Interactive simulations to support quantum mechanics instruction for chemistry students

Supporting Information

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SI1. Syllabus of quantum mechanics topics and simulations used in the Physical Chemistry course

The introduction to quantum mechanics described in the article is taught as part of a traditional lecture-based second year physical chemistry course and consists of 12 lectures. Simulations used in the lectures are demonstrated by the instructor. These simulations are mainly employed to support and visualize concepts in quantum mechanics that are new to many students and with which they are not familiar. The visualizations aim to support the explanations of the course content introduced in the lecture and to help students develop conceptual understanding of key ideas such as eigenvectors, wavefunctions and probability densities, quantum tunnelling, etc.

In what follows, we provide a brief syllabus of topics broken down by lecture and the simulations used by the instructor. Simulation titles are in italics, with the short title used on the website where different in parentheses. The simulation URLs are listed at the end of this section. The time spent with the simulations is typically 5-10 minutes where used during a 50 minute lecture. Students are encouraged to use the simulations and to explore them in more detail along with the lecture notes outside of class time.

Lecture 1: Introduction to classical mechanics

- Linear momentum
- Newton's Second Law
- Kinetic energy
- Potential energy and force
- Total energy

Lecture 2: Classical mechanics

- Harmonic oscillator
- Angular momentum
- Kinetic energy of rotation
- Summary of classical mechanics
- Atomic models based on classical mechanics and their failure

Lecture 3: Wave-particle duality

- Further failures of classical mechanics: black body radiation
- Quantization of photon energy (Planck)
- What is light?
- What are waves?
- Wave particle duality in the case of electromagnetic radiation
- Davisson and Germer experiment: wave character of particles
- de Broglie wavelength of particles
- Electron diffraction from single crystal surfaces (LEED)

Lecture 4: Schrödinger equation (I)

- Dynamics of microscopic systems

- Operators, eigenfunctions and eigenvalues
  Graphical representation of eigenvectors[1] *(Eigenvectors and Eigenvalues) simulation*
- Position and momentum operators
- Meaning of the wavefunction (Born interpretation)
- Normalization of the wavefunction
- Superposition and expectation values
- Collapse of the wavefunction
  Successive energy measurements[2] *simulation*

Lecture 5: Schrödinger equation (II)

- Eigenstates and eigenvalues for a given system
- Uncertainty principle
  Heisenberg Uncertainty Principle[3] *simulation*
- Complementarity of operators
- Classical particle in a 1D box with infinitely high walls
  Probabilistic analysis of a mass-spring system[4] *(Classical Oscillator) simulation*
- Quantum particle in a 1D box with infinitely high walls
  The one-dimensional particle in a box[5] *(1D particle in a box) simulation*

Lecture 6: One- and two-dimensional quantum systems

- Particle in a 2D box with infinitely high walls; degeneracy
  Energy eigenfunctions of the two-dimensional infinite well[6] *(2D Infinite Well) simulation*
- One particle in a 2D square box versus two particles in a 1D box
  Comparison of one particle in a two-dimensional well and two particles in a one-dimensional well[7] *(1D and 2D Infinite Well) simulation*
- Symmetric and antisymmetric wavefunctions
  Fermions and bosons in a one-dimensional infinite square well[8] *(Fermions and Bosons) simulation*
- Particle in a 1D box with walls of finite height
  Comparison of bound states for the infinitely-deep and finite-depth square well[9] *(Comparison Infinite Finite Well) simulation*
- Tunnelling
  Quantum tunneling[10] *simulation*

Lecture 7: H atom (I)

- Hamiltonian for the H atom
- Spherical polar coordinates
  The volume element in spherical polar coordinates[11] *(Spherical Polar Coordinates) simulation*
- Schrödinger equation in polar coordinates
- Wavefunction of the electron: angular part
- Rotation in three dimensions: particle on a sphere

- Spherical harmonics
  Spherical harmonics[12] *simulation*
- Representation of wavefunctions

Lecture 8: H atom (II)

- Wavefunction of the electron: radial part
- Effective potential of an electron in the hydrogen atom
- What do orbitals look like?
  Atomic orbitals[13] *(Hydrogen orbitals) simulation*
- Radial solutions, radial distribution functions
  Radial distribution functions and electron densities for hydrogen electron orbitals[14] *(Radial Distribution Functions) simulation*
- Representation of orbitals
- Energy eigenvalues
- Hydrogenic atoms
- Atomic orbitals and quantum numbers
- Shells and subshells

