Open-Access, Interactive Explorations for Teaching and Learning Quantum Dynamics

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S *Supporting Information*

ABSTRACT: While the research field of quantum dynamics (QD) benefits from advances in modern computational power, the educational field of QD paradoxically does not. We have developed an open-access, interactive, electronic notebook that leverages a user-friendly interface to engage a new generation of visual learners with QD. We begin each topic (e.g., adiabaticity, light−matter interactions, and relaxation processes) with essential questions, issues, and background that orient the learner; we then move directly to visual explorations of the phenomena, where the learner can immediately manipulate parameters that control and drive the physics. This notebook requires only a computer that can run Wolfram's computable document format (CDF) files (both the notebook and CDF player are free) and enables learning in a variety of contexts and grade levels: flipped classrooms, small groups, and high school students through advanced researchers. Without sacrificing rigor, *Quantum Dynamics...with the Dynamics!* (QDWD) aims to develop physical intuition and is built in the spirit of hands-on experimentation with immediate and visual results. The hierarchical structure of QDWD lends itself to differentiated instruction, where a motivated or advanced student can explore the computer code, mathematical formalism, and underpinning physics.

KEYWORDS: *Hands-On Learning/Manipulatives, Inquiry-Based/Discovery Learning, Quantum Chemistry, Theoretical Chemistry, Upper-Division Undergraduate, Graduate Education/Research, Kinetics, Physical Chemistry, Computer-Based Learning, Distance Learning/Self Instruction*
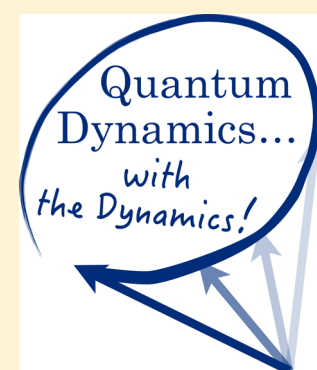
INTRODUCTION

Traditional passive instruction can impart limited conceptual understanding, even for introductory physics courses on Newtonian mechanics.[1] Introductory treatments of quantum mechanics usually focus on stationary states, or "quantum statics." However, numerous essential phenomena, including vision and photosynthetic energy transduction, involve nonstationary quantum states that evolve in time.[2,3] The study of such quantum dynamical phenomena requires dynamics and thus a purposeful departure from the static nature of textbooks. However, teaching quantum dynamics (QD) lacks an accessible and intuitive means to convey, to visualize, and to explore these processes. Motivated by the growing number of nontraditional resources for STEM education,[4−15] we have developed a conceptual tool, called *Quantum Dynamics...with the Dynamics!* (QDWD), that promotes deepened learning and intuition building by guiding students through a series of interactive explorations of QD phenomena (see Figure 1).

QDWD explores 2- and 3-level system dynamics, classical kinetics, sudden versus slow change, control of quantum transitions (Fermi's golden rule, adiabatic passage, the quantum Zeno effect), mixed versus pure states, and relaxation processes (described by the density matrix formalism). QDWD promotes hands-on, interactive manipulation of key parameters that govern quantum processes and develops intuition for how these parameters influence the dynamics. Student exploration is guided through *Directed Exploration* callouts, and the learner receives immediate visual feedback concerning the effects of the parameters on the dynamics. The learner can also discover limiting dynamical cases that are popular in the static textbooks without being constrained to these limited, special cases. QDWD is freely available for download via the Supporting Information. (For the best viewing experience, we recommend also installing the associated fonts.)

