INTERACTIVE SIMULATIONS FOR THE LEARNING AND TEACHING OF QUANTUM MECHANICS CONCEPTS

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Abstract
Since 2009, we have been developing and evaluating interactive simulations with accompanying activities for the learning and teaching of quantum mechanics concepts at university level. The QuVis simulations build on education research and our lecturing experience, and aim to specifically target student areas of difficulty in quantum mechanics. Simulations are available on a wide range of topics from introductory to advanced level quantum mechanics.
This article gives an overview of the three collections of QuVis simulations developed so far. These include simulations for physics students, simulations for physical chemistry students studying introductory quantum mechanics and simulations to support a new introductory quantum mechanics curriculum based on two-level systems. Evaluation with students plays a decisive role in optimizing the educational effectiveness of the simulations and activities. We describe methods used to refine and further develop the resources. We give examples of revisions based on outcomes of individual student observation sessions.

1. Introduction

Interactive simulations can help students to engage with and explore physics topics through high levels of interactivity, prompt feedback and multiple representations of physics concepts (Podolefksy 2010). They can give students visual representations of abstract concepts and microscopic processes that cannot be directly observed. Well-designed interactive simulations promote engaged exploration, where students actively explore and make sense of the phenomena shown led by their own questioning. Careful design of simulations in terms of affordances (actions that are available) and constraints (features that restrict actions) can make simulations effective through implicit scaffolding of students' exploration. Due to its often abstract ideas far removed from everyday experience and counterintuitive results, interactive simulations can be particularly useful to help students learn quantum mechanics. Research-based simulations for the learning and teaching of quantum mechanics have been developed and shown to enhance student understanding (see e.g. Goldberg 1967, Schroeder 1993, Steinberg 1996, Zollman 2002, Belloni 2006, Singh 2008, McKagan 2008, Zhu 2012).

The Quantum Mechanics Visualization Project QuVis (www.st-andrews.ac.uk/physics/quvis) consists of research-based interactive simulations and accompanying activities for the learning and teaching of quantum mechanics concepts at university level (Kohnle 2012). Simulations make use of previous work on developing educationally effective simulations and research on student difficulties with quantum mechanics, and are informed by our lecturing experience. They aim to specifically target student misconceptions and areas of difficulty in quantum mechanics. Many simulations cover topics not found elsewhere. As described in section 2, one collection of QuVis simulations aims to make topics typically covered at the advanced level accessible to a first course in quantum physics. These simulations are embedded in a full online course including texts and problems.

Each simulation includes two views, the "Controls" view with the interactive elements and the "Step-by-step Explanation" view that explains key points with animated highlighting and includes step controls. Through the text explanations, simulations aim to be self-contained instructional tools. Simulations have been coded in Adobe Flash, with Mathematica used for graphics where needed. The majority of simulations include an accompanying activity. Depending on simulation context, activities aim to help students build mental models of quantum mechanics concepts, use the simulations to collect and interpret data, and to make connections between multiple representations. They promote guided exploration and sense-making and provide scaffolding to progress from simpler to more complex situations. Simulations and activities are freely available from the QuVis website and can be played or downloaded from this site. Full solutions to activities are available to instructors.

In what follows, we give an overview of the simulations and describe features that make them effective for learning (section 2). Section 3 describes the methods used for refinement of simulations and activities and gives examples of outcomes based on individual student observation sessions. Section 4 outlines future plans.

2. Overview of the simulations

The QuVis website includes three collections of resources: simulations for physics students, simulations for physical chemistry students studying introductory quantum mechanics and simulations to support a new introductory quantum mechanics curriculum based on two-level systems.

2.1 Simulations for physics students

This collection of simulations covers a wide range of topics, with currently 50 simulations available. The majority of simulations are aimed at the intermediate level, covering topics such as wave packets, energy eigenstates and superposition states in one-dimensional potentials, measurement and wave function collapse, one-dimensional scattering, expansion in eigenstates, time-independent perturbation theory and spin and angular momentum. A smaller number of simulations are aimed at the introductory level (such as the probabilistic analysis of classical systems) and the more advanced level (such as the density matrix, spin clusters and spin chains).

2.2 Simulations for physical chemistry students

Chemistry students may have less mathematical background than physics students, so visualization may play an even more important role in helping these students learn quantum mechanics concepts. In order to extend the resources to be more useful to chemistry students studying introductory physical chemistry, we modified existing simulations by removing or adding functionality and tailoring explanations, developed new simulations and developed accompanying problems sets aimed at chemistry students. Topics of the simulations link to Atkins' "Physical Chemistry" textbook, with most simulations developed so far focussing on basic quantum theory. Simulation topics include one-dimensional potentials, the Heisenberg Uncertainty Principle, multi-particle wave functions, the hydrogen atom, many-electron atoms, angular momentum and valence-bond theory. There are currently 18 simulations available in this collection.