Lecture 9: Spin

- Angular momentum in quantum mechanics
  Semi-classical vector model of orbital angular momentum[15] *(Vector Model Angular Momentum) simulation*
- Stern Gerlach experiment
  Experimental proof of spin angular momentum: The Stern-Gerlach experiment[16] *(Experimental Proof of Spin) simulation*
- Spin quantum number
- Spin orientations
- Spin ½ and spin 1 particles (fermions and bosons)
- Quantum numbers to define the state of an electron in a H atom
- Spectroscopic transitions and selection rules

Lecture 10: The structure of many-electron atoms

- Orbital approximation
- The He atom
- Pauli exclusion principle
- Electron configuration of C and O
- Hund's maximum multiplicity rule
- Third row of the periodic table
- Fourth row of the periodic table
- Building up principle
- Shielding
- Ionization energies

Lecture 11: The spectra of complex atoms

- Hamiltonian for He

- Singlet and triplet states – electron correlation
- Spin-orbit coupling
- Fine structure

Lecture 12: Term symbols and selection rules

- Total orbital angular momentum
- Multiplicity
- Total angular momentum
- Term symbols
- Selection rules

The Physical Chemistry course has bi-weekly assessed homework problems. Two of the homework assignments relate to the quantum mechanics part of the course. The following three homework problems incorporate simulations:

Homework problem on complementary: This problem first considers complementary using translations and rotations of a cuboid along different axes. The problem then asks students to show mathematically that the momentum and position operators are complementary. Using the *Heisenberg Uncertainty Principle*[3] simulation, it asks students to explain what this result means physically, and to consider whether momentum and position operators acting along different axes are also complementary.

Homework problem on the one-dimensional particle in a box: Using *The one-dimensional particle in a box*[5] *(1D particle in a box)* simulation, this problem asks students to sketch the potential, the first three energy values and corresponding wave functions and probability distributions. It asks for the physical interpretation of the probability distribution. It then asks students to show mathematically that the wave functions are eigenfunctions of the Hamilton operator, and to show how the boundary conditions and normalization condition determine the amplitude and the wave number of the wave functions.

Homework problem on the Bohr / de Broglie standing wave model of the hydrogen atom: Using *The Bohr model of the hydrogen atom*[17] *(Bohr model I)* simulation, this problem asks students to derive an expression for the allowed energy values in the hydrogen atom electron assuming a classical circular orbit. The length of the orbit needs to be a multiple of the de Broglie wavelength, leading to a quantization condition for the allowed energy levels.

1. Graphical representation of eigenvectors. http://www.st-andrews.ac.uk/physics/quvis/simulations_html5/sims/EigenvectorsAndEigenvalues/Eigenvectors_and_Eigenvalues.html (accessed Dec 2016).
2. Successive energy measurements. http://www.st-andrews.ac.uk/physics/quvis/simulations_html5/sims/EMeasurement/EMeasurement.html (accessed Dec 2016).

3. Heisenberg Uncertainty Principle. http://www.st-andrews.ac.uk/physics/quvis/simulations_phys/ph10_Heisenberg_Uncertainty_Principle.html (accessed Dec 2016).
4. Probabilistic analysis of a mass-spring system. http://www.st-andrews.ac.uk/physics/quvis/simulations_html5/sims/ClassicalOscillator/ClassicalOscillator.html (accessed Dec 2016).
5. The one-dimensional particle in a box. http://www.st-andrews.ac.uk/physics/quvis/simulations_html5/sims/infwell1d/infwell1d.html (accessed Dec 2016).
6. Energy eigenfunctions of the two-dimensional infinite well. http://www.st-andrews.ac.uk/physics/quvis/simulations_html5/sims/infwell2d/infwell2d.html (accessed Dec 2016).
7. Comparison of one particle in a two-dimensional well and two particles in a one-dimensional well. http://www.st-andrews.ac.uk/physics/quvis/simulations_chem/ch11-Comparison-particles.html (accessed Dec 2016).
8. Fermions and bosons in a one-dimensional infinite square well. http://www.st-andrews.ac.uk/physics/quvis/simulations_html5/sims/FermionsBosons/FermionsBosons.html (accessed Dec 2016).
9. Comparison of bound states for the infinitely-deep and finite-depth square well. http://www.st-andrews.ac.uk/physics/quvis/simulations_phys/ph18_Comparison_Infinite_Finite_Well.html (accessed Dec 2016).
10. Quantum tunneling. http://www.st-andrews.ac.uk/physics/quvis/simulations_phys/ph16_Quantum_Tunnelling.html (accessed Dec 2016).
11. The volume element in spherical polar coordinates. http://www.st-andrews.ac.uk/physics/quvis/simulations_chem/ch05_Spherical_Polar_Coordinates.html (accessed Dec 2016).
12. Spherical harmonics. http://www.st-andrews.ac.uk/physics/quvis/simulations_phys/ph45_Spherical_Harmonics.html (accessed Dec 2016).
13. Atomic orbitals. http://www.st-andrews.ac.uk/physics/quvis/simulations_chem/ch09_Hydrogen_Orbitals.html (accessed Dec 2016).
14. Radial distribution functions and electron densities for hydrogen electron orbitals. http://www.st-andrews.ac.uk/physics/quvis/simulations_chem/ch08_Radial_Distribution_Functions.html (accessed Dec 2016).
15. Semi-classical vector model of orbital angular momentum. http://www.st-andrews.ac.uk/physics/quvis/simulations_chem/ch15-Vector_Model.html (accessed Dec 2016).
16. Experimental proof of spin angular momentum: The Stern-Gerlach experiment. http://www.st-andrews.ac.uk/physics/quvis/simulations_chem/ch14-Experimental-proof-spin.html (accessed Dec 2016).