(THE LACK OF) CURRENTLY AVAILABLE TOOLS TO TEACH QD

Interestingly, the majority of currently available, interactive modules focusing on quantum mechanics deal almost exclusively with quantum statics and often require some amount of programming.[6] The few examples of computer-based QD modules utilize mainly static graphical frameworks or snapshots, and the student must overcome a "coding barrier" to manipulate and to visualize the physical principles.[7] QD concepts are often non-intuitive; as such, any pedagogical attempt to help the learner develop a picture of the dynamics is valuable (see, e.g., ref 16). Previous undertakings have not yet fully capitalized on modern computational power to bring real-time dynamics to the fingertips of students.[17] Many lack a unified, user-friendly interface.[18] QDWD is an attempt to leap past these technical and
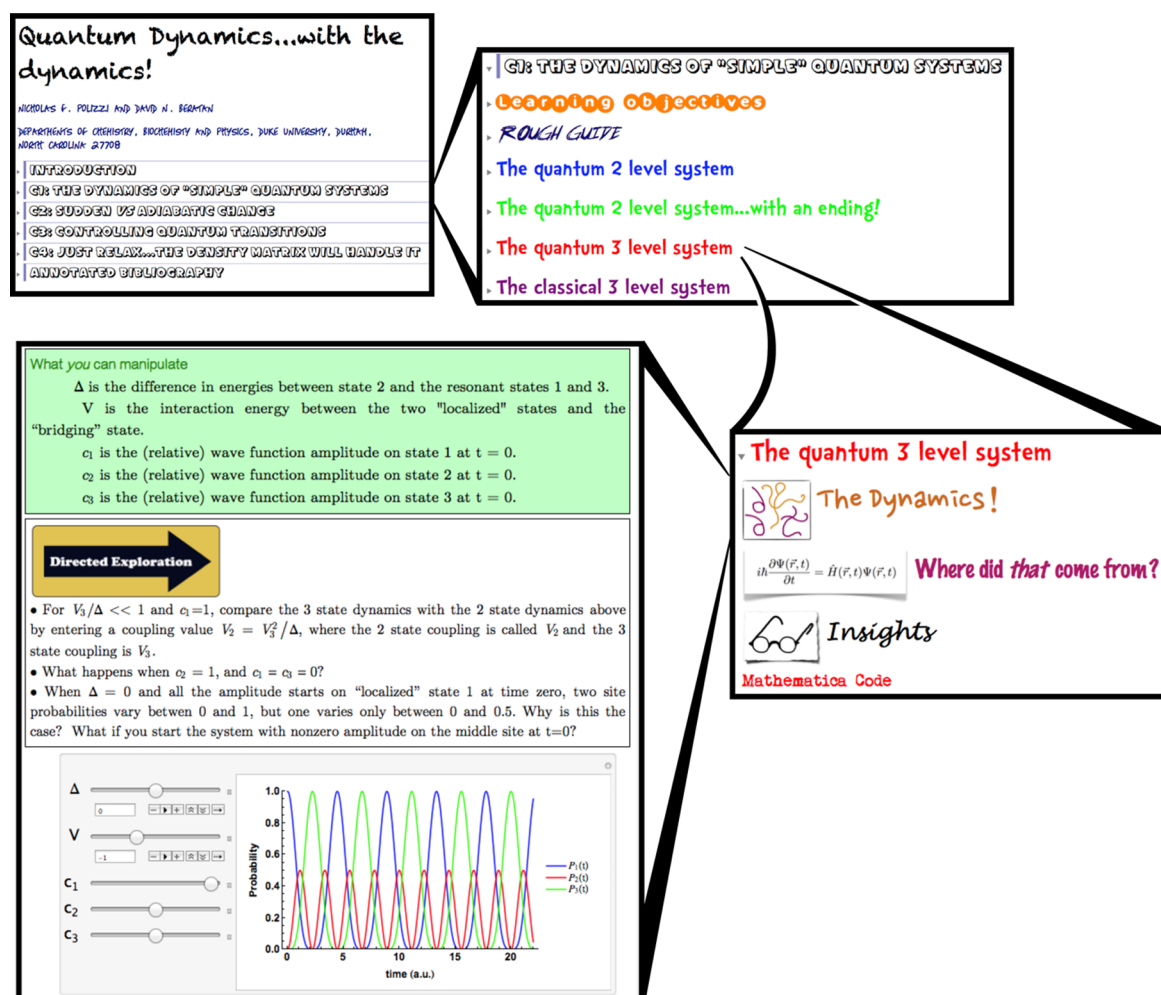
Figure 1. Organization of *Quantum Dynamics...with the Dynamics!* Each unit (C1, C2, etc.) houses learning objectives, a *Rough Guide*, and several quantum systems. Within each quantum system are interactive modules that allow the learner to interface with the physics before she meets any mathematical formalism or computer code. We guide learner investigation of these manipulatable plots via *Directed Exploration* callouts.

visual hurdles to enable learning, in the framework of an integrated, stand-alone, open-access package.

