exchange and the ComPADRE Portal to the National Science Digital Library. Both of these projects use technologies that encourage community development and collaboration. Using these tools, faculty can create learning experiences, share and discuss their content with others, and combine resources in new ways. Examples of the available content and tools are given, along with an introduction to accessing and using these resources.

Since its inception in the 1920's, quantum mechanics has been essential for advancements in fields that require an accurate description of atomic and sub-atomic phenomena. Advances in atomic, nuclear, and solid-state physics and most of chemistry are a direct result of our understanding and application of quantum mechanics. The laser is an obvious practical example. The ubiquitous solid state laser is based on simple quantum principles. These quantum systems now appear in grocery stores (scanners), operating rooms (laser surgery), entertainment devices (CD and DVD players), and even toys for pets. Similarly, the understanding of quantum theory is crucial for medicine with the advent and use of modern diagnostic techniques (*e.g.* PET scans and MRIs) based on quantum phenomena. Modern electronic devices, advanced nano-structure materials, and the latest in cryptography are all examples of how quantum theory is relevant to technology.

The importance and relevance of quantum theory is reflected in the physics and chemistry curricula. Students see aspects of quantum mechanics in their introductory, intermediate, and advanced courses. The teaching of quantum mechanics at the introductory level is as important as the advanced level because of the audience. For many students, this will be the only time that they will have a chance to learn about the science responsible for many of the products that shape their lives. Of course, for the physics and chemistry students who will become the scientists of the future, understanding quantum theory is essential for making new fundamental and applied discoveries.

Despite the importance of quantum theory, its teaching and learning is a difficult endeavor. To develop a conceptual "feel" for quantum systems, students must grasp the properties and time evolution of abstract objects and operators in an abstract vector space and then connect them to familiar measurable quantities such as position or energy. The most basic quantum dynamics is challenging because of the two very different and non-trivial time dependences of the theory; that of an isolated quantum system and that of "observations". Providing help for students trying to understand these systems, and faculty teaching them, is the goal of the projects described in this article.

I. Time-Dependence: A Learning Challenge

In quantum courses, "time dependence" often refers to the deterministic evolution governed by the Schrödinger equation. This separable partial differential equation is usually solved by finding eigenstates of the spatial term, the time-independent Schrödinger equation (TISE), then incorporating the time-dependent phase $\Psi_n(r,t) = \psi_n(r)e^{-iE_n t}$. The solutions to the TISE, the energy eigenstates, contain the physics of the problem including boundary conditions, potentials, and interactions. Any arbitrary state can be constructed from a superposition of energy eigenstates:

$$\Psi(\mathbf{r},t) = \sum_{n=1}^{\infty} c_n \psi_n(\mathbf{r}) e^{-iE_n t/\hbar} \qquad (1)$$

A fundamentally different time dependence is the result of measurements on a quantum-mechanical system and is much more abstract. The canonical interpretation of quantum theory holds that the time evolution due to measurements, the change in the system and measuring device from before the measurement to afterwards, is fundamentally probabilistic. An energy measurement on an ensemble of quantum systems, all in the state given by Eq. (1), will yield the results E_n with the probabilities $|c_n|^2$. With the measurement, the wave function "collapses" into the corresponding energy eigenstate. Measurements of other quantities yield similar changes in quantum systems, and differences in eigenstates of incompatible observables result in uncertainty relations.

It is important for students to build a cohesive mental model of quantum dynamics to understand the complex nature of quantum-mechanical time evolution and measurement. This model building is complicated because of our unfamiliarity with the quantum world. Styer has pointed out that if proper and correct quantum visualizations are not presented to students, they create incorrect visualizations that hinder their understanding of quantum-mechanical systems [Styer, 2000]. If used well, simulations that properly display quantum-mechanical time development and the results of quantum-mechanical measurement play an important role in the teaching and learning of quantum theory. Pedagogy that integrates these simulations with student activities and assessments is the key to helping students build an understanding of quantum phenomena.