2.3 Simulations for a new introductory quantum mechanics curriculum

Recent developments include a collection of 17 simulations with accompanying activities as part of the Institute of Physics (IOP) Quantum Physics resources available at quantumphysics.iop.org and on the QuVis website (Kohnle 2014). The IOP resources consist of learning and teaching materials (texts, simulations and activities) for a novel approach to a first course in university quantum mechanics starting from two-level systems. This approach immediately immerses students in inherently quantum mechanical aspects by focusing on experiments that have no classical explanation. It allows from the start a discussion of interpretative aspects of quantum mechanics and quantum information theory. The resources are freely available (but require registration) with multiple paths through the material. Texts have being written by researchers in quantum information theory and foundations of quantum mechanics. The simulations cover the topics of linear algebra, fundamental quantum mechanics concepts, single photon interference, the Bloch sphere representation, entanglement, local hidden variables and quantum information.

Fig. 1 shows a screenshot of the *Superposition states and mixed states* simulation from this collection. This simulation allows students to use a Stern-Gerlach apparatus that can be oriented along two orthogonal axes to investigate whether they can experimentally distinguish mixed states and superposition states. Students can choose different input spin states, which include a superposition state, a corresponding mixed state and two unknown input states (see the "Input particles" panel in Fig. 1). The simulation shows the individual input spin states and spin measurement outcomes, and the experimentally determined and theoretical outcome probabilities mathematically and graphically.

Simulations aim to help students make connections between multiple representations by using physical, mathematical and graphical representations, with consistent representations across different simulations. In the *Superposition states and mixed states* simulation, flashes are used to help students make connections between the measurement outcome on the screen and the outcomes shown in the "Number of measurements" panel. Colour is used to help students differentiate between the two measurement outcomes. Colour is also used to link the number of measurement outcomes to their respective observed and theoretical detection probabilities as shown mathematically and graphically (the three right-hand panels in Fig. 1).
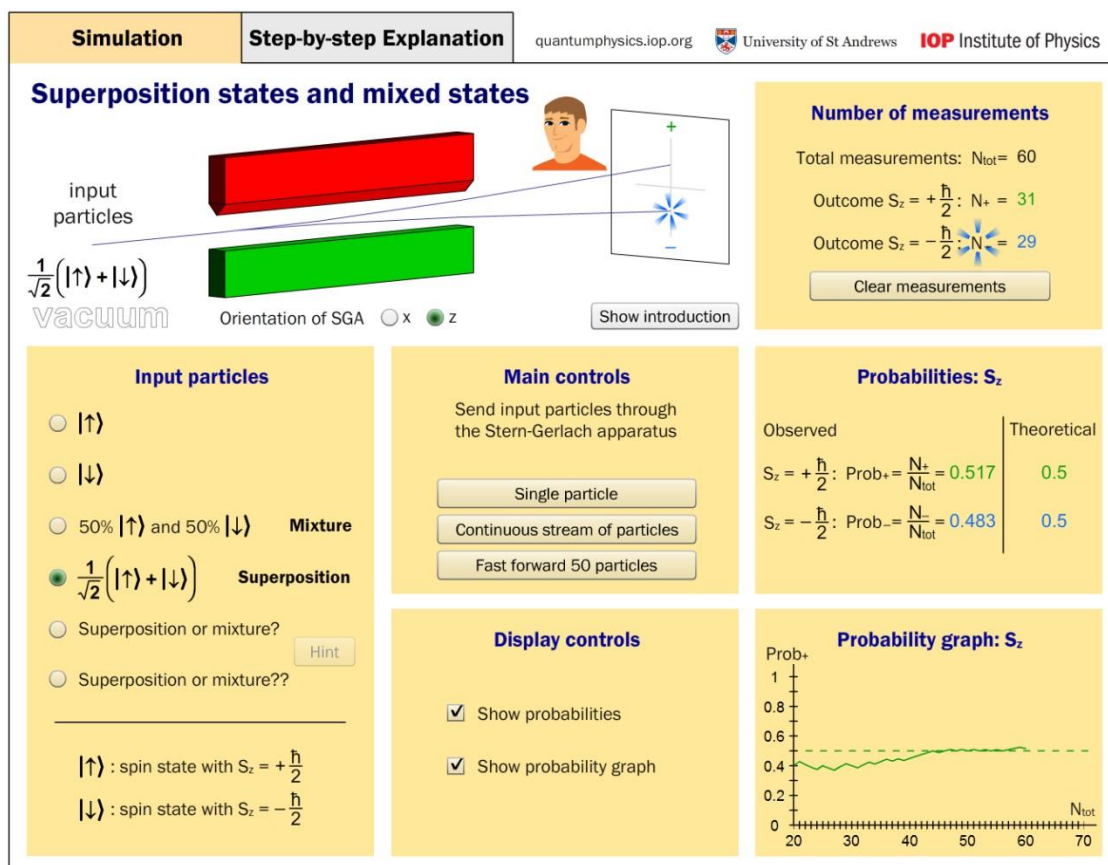
Figure 1: A screenshot of the "Superposition states and mixed states" simulation. This simulations allows students to investigate whether they can experimentally distinguish mixed states from superposition states.