TARGET AUDIENCE AND PROJECTED USE

QDWD is a suitable tool to use as part of an introductory course in chemistry or physical chemistry, as well as in more specialized graduate courses in QD or spectroscopy. The material is intended to be accessible to members of a diverse community of learners, from high school students to university faculty.

We have employed QDWD in a number of contexts: as a demonstration lecture in the 2014 Bioelectronics Workshop at the Majorana Centre in Erice, Italy; as a means to activate a flipped graduate class in QD at Duke; and in colloquium lectures. We have received enthusiastic feedback supporting the development of further guided visualizations tailored to a growing community of visual thinkers and learners. We foresee using QDWD as a teaching tool to activate flipped classroom activities, to promote self-guided independent study, to supplement traditional lectures, to catalyze team-based discussion, to contextualize standard textbooks, and to facilitate the transition from textbook learning to independent research. We also anticipate using QDWD in formative and summative assessments of student learning. For example, teachers can monitor student interaction with the material in a classroom setting and can ask students to

provide answers to the questions posed in *Directed Exploration* callouts. A final project could involve student adaptation of the provided code within *Mathematica* (which requires a license) to explore a new system.

LEARNING OUTCOMES

Through QDWD, students will be able to identify and to relate the key parameters that drive the time evolution of quantum systems. Students may also synthesize new ideas from learned ones by splicing and editing the provided *Mathematica* code. (Code tinkering does require a *Mathematica* license. Alternatively, open-source, python-based coding platforms could be used, but would require additional programming expertise.) Learners may map problems in the scientific literature onto the simplified models developed in QDWD. For example, the 3-level system dynamics module (see Figure 2) is directly related to protein-mediated electron transfer problems. Students and researchers thus position themselves to better evaluate and understand the scientific literature.

ORGANIZATION OF *QUANTUM DYNAMICS...WITH THE DYNAMICS!*

QDWD contains four units, labeled C1, C2, C3, and C4 (Figure 1). Figure 1 shows that each unit contains learning objectives and
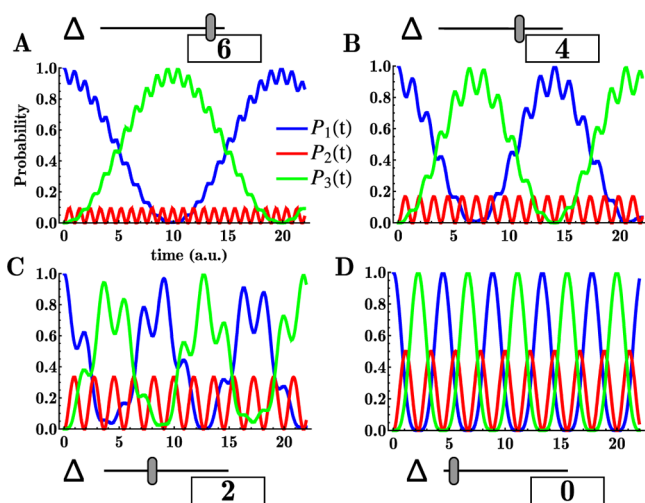
Figure 2. Depiction of a user-controlled plot of oscillatory 3-level dynamics. Explicitly shown is one of several slide bars, with its associated value, that the learner may manipulate. The learner sees how the energy gap (Δ) between the "bridging" state 2 (red) and the energy-degenerate states 1 and 3 (blue and green, respectively) affects the population transfer dynamics. Panels A–D show the transition from "off-resonant" (A) to "resonant" (D) dynamics. Other parameters not explicitly displayed are the electronic coupling and the initial amplitudes of each state.