2. History and Research on Pedagogical Simulations in Quantum Mechanics

Computer-based visualizations can play an important pedagogical role in the teaching of physics on a variety of levels and topics [Dancy and Beichner, 2005; Finkelstein et al., 2005] and quantum mechanics is no exception [Belloni and Christian, 2003]. The use of computers to display quantum-mechanical dynamics began in 1967 when Goldberg and his collaborators [Goldberg et al., 1967] created one of the first computer-generated images of the scattering of Gaussian wave packets off of wells and barriers. Probability densities were computed, displayed on a cathode-ray tube, photographed, and the successive frames turned into a movie. Later the "picture" books of Brandt and H. Dahmen [Brandt and Dahmen, 2001] and the *Visual Quantum Mechanics* books by Thaller [Thaller, 2000] continued this approach, including more scenarios depicting time development with successive images or using *QuickTime* movies, respectively. Michielsen and De Raedt have developed a web-based tutorial using similar animations to illustrate the theory [Michielsen and De Raedt, 2008].

Although these illustrations provide students with a new and unique view of quantum systems, they are limited because the student can neither change the dynamics nor get a sense of the underlying calculations. The transition from movies to user-controlled simulations was accomplished by the Consortium for Upper-level Physics Software (CUPS) Series quantum mechanics book by Hiller, Johnston, and Styer [Hiller et al., 1995], and more recently by the book *Physlet Quantum Physics* [Belloni et al., 2006]. Both use computer-based interactive simulations to aid students' conceptual understanding. Zollman and co-workers used computer-based experiments as part of a curriculum to introduce quantum physics to high school teachers and students [Zollman et al., 2002]. More recently the Open Source Physics Project (OSP) has created dozens of simulations for the teaching of quantum mechanics based on open source Java programs. While there are many other programs, applications, and applets available simulating quantum mechanics, these particular efforts are noteworthy because of the close connections between simulations, learning goals, and student activities. Teaching with technology but without a sound pedagogy is unlikely to yield significant educational gain [Beichner, 1997]. Without help, students view computer simulations uncritically and do not assess the simulation's validity and conceptual foundation [Chi et al., 1981; Larkin et al., 1980; van Heuvelen, 1991]. Pedagogy and assessment are important for productive use of these computational resources.

The goal for pedagogical quantum simulations is to improve the conceptual understanding of quantum mechanics that is surprisingly lacking in students at all levels [Singh et al., 2006]. The methods of physics education research (PER) have been used to investigate difficulties in student learning in quantum courses [Zollman, 1999; Singh, 2001; Wittmann et al, 2003; Singh, 2004; Singh, 2005; Styer, 1996]. Studies have shown that in physics and chemistry courses there is very little difference between undergraduate and graduate conceptual understanding of quantum mechanics [Cataloglu and Robinett, 2002]. Students, regardless of their background and level, struggle to grasp quantum time development and measurement. What they do understand, such as the time dependence of energy eigenstates, is often inappropriately generalized to more complicated situations, such as the time dependence of superpositions of energy eigenstates.

PER researchers are creating materials aimed at improving student understanding and computer simulations are playing a central role. For example, researchers from the University of Maryland and University of Maine [Wittman et al., 2002; Bao and Redish, 2002] have developed twelve group-learning tutorials as part of their *New Model Course in Quantum Mechanics*. These tutorials make use of simulations including Physlets [Belloni, 2006]. While PER is making strides in this field, results suggest that the techniques and technology used in introductory or modern physics for teaching quantum mechanics need to be augmented to more properly represent the specialized nature of the teaching of quantum mechanics to more sophisticated students.

This article describes Open Source Physics (OSP), an effort to improve pedagogical software for intermediate and advanced classes, and the resources for quantum mechanics education that are being developed as a part of this effort. The guiding paradigm is similar to much of modern software development; that an open community using and developing a code base is more efficient and effective than a small, closed group of programmers. This open access approach is as important for the reuse and repurposing of the pedagogical resources connected with the simulations as it is for the computer code. Students and teachers need resources that they can tailor to their needs and specific learning context. Physlets, scriptable java applets for introductory physics topics, provide an example of the power of tools designed for reuse [Christian and Belloni, 2001; Christian and Belloni, 2004]. Although not open source, the built-in javascript connections of these programs have made them a world-wide standard for the creation of simulation-enabled curricular pedagogies. The work of Duffy [Duffy, 2008] and Schneider [Schneider, 2008] are examples.