17. The Bohr model of the hydrogen atom. http://www.st-andrews.ac.uk/physics/quvis/simulations_chem/ch16_Bohr_model.html (accessed Dec 2016).

SI2. Research-based simulation design and refinement

The QuVis simulation development is an iterative process informed by student difficulties with quantum mechanics and student feedback on initial versions of the simulation (see reference 1 and the articles listed under the "Research" section of the QuVis website[2] for more details on the design and evaluation process). The simulation topics and learning goals are defined by our teaching experience and the literature on student difficulties with quantum mechanics. The learning goals determine the visualizations shown, the controls available and their ranges. Simulations typically focus on a single concept, and avoid additional material to keep the simulation as simple as possible. The simulation layout follows guidelines of interaction design[3], e.g. using intuitive controls that have the same look-and-feel across simulations, keeping the startup view simple to encourage exploration, avoiding extraneous material not linked to the intended learning goals and organizing similar controls into groups. Simulations make use of so-called implicit scaffolding[4], e.g. guiding students towards the learning goals through the controls available and their layout. For example, controls are typically explored (in the Western world) from top to bottom and left to right. Simulations make use of this fact by organizing controls so that students progress from simpler to more complex situations as they explore the simulation. Including small puzzles can enhance student engagement and exploration with a simulation[5]. Most of the new HTML5 simulations include a second challenges tab. These challenges are aligned with the learning goals and are ordered in terms of increasing difficulty.

After the initial drafting, simulations are coded by undergraduate students, who inform the development process by making suggestions for revisions from their perspective. After coding and activity development, we typically run a small number of individual observation sessions with student volunteers. In these sessions, students are first asked to freely explore the simulation and "think aloud", e.g. describe what they are looking at, what they are making sense of, what questions they are asking themselves and what they are finding confusing. Once students feel they have finished exploring the simulation, they work on the accompanying activity. Finally, students answer survey questions on their experience of using the simulation and make suggestions for improvement. We use screencapture and audiorecording in these sessions as well as making detailed observation notes. These sessions typically lead to minor revisions of the simulation and activity based on aspects found confusing and students' suggestions for improvement. We often include minor revisions in between observation sessions to assess their impact. After revisions from the observation sessions have been incorporated, we run in-class trials with simulations. For the in-class trials, we assess how well students completed the activity questions, and often ask students to complete the same survey questions on their experience of using the simulations as for the individual interviews. In some cases (but not for the simulations described in the main

article), we also make use of pre- and post-test questions that students answer prior to and after working with a simulation. Student feedback from the in-class trials often points to further minor revisions of the simulation and the activity which are then incorporated.

1. Kohnle, A. Research-based interactive simulations to support quantum mechanics learning and teaching. Proceedings of the 2014 GIREP-MPTL Conference, Palermo, Italy, July 7 - 12, 2014; Fazio, C., Mineo, R. M. S., Eds.; Università degli Studi di Palermo: Palermo, Italy, 2015; pp 29-40. http://www1.unipa.it/girep2014/proceedings/Chapter%201.pdf (accessed Dec 2016).
2. Research section of the QuVis website. http://www.st-andrews.ac.uk/physics/quvis/research.html (accessed Dec 2016).
3. Saffer, D. *Designing for Interaction*, New Riders: Berkeley, 2010.
4. Adams, W. K.; Reid, S.; LeMaster, R; McKagan, S. B.; Perkins, K. K.; Dubson, M. & Wieman, C. E. A Study of Educational Simulations Part II - Interface Design. *Journal of Interactive Learning Research* **2008**, 19 (4), 551-577.
5. Adams, W. K.; Reid, S.; LeMaster, R; McKagan, S. B.; Perkins, K. K.; Dubson, M. & Wieman, C. E. A Study of Educational Simulations Part I - Engagement and Learning. *Journal of Interactive Learning Research* **2008**, 19 (3), 397-419.