Box 1. Description of the Hierarchical Structure of *Quantum Dynamics...with the Dynamics!*

Learning Objectives. We explain the motivation for learning this particular topic. We frame the discussion in terms of essential questions and understandings.[19]

Rough Guide. Here we distill decades of textbook quantum mechanics into a page or so. In addition to the classics[20–29] and recent excellent graduate texts that emphasize QD,[30–33] our aim is to prompt the reader with a minimal amount of formalism, to be used as a jumping-off point for exploration, but not to restate what is described so well and so often by others. We also suggest further readings for delving deeper, which is essential for differentiated learning.[19]

The Dynamics! This is the heart of QDWD. Here we embed objects (often plots) that can be manipulated by the learner via slide bars or by typing specific numerical values. The learner visualizes the interplay among key parameters by direct, real-time manipulation. We guide such exploration via introductory notes and callout sections entitled *What you can manipulate* and *Directed Exploration* (see Figure 1).

Surprises. When appropriate, we add statements that emphasize counterintuitive physical findings in this section.

Where did *that* come from? Here we derive the formalism that governs the dynamics. At this stage, the learner is in a position to make meaningful connections among the equations and the physical relationships derived from her earlier exploration.

Insights. To reinforce ideas and to promote the transfer of core concepts,[19] we emphasize key understandings and take-home messages.

***Mathematica* code.** We display the annotated code that was used to generate the interactive plots. The code can be modified and redeployed for a variety of research and pedagogical uses.
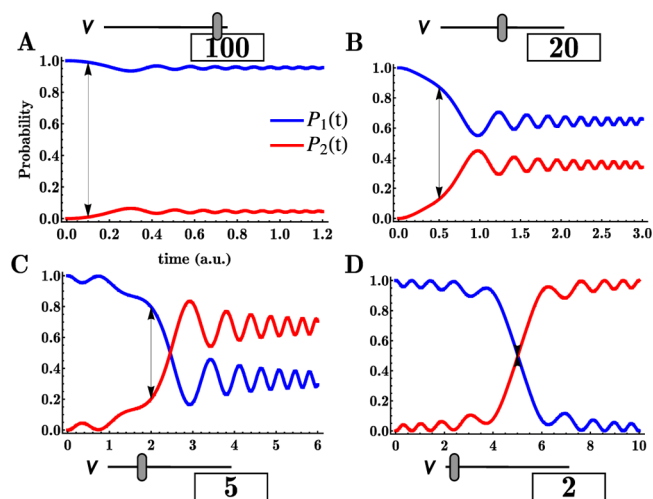
a so-called *Rough Guide*. These items orient the student toward the learning goals and key background materials, respectively, and are followed by several QD systems that the learner can explore. The didactic treatment of each QD system is divided into several parts, beginning with *The Dynamics!* Clicking on this header reveals several interactive calculations, embedded within probing questions and specific background material. Each module within QDWD includes callouts entitled *What you can manipulate* and *Directed Exploration*, where the learner is encouraged to explore the parameter space in a way that aims to reveal core concepts. Figure 2 depicts how the learner interfaces with such a calculation, in particular with the quantum 3-level system. Box 1 describes each section in more detail.

Each part listed in Box 1 aims to transfer and reinforce key ideas. Only after the learner interfaces with *The Dynamics!* do we explain the formalism that drives these processes (in Where did *that* come from?). In this way, the learner develops a visual understanding onto which she can map the more formal equations. We aim to keep the formalism to a minimum and to refer the reader to the classic textbooks[20–29] for supplementary reading. The learner then is exposed to *Insights* that recapitulate important relationships and provide additional context for the previous investigations. Finally, the learner can look "under the hood" at the computational code that drives the interactive computations. At this stage, the learner is reacquainted with the dynamical objects at a deeper level. Often the code used is relatively simple, employing the tools of *Mathematica*. This tactic encourages its easy repurposing without much fear of the intricacies associated with programming. This "part–whole–part" iteration[19] is uniformly applied throughout QDWD, providing a consistent platform for deep exploration of QD concepts. Figure 3 shows another such quantum system (related to sudden vs slow change) to which the "part–whole–part" iteration is applied in C2 of QDWD.