To be effective, these resources must be disseminated as widely as possible to encourage access, sharing, and development. The ComPADRE Pathway of the National STEM Digital Library (NSDL) is helping in this effort. ComPADRE provides an online catalog of educational resources, almost all open access materials, where developers, educators, and students can share their work, rank and comment on materials in the catalog, and build personal collections that meet their own needs. Built on top of this catalog are specialized collections of materials designed for particular groups of users. The Quantum Exchange, an online collection of learning resources for quantum physics, makes use of many of the resources described here. The OSP quantum materials are an important part of the Quantum Exchange and, at the same time, ComPADRE and the Quantum Exchange can help disseminate the OSP results. Furthermore, through ComPADRE, the OSP resources are shared with the NSDL and connected to ComPADRE's four professional society sponsors, the American Association of Physics Teachers, the American Physical Society, the American Astronomical Society, and the Society of Physics Students, providing greater opportunities for attracting attention to these high quality quantum education resources. In fact, ComPADRE has recently created a collection specifically for all OSP materials to take advantage of the library's database, library, and dissemination tools.

3. Open Source Physics: Overview of Project, Library, Tools, and Examples

The Open Source Physics (OSP) project promotes the innovative and effective uses of computation, computer-based curricular materials, and computer modeling through the integrated use of open source programs and models. Our material is based on (1) a consistent object-oriented Java library that is distributed under the GNU General Public License (GPL), (2) a computational physics textbook that uses a physics-first approach to motivate numerical algorithms and computer programming, and (3) high-level authoring and modeling tools that allow non-programmers to build, explore, edit, and distribute ready to run models. Although the modeling instruction method [Hestenes, 2008] can be used without computers, the use of computers allows students to study problems that are difficult and time consuming, to visualize their results, and to communicate their results with others. The combination of computer programming and modeling, theory, and experiment can achieve insight and understanding that cannot be achieved with only one approach.

The OSP library is the basis for OSP curricular material. The library contains numerical methods, user-interface components, visualization tools, and an XML framework. The library's source code and numerous examples are distributed under the GNU General Public License (GPL). *An Introduction to Computer Simulation Methods* by Harvey Gould, Jan Tobochnik, and Wolfgang Christian [Gould et al., 2007] uses this library to teach programming in the context of learning physics. This book does not discuss syntax or programming for its own sake but stresses the science and encourages student experimentation. The development of good programming habits is done by example.

It is not necessary to become expert in programming to use the programs in *An Introduction to Computer Simulation Methods.* Compiled versions of these programs are available and run on any Java-enabled computer. In addition, we are currently modifying and adapting these programs for use in other contexts. For example, we have created a suite of programs based on algorithms described in the book to help students develop an understanding of the time dependence of quantum mechanical states. These programs are based on the superposition principle outlined in Eq. (1). The simplest is called **QM Superposition** and is shown in Figure 1. It displays the time evolution of the position-space wave function, $\Psi(x,t)$, using an energy eigenstate expansion. In the example shown in Figure 1, the simulation shows a two-state superposition in a harmonic oscillator, $V(x)=x^2/2$. Because time-dependent wave functions are complex, the program must display complex functions. We depict the