Several simulations aim to help students develop quantum models and transition students away from classical perspectives by using comparisons between classical and quantum systems. The activity to the *Superposition states and mixed states* simulation asks students whether they encounter similar mixtures of objects in their everyday experience, and helps students make sense of the difference between quantum superposition and classical mixtures.

Simulations provide an intuitive interface that uses interactive controls such as sliders, buttons and tick boxes that are familiar to students. Controls and depictions of experimental apparatus have a similar look-and-feel across all simulations. Layout makes use of the fact that controls are typically explored top to bottom and left to right. The initial configuration is kept simple and includes an introductory text to encourage exploration and avoid overwhelming students. To reduce complexity and focus on fundamental ideas, simulations depict idealized and simplified situations. Some of the simulations aim to help students develop mental models by making the invisible visible, such as depicting single photons. As shown in Fig. 1, some of the simulations allow students to collect data to see how quantum-mechanical quantities are determined experimentally. These simulations can help students understand inherent statistical fluctuations by showing how the experimental quantities approach the theoretically predicted values in the limit of a large number of measurements. For the simulations where students collect data, a "Clear measurements" button allows students to reset the simulation.

3. Evaluation and refinement

Feedback from students at the appropriate level is vital to ensure simulations and activities are effective for learning. We have used the following evaluation methods to iteratively refine the simulations:

- End-of-course student surveys on attitudes towards and use of the simulations
- Surveys focusing on individual simulations asking about clarity, ease-of-use and aspects found confusing, completed by students directly after working with a simulation

- A conceptual diagnostic survey to assess learning gains of topics for which students had used simulations
- In-class observations of students working with simulations
- Individual observation sessions with student volunteers using screencapture and audiorecording
- Assessing learning gains using pre- and post-tests
- A small number of comparative studies

In what follows, we give three examples of revisions based on outcomes of individual student observation sessions (42 hours in total with 19 student volunteers) of the IOP Quantum Physics simulations (see also Kohnle 2013). In these sessions, students first interacted freely with a simulation and then worked on the activity for that simulation. Students were asked to "think aloud", e.g. to describe what they were seeing and making sense of and what they were finding confusing. Data were analyzed for common difficulties with content, interface and activity. This led to revisions of simulations and activities, included in all resources wherever appropriate.

For the *Superposition states and mixed states* simulation (Fig. 1), we found that students initially had difficulty understanding the mixed state. We revised the simulation so that the state of each input particle is shown in the graphics window. Thus, for the mixed state, the simulation now shows a random sequence of spin-up and spin-down input states. This allows students to make connections between the input state and the measurement outcome seen as a flash on the screen. For the superposition state, the simulation now shows a sequence of identical input states. We found that this revision helped students make sense of the difference between mixed states and superposition states.

Previous studies on developing educationally effective simulations show that including small puzzles or challenges in simulations can encourage prolonged engagement and inquiry (Adams 2008, Podolefsky 2010). To be productive, challenges need to be aligned with the learning goals of the simulation. We have incorporated small challenges into several simulations, e.g. the two unknown input states shown in Fig. 1. In the observation sessions, students often tell us that they particularly enjoy these challenges. Our studies show the importance of scaffolding the challenges in terms of students having other examples in the simulation for comparison, and in some cases providing a Hint button that brings up additional help but does not contain the solution. Activities also scaffold the challenges; the activity to the *Superposition states and mixed states* simulation first asks students to focus on the known input states and only later asks them to apply what they have learned to tackle the challenges.

The personalization principle is an important aspect of designing effective e-learning resources. This includes personalized language and on-screen characters (Clark 2011). Initially, the introductory text and text explanations were impersonal and did not include learning goals. One student commented in an observation session "I think the introduction [introductory text] made sense by itself. But I don't really think it relates to what you are doing very well. In the introduction it talks about what observer A could see..." Thus, we revised the text of all simulations to be more personal to students using formulations such as "You can send particles through the experiment...". Many simulations now explicitly state the learning goal in the introductory text. For the *Superposition states and mixed states* simulation, the introductory text states "Your goal is to determine whether or not you can experimentally distinguish mixed states from superposition states." We also added images of observers into the simulations where applicable, as shown in Fig. 1.

4. Conclusions and future steps

We have given an overview of the QuVis simulations and described features that make them effective for learning. We have stressed the key importance of student feedback in ensuring resources are effective for learning, and described methods used to iteratively refine simulations and activities.

We are currently developing HTML5 versions of the simulations suitable for touchscreens, and are carrying out observation sessions to optimize interface design for devices with smaller screens. We are conducting further evaluation studies using simulations in courses with students at multiple institutions, and assessing learning gains through a combination of pre- and post-testing, survey questions and some comparative studies. We will optimize and further develop simulations and activities based on this evaluation.

We plan further work on how best to visualize photon superposition and entangled photon pairs, with the aim of devising visualizations that help students develop productive mental models. We plan further development of more open activities that encourage exploration and discussion, and activities that are inherently collaborative in nature. We plan the development of simulations that incorporate game-like features to enhance motivation. We also plan simulations on further topics, with a particular focus on quantum information theory.

Acknowledgements

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