Figure 3. Speeding through degeneracy. Explicitly shown is one of several slide bars, with its associated value, that the learner may manipulate: the speed (v) by which the energy of state 2 decreases [$E_2(t) = \Delta - vt$]. Other manipulatable parameters not displayed are the initial energy offset between states 1 and 2 ($\Delta = 10$), the electronic coupling ($V = -1$), and the initial amplitudes ($c_1 = 1$, $c_2 = 0$) of each state. The double-sided black arrow denotes the time where the two energy levels are degenerate. After this time, the energy of state 2 continues to decrease with speed v. The energy of state 1 is fixed at 0. The system dynamics are computed numerically in *Mathematica*.

■ CONCLUSION

QDWD provides a first step toward teaching QD to visual learners. Further development of a video game platform could address a host of accepted good teaching practices by creating opportunities for continuous feedback and accumulation of rewards to track progress.[34] As with video games, QDWD provides students with a safe place to explore, to fail, and to

succeed. However, no one medium has a monopoly on providing learning opportunities; effective learning requires diversity.[35] Textbooks, electronic materials, and video games each are likely to play important and complementary roles in teaching quantum mechanics and dynamics. We have developed QDWD as an open-access tool that utilizes hands-on visualization to facilitate the transfer of key ideas in QD, a subject that explains the molecular underpinnings of vision, DNA repair, and solar energy conversion.[2]

ASSOCIATED CONTENT

Ⓢ Supporting Information

The Supporting Information is available on the ACS Publications website at DOI: 10.1021/acs.jchemed.5b00662.

> *Quantum Dynamics...with the Dynamics!* provided as a CDF file and associated fonts (ZIP)

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Notes
The authors declare no competing financial interest.

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REFERENCES

(1) Hake, R. R. Interactive-engagement versus traditional methods: A six-thousand-student survey of mechanics test data for introductory physics courses. *Am. J. Phys.* **1998**, *66* (1), 64−74.

(2) Migliore, A.; Polizzi, N. F.; Therien, M. J.; Beratan, D. N. Biochemistry and Theory of Proton-Coupled Electron Transfer. *Chem. Rev.* **2014**, *114* (7), 3381−3465.

(3) Rando, R. R. The Biochemistry of the Visual Cycle. *Chem. Rev.* **2001**, *101* (7), 1881−1896.

(4) Briggs, W.; Cochran, L.; Gillett, B. *Calculus: Early Transcendentals*, 2nd ed.; Pearson: London, 2015.

(5) Cass, M. E.; Rzepa, H. S.; Rzepa, D. R.; Williams, C. K. The use of the free, open-source program Jmol to generate an interactive web site to teach molecular symmetry. *J. Chem. Educ.* **2005**, *82* (11), 1736−1740.

(6) *Symbolic Mathematics Documents for Physical Chemistry*. http://www.chemeddl.org/alfresco/service/org/chemeddl/symmath/frameset?guest=true (accessed June 2015).

(7) Ellison, M. D. Femtochemistry. *J. Chem. Educ.* **2003**, *80* (5), 581.

(8) Freasier, B.; Collins, G.; Newitt, P. A web-based interactive homework quiz and tutorial package to motivate undergraduate chemistry students and improve learning. *J. Chem. Educ.* **2003**, *80* (11), 1344−1347.

(9) Georgios, T. Teaching and Learning Physical Chemistry: A Review of Educational Research. In *Advances in Teaching Physical Chemistry*; American Chemical Society: Washington, DC, 2007; Vol. *973*, pp 75−112.

(10) Lay, D. *Mathematica Manual for Linear Algebra and Its Applications*, 4th ed.; Pearson: London, 2012.

(11) Tanner, J. J. A computer-based approach to teaching quantum dynamics. *J. Chem. Educ.* **1990**, *67* (11), 917.