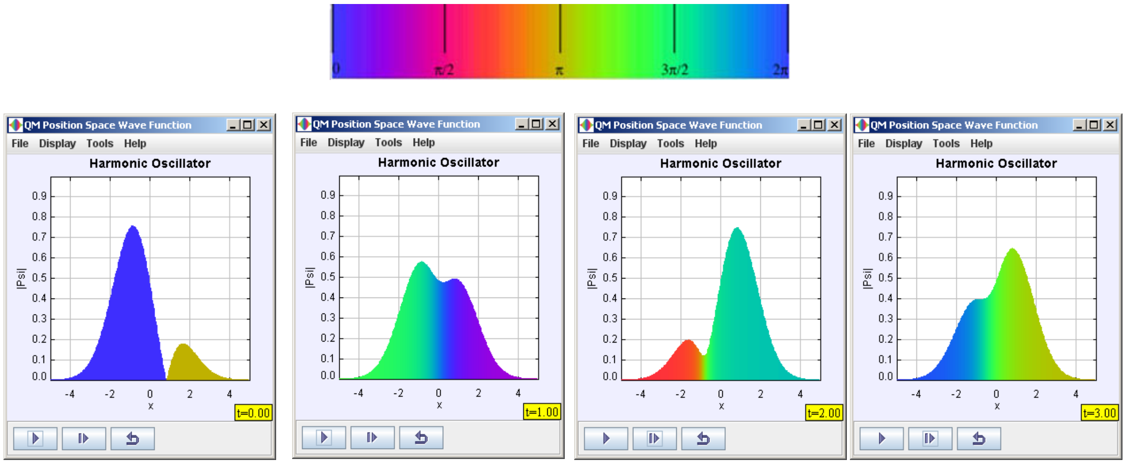

Figure 1: *The QM Superposition program showing the wave function for a two-state superposition in a harmonic oscillator. The initial state and potential energy well can be customized to almost any state or well. The legend at the top maps the color of the wave function into phase of the complex functions. This program is available at: http://www.compadre.org/OSP/items/detail.cfm?ID=6798 .*

phase of the wave function with the colors shown on the color strip. The simulation is controlled by three buttons, play/pause, step, and reset.

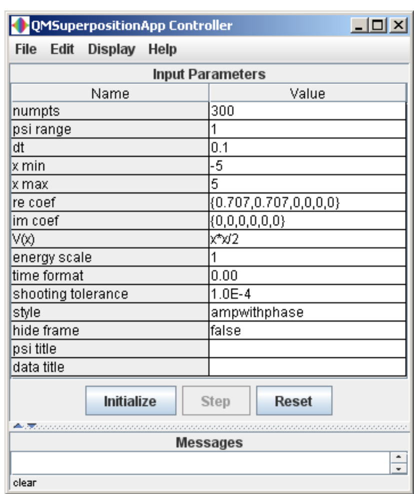

Figure 2: *The QM Superposition control panel allows parameters to be changed and saved. The Initialize button switches the program to run mode where the buttons change to Run, Step, and New. The New button allows the user to enter new values and re-run the simulation.*

The **QM Superposition** program can be customized to show different superposition states in different potential energy functions. The **Display | Switch GUI** menu item changes the user interface as shown in Figure 2. The energy eigenfunctions and energy eigenvalues are determined based on the user-defined potential energy function, $V(x)$. Besides arbitrary functions, there are hard-coded analytic solutions provided for the infinite square well (**well**), harmonic oscillator (**sho**), and the infinite square well with periodic boundary conditions (**ring**). Depending on the potential energy function and the set of expansion coefficients provided, a superposition is created and the dynamics of the state displayed.

To enable the creation and sharing of a wide range of pedagogical exercises, OSP programs save their data in XML data files that can be examined and edited by users. For example, the parameters in Figure 2 can be stored and then loaded into the simulation at another time. Listing 1 shows how the wave function expansion coefficients for **QM Superposition** are set in the relevant property tags. The names of properties match the physics so that their meaning is easily deduced. The ease with which these programs can be modified means that they can be adapted for other uses, for example in an introductory or physical chemistry course.

```
<?xml version="1.0" encoding="UTF-8"?>
<object class="org.opensourcephysics.controls.OSPApplication">
   <property name="control" type="object">
   <object class="org.opensourcephysics.controls.AnimationControl">
      <property name="initialize_mode" type="boolean">false</property>
      <property name="numpts" type="string">300</property>
      <property name="psi range" type="string">0.1</property>
      <property name="dt" type="string">0.1</property>
      <property name="x min" type="string">-5</property>
      <property name="x max" type="string">5</property>
      <property name="re coef" type="string">{0.707,0.707,0,0,0,0}</property>
      <property name="im coef" type="string">{0,0,0,0,0,0}</property>
      <property name="V(x)" type="string">sho</property>
      <property name="energy scale" type="string">1</property>
      <property name="time format" type="string">0.00</property>
      <property name="style" type="string">phase</property>
      <property name="hide frame" type="boolean">false</property>
   </object>
   </property>
   <property name="model" type="object">
   <object class="org.opensourcephysics.davidson.qm.QMSuperpositionApp"/>
   </property>
</object>
```

__Listing 1:__ An XML description of a quantum-mechanical superposition. Pairs of opening and closing property tags specify initial conditions such as the wave function's real and imaginary expansion coefficients.