SI3. General guidelines for simulation use

QuVis simulations can be used flexibly in a wide range of learning environments. In this section, we give recommendations for simulation use based on our experience in the physical chemistry course described in the article as well as several physics courses at the University of St Andrews. In these courses, simulations are used as virtual demonstration experiments in lecture-based classes, in computer classroom workshops and as homework assignments.

Simulations can be used as virtual demonstration experiments either to introduce a new concept or to deepen students' understanding of a concept. In both cases, we first explain what is being represented and displayed in the simulation. If the simulation is being used to introduce a new concept, we ask students to observe what happens when a certain parameter is changed and to note down their observation. The instructor then uses this observation to introduce and explain underlying concepts. If the simulation is being used to deepen students' understanding, we often ask students to predict the outcome of changing a certain parameter or the outcome of an experiment set up in the simulation. Students are asked to discuss their prediction in small groups. We sometimes use multiple choice questions for students to vote on their prediction. The instructor then shows the outcome with the simulation, and discusses underlying reasons for this outcome.

Simulations can be used in computer classroom workshops, where students work on the activity associated with a simulation with facilitator support. Simulation activities are kept intentionally short so that they can be completed in a single hour-long period. We have run such workshops with students working individually

and in pairs at a computer. Our experience is that asking students to work collaboratively enhances discussion between students about the displayed quantities and the relationships between them.
We also use simulations as homework assignments. Students are asked to write out their answers (or type them into an online form) to the activity associated with a simulation. Students receive feedback on their work or discuss the solutions in small groups with a facilitator.
Our experience and that of other studies is that a first phase of free exploration increases engagement with a simulation.[1,2] Thus, the simulation activities often ask students to have a play with the simulation first and note down some things they have found out before answering the rest of the activity questions. Most of the newly developed HTML5 simulations have a second Challenges tab. The challenges are aligned with the learning goals of the simulation and allow students to assess their understanding. For all simulations with a Challenges tab, the last activity question asks students "Which of the Challenges did you find most difficult and why? Explain how you solved this challenge. If none of the Challenges were difficult, choose the one you found most interesting and explain how you solved it." This questions aims to increase student engagement with the challenges.

1. Kohnle, A. Research-based interactive simulations to support quantum mechanics learning and teaching. Proceedings of the 2014 GIREP-MPTL Conference, Palermo, Italy, July 7 - 12, 2014; Fazio, C., Mineo, R. M. S., Eds.; Università degli Studi di Palermo: Palermo, Italy, 2015; pp 29-40. http://www1.unipa.it/girep2014/proceedings/Chapter%201.pdf (accessed Dec 2016).
2. Moore, E. B.; Herzog, T. A. & Perkins, K. K. Interactive simulations as implicit support for guided-inquiry. *Chem. Educ. Res. Pract.* **2013**, 14, 257-268.

SI4. Website features and navigation

Simulations can be run online from the QuVis website[1] or downloaded for offline use. Simulations can be selected for online use by clicking on the thumbnail images. For the HTML5 simulations we recommend using Internet Explorer, Firefox, Chrome or Safari browsers.
Simulations can be downloaded by clicking on the download icon below the thumbnail images. The Flash simulations consist of a single .swf file that can be run in a browser if Adobe Flash Player is installed. The HTML5 simulations are downloaded as a single .zip file, from which the files first need to be extracted. Once this is done, the simulation can be run by opening the .html file in the main directory in a browser window.
The majority of simulations come with an accompanying activity, which aims to guide students' exploration and help students make sense of the displayed quantities and make connections between physical, graphical and mathematical representations. The accompanying activity for a simulation (without solutions) can be downloaded as a pdf file by clicking on the pdf icon below the thumbnail image.

The activity with solutions is password-protected, and can be downloaded as an editable Word file by clicking on the lock icon below the thumbnail images. Instructors can obtain the activity solutions via an email request.[2] Instructors are welcome to modify activities as needed to suit their context.
The website includes several navigation features to find simulations on given topics. The left-hand navigation panel allows users to select one or more topics and the simulation level (introductory or advanced), and displays all simulations meeting these criteria. Simulations can be sorted alphabetically via a short title (given in parentheses in the article and in section SI1) or chronologically, i.e. with the most recently developed simulations shown at the top of the page. The top navigation bar includes a search box. A simulation with a known title can be found by typing part or all of the title into the search box. Note that the search will only bring up simulations that can be run on a given device, e.g. Flash simulations are not displayed on touchscreen devices.

1. The QuVis Quantum Mechanics Visualization project. http://www.st-andrews.ac.uk/physics/quvis (accessed Dec 2016).
2. Instructors interested in obtaining the password for the activity solutions are requested to email quvismail@st-andrews.ac.uk.