(12) Yang, E. M.; Greenbowe, T. J.; Andre, T. The effective use of an interactive software program to reduce students' misconceptions about batteries. *J. Chem. Educ.* **2004**, *81* (4), 587−595.

(13) Zielinski, T. J. Introducing JCE LivTexts: Physical Chemistry. *J. Chem. Educ.* **2005**, *82* (12), 1880.

(14) Zielinski, T. J.; Hanson, D. M. Particle-in-a-Box Dynamics. *J. Chem. Educ.* **2007**, *84* (7), 1232.

(15) da Silva Júnior, J. N.; Sousa Lima, M. A.; Sousa, E. H. S.; Oliveira Alexandre, F. S.; Leite Júnior, A. J. M. KinChem: A Computational Resource for Teaching and Learning Chemical Kinetics. *J. Chem. Educ.* **2014**, *91* (12), 2203−2205.

(16) Bernd, T. *Visual Quantum Mechanics: Selected Topics with Computer-Generated Animations of Quantum-Mechanical Phenomena*; Springer-Verlag: New York, 2000.

(17) Brandt, S.; Dahmen, H. D. *Picture Book of Quantum Mechanics*, 4th ed.; Springer-Verlag: New York, 2012.

(18) *Introduction to Chemical Bonding - Java3D Applets*. http://www.fh.huji.ac.il/~nsh75/ (accessed October 2015).

(19) Wiggins, G.; McTighe, J. *Understanding by Design*, 2nd ed.; Association for Supervision and Curriculum Development: Alexandria, VA, 2005.

(20) Atkins, P. W.; Friedman, R. S. *Molecular Quantum Mechanics*, 3rd ed.; Oxford University Press: New York, 1997.

(21) Cohen-Tannoudji, C.; Diu, B.; Laloë, F. *Quantum Mechanics*, 2nd ed.; Wiley-Interscience: Paris, France, 2006.

(22) McQuarrie, D. *Quantum Chemistry*, 2nd ed.; University Science Books: Sausalito, CA, 2007.

(23) Merzbacher, E. *Quantum Mechanics*, 3rd ed.; Wiley: New York, NY, 1998.

(24) Sakurai, J. J. *Modern Quantum Mechanics*. Addison-Wesley: Reading, MA, 1994.

(25) Schatz, G. C.; Ratner, M. A. *Quantum Mechanics in Chemistry*; Prentice-Hall: Englewood Cliffs, NJ, 1993.

(26) Schiff, L. I. *Quantum Mechanics*; McGraw-Hill: New York, 1968.

(27) Shankar, R. *Principles of Quantum Mechanics*, 2nd ed.; Springer: New York, 1994.

(28) Griffiths, D. J. *Introduction to Quantum Mechanics*; Pearson Prentice Hall: Upper Saddle River, NJ, 2004.

(29) Nitzan, A. *Chemical Dynamics in Condensed Phases: Relaxation, Transfer and Reactions in Condensed Molecular Systems*; Oxford University Press: New York, 2006.

(30) Bittner, E. *Quantum Dynamics: Applications in Biological and Materials Systems*; CRC Press: Boca Raton, FL, 2009.

(31) Hamm, P. *Principles of Nonlinear Optical Spectroscopy: A Practical Approach*; University of Zurich:Zurich, 2005. http://www.mitr.p.lodz.pl/evu/lectures/Hamm.pdf (accessed July 2015).

(32) Tannor, D. J. *Introduction to Quantum Mechanics: A Time-Dependent Perspective*; University Science Books: Herndon, VA, 2006.

(33) Tokmakoff, A. *Time-Dependent Quantum Mechanics and Spectroscopy*. http://tdqms.uchicago.edu/page/tdqms-notes (accessed November 2015).

(34) Mayo, M. J. Video Games: A Route to Large-Scale STEM Education? *Science* **2009**, *323* (5910), 79−82.

(35) Greenfield, P. M. Technology and Informal Education: What Is Taught, What Is Learned. *Science* **2009**, *323* (5910), 69−71.