Additional programs based on the superposition principle are available. For example, there are four OSP programs that simulate quantum-mechanical measurements. The program shown in Figure 3, **QM Measurement**, simulates the measurement of energy, position, or momentum. The other three programs only allow the measurement of one observable (e.g. just energy). The measurement of energy is done exactly, with the result of the measurement determined by the amplitudes of the energy eigenstates. The measurements of x and p are done to a finite uncertainty that can be changed. An ensemble measurement on identical states can be performed using the reset button, which resets the simulation back to its original state. This simulation is pedagogically powerful because, after measurements, the program displays the time evolution of the position-space wave function, $\Psi(x,t)$, using an energy eigenstate expansion and the momentum-space wave function, $\Phi(p,t)$, using a Fourier transform. Students easily see the differences in the results of measurements.

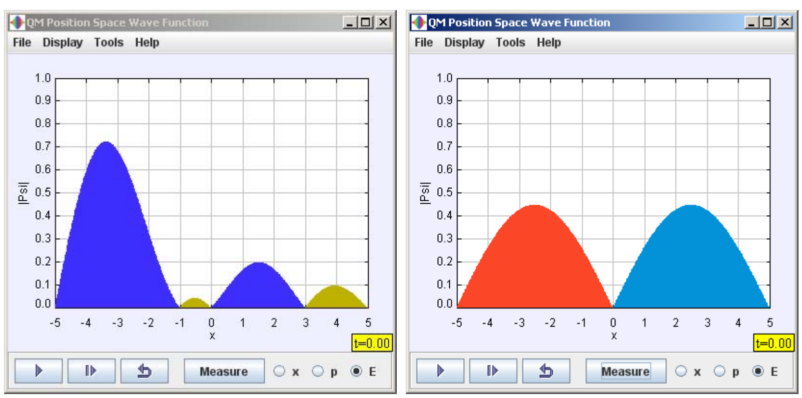

__Figure 3:__ The QM Measurement program showing the position-space wave function and the interface for measuring E, x, or p. The initial state and potential energy well can be customized to almost any state or well. The initial state (left) has its energy measured, collapsing it into an energy eigenstate (right). This program is available at: <u>http://www.compadre.org/osp/items/detail.cfm?ID=6814</u>

Additional programs share the same interface but model other quantum-mechanical concepts and display different data. These concepts include:

- **Probability** which adds a graph showing the probability density
- **Expectation X** which adds a graph showing the expectation value of position

- **Expectation P** which adds a graph showing the expectation value of momentum
- **Carpet** which adds a space-time graph of the wave function dynamics
- **FFT** which adds a graph of the wave function in momentum space
- **Momentum Carpet** which adds a momentum-time graph of the wave function dynamics
- **Wigner** which adds a graph of the quasi-phase space (x-p) distribution

A second approach to using OSP material is to use a high-level authoring and modeling tool that builds programs with minimal programming. *Easy Java Simulations* (EJS) [Esquembre, 2008] is an Open Source Physics application that enables both programmers and novices to quickly and easily prototype, test, and distribute packages of Java simulations. It is well suited for education because it is simple to use and combines authoring with powerful modeling tools. Its dynamic and highly interactive user interface greatly reduces the amount of programming required to implement an idea. Even experienced programmers find EJS useful, because it is faster and easier to:

- Develop a prototype of an application in order to test an idea or algorithm,
- Create user interfaces without programming,
- Create models whose structure and algorithms non-programmers can inspect and understand,
- Encourage students or colleagues (who may be new to Java) to create their own simulations,
- Quickly prepare simulations to be distributed as applets or as standalone programs,
- Create a package containing multiple programs and the associated curricular material.

Figure 4 shows an EJS simulation of quantum mechanical tunneling through a Dirac delta function potential. Delta function tunneling can be described analytically but the resulting wave function is difficult to visualize without animation. The amplitude and phase of the state vary in both space and time. Well-designed computer models showing analytical solutions are useful because they reinforce the mathematics and provide feedback about the model's correctness and applicability.

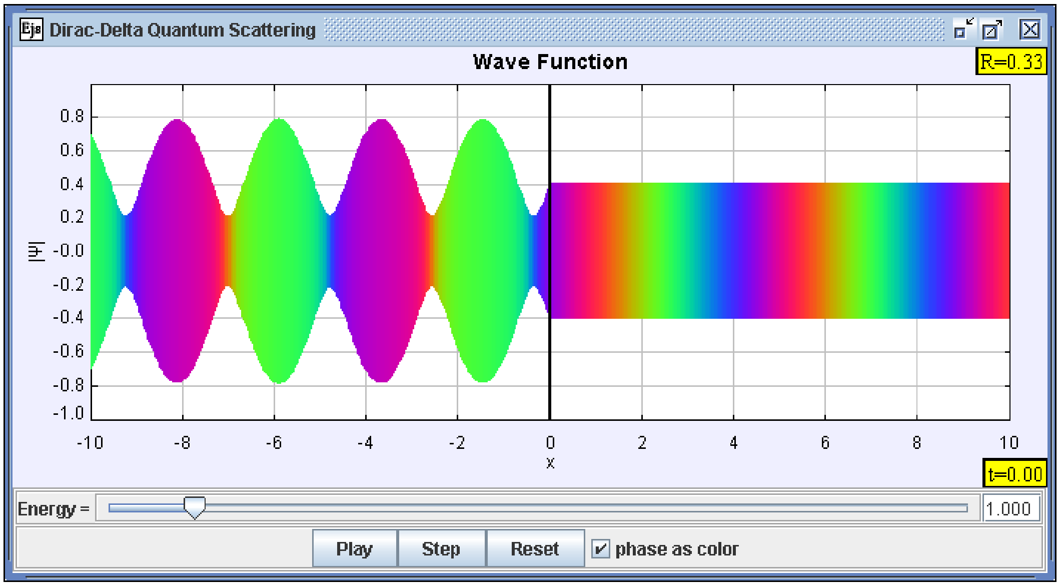

Figure 4: *EJS model of quantum scattering due to a 1D delta function. The simulation provides visual illustrations of an analytically solvable model and allows students to explore the system in both time and the energy of the scattering state. This model is available at: http://www.compadre.org/osp/items/detail.cfm?ID=6990*

4. Newly Accessible Physics

The increasing power of computers allows simulations of more interesting and complicated phenomena. Wave packet dynamics is an excellent example. Schrödinger first proposed a localized wave packet solution to his wave equation to connect classical and quantum mechanics. Over the last 30 years quantum-mechanical wave packets and their revivals, the fact that certain bound-state wave packets reform to their original shape in a predictable way, have received considerable theoretical attention and experimental verification.

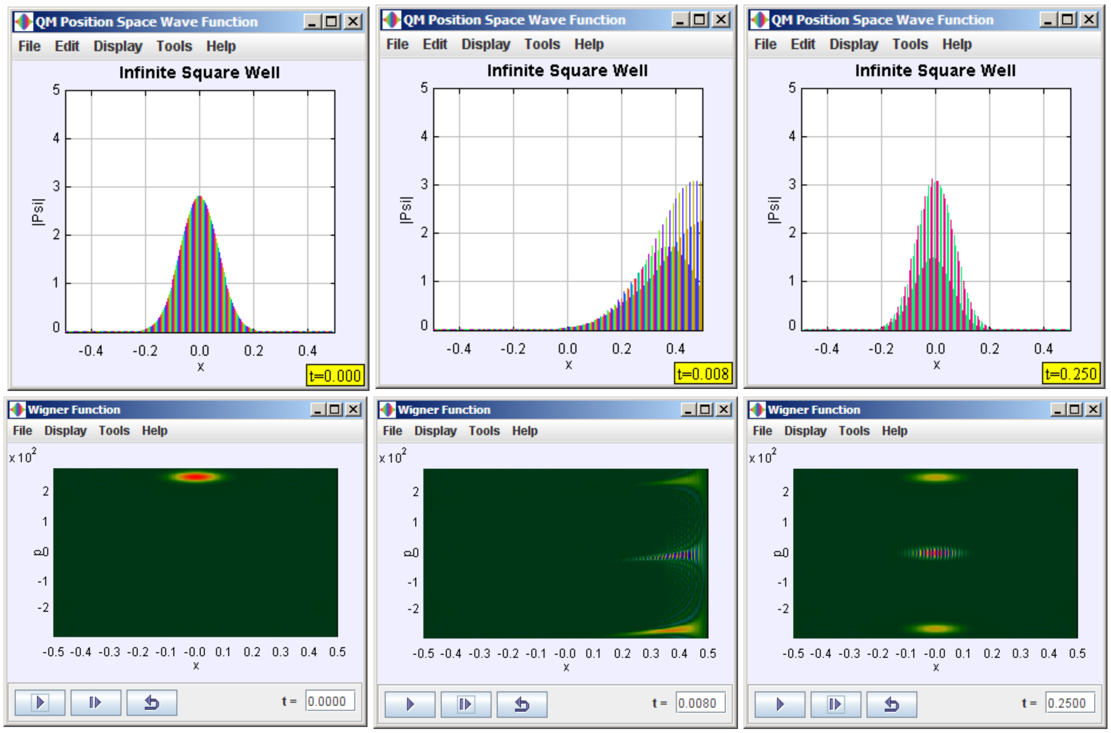

Figure 5: *The QM Wigner program showing the position-space wave function (top) and the Wigner quasi-phase-space representation (bottom). The initial state is a Gaussian (left). The middle images show the quantum bounce with the left wall of the well. The images on the right depict a fractional revival in which two mini wave packets appear on top of each other. The two wave packets can be observed separately with the Wigner function as shown. This program is available at:* *http://www.compadre.org/osp/items/detail.cfm?ID=6813*

OSP tools allow the construction of wave packets, such as the one shown in Figure 5, and the exploration of their evolution in time. Theoretical research has most often focused on wave packets in the infinite square well because of the two well-defined time scales: the classical “bounce” time and the quantum revival time. The first bounce of the initially localized quantum state against one wall occurs at one quarter of the classical period of oscillation. Investigation of the bounce illustrates the similarities and differences between the classical and quantum-mechanical systems. On a considerably longer time scale, the well-known exact and fractional revivals occur in the infinite square well. At revivals, the wave packet or copies of the original wave packet, sometimes called mini-packets or clones, reform long after the original packet has spread throughout the well. Student exploration of this behavior can be an excellent exercise on the time dependence of quantum states and results of the expansion in energy eigenstates. The added visualization of the quasi-phase space through the Wigner function gives another picture of the real-space and momentum-space evolution of quantum states and provides a high-level visualization technique to be used in analyzing the system.

5: Pedagogy: Tutorials and Worksheets Connected to OSP Simulations

OSP simulations connected with proven pedagogical approaches lead to more effective learning in quantum mechanics courses. When integrated with carefully constructed, research-informed curricular materials, interactive computer-based simulations can help reduce students' cognitive load [Sweller, 1994] by providing scaffolding and visuals that assist in conceptual understanding and problem solving. In addition, well-written exercises supported by computer-based simulations can help confront students' misconceptions and provide the cognitive dissonance, the incompatibility between the students' viewpoint and the results of the correctly modeled simulation, which is useful in improving understanding. Tutorials are a pedagogical approach that is particularly suited for the challenging task of teaching quantum physics [McDermott et al., 2002]. In tutorials, student difficulties and misconceptions are first brought to the forefront via specially designed tasks and questions. Once misconceptions are clearly identified, students are carefully guided to the correct answer. Successive tasks are made progressively more difficult as the tutorial's assistance is gradually taken away. Computer simulations are of particular importance for quantum tutorials because of the lack of traditional experiments and demonstrations.

QuILT (Quantum Interactive Learning Tutorials) is a set of tutorials designed for quantum topics. These tutorials are based on written materials from Chandralekha Singh and add the visualization possible through simulations from the OSP Project [Singh, 2006]. These activities:

- Address cognitive issues and are based upon physics education research,
- Actively engage students in the learning process through predictions and feedback,
- Employ visualization tools to help students build physical intuition about quantum processes,
- Bridge the gap between the abstract quantitative formalism and qualitative understanding,
- Consist of stand-alone modular units that can be used in any order that is convenient,
- Are designed to be used as supplements to lectures, as homework, or as a self-study tool.

Participants in the OSP Project have developed other materials using a tutorial format. These resources cover a range of topics including energy eigenfunction shape and time dependence, quantum-mechanical time development of general states, and quantum-mechanical measurement. These materials, simulations, xml parameter files, and pedagogy, are delivered in single Java Archive (jar) files that are compact and easily downloaded, opened, and run. The packages can also be copied and modified for needs specific to a particular class. In addition, separate editable worksheets are provided so that individual instructors may develop and distribute assignments in formats other than the complete packages. All of these materials are freely available through the OSP website for download and use [Open Source Physics, 2008].

6: Dissemination and Participation

The Open Source project is working to increase the awareness and use of the OSP resources through collaboration with the NSDL's Physics and Astronomy Pathway, ComPADRE [Compadre, 2008]. The ComPADRE project supports teachers and learners in a broad range of topics and levels of Physics and Astronomy through the development of community-specific resource collections. Each of these collections are developed and maintained by an editor and other members of the community. Through the technical infrastructure of ComPADRE, and regular discussions between the editors, each of these collections is strengthened by the ability to share resources and tools with all of the other ComPARE communities.

Figure 6: *Personal filing cabinet on the Quantum Exchange. Folders and sub-folders can be created to organize resources and annotations written*

to describe the materials and their use. Folders can be either private or public.

The Quantum Exchange [Quantum Exchange, 2008] is the ComPADRE collection where the OSP quantum pedagogical resources are being incorporated. This collection is focused on providing resources that can help students understand the abstract, non-classical aspects of quantum theory described above. The OSP materials are featured in the collection because of their connection between pedagogy and interactive computer simulations. The catalog includes other simulations, more traditional pedagogical materials such as notes and homework problems, and references on effective teaching of quantum mechanics. Through the ComPADRE interface, these different resources can be connected where appropriate. For example, online lecture notes on spin physics and a simulation of the Stern-Gerlach experiment can be related through their ComPADRE records. In particular, every registered ComPADRE user has a personal filing cabinet to gather, organize, and annotate their favorite resources, such as shown in Figure 6. As with all ComPADRE collections, registered users are also able to recommend materials for consideration by the editor, comment on materials, and share folders from their filing cabinets with other users. Through modification in the OSP curricular resources and the ComPADRE submission process, faculty teaching different topics can easily share their work.

The connection between OSP and ComPADRE is also being leveraged to help both projects grow. The connections between ComPADRE and other digital libraries provide avenues for spreading the word about the OSP resources. The harvesting of ComPADRE records by the NSDL is particularly important for this dissemination. Workshops and presentations by both groups publicize their materials and collaboration. Of course these connections also improve the rankings of resources by web search engines. In the near future an OSP-specific collection will be available on ComPADRE that will include all topics in physics. This will also provide a core set of quality pedagogical resources to develop new collections similar to the Quantum Exchange and expand existing collections. ComPADRE is also working with other curriculum developers to expand the depth and breadth of the library.

We encourage all those involved in quantum education to try the resources described here. They are available through both the OSP web site on ComPADRE and the Quantum Exchange. The power of open source and open access resources is the feedback that comes from the community of users. Comments and suggestions are welcome and contributions are greatly appreciated. Most importantly, we hope that the materials presented here will help students develop a deeper understanding and appreciation of quantum mechanics.

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