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Implementing New Educational Platforms in the Classroom: An Interactive Approach to the Particle in a Box Problem

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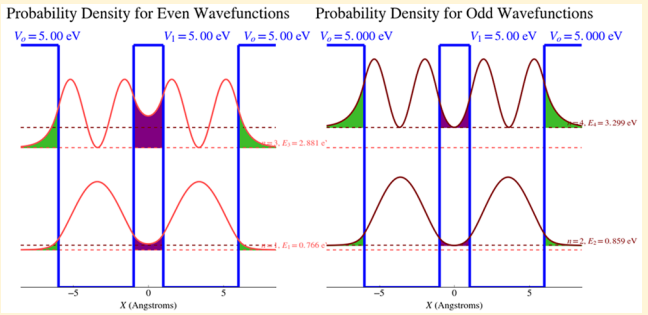
Supporting Information

ABSTRACT: The ready availability of interactive platforms has produced a new generation of students able to utilize computer-based learning tools with ease and comfort. The potential to better "explore by yourself" the lecture material permits students to have an enhanced learning experience and stimulates them to tinker with equation parameters generating insightful figures or animations. Used in the classroom, it emboldens students to have a deeper comprehension of complex derivations or mathematical expressions. We illustrate the power of interactive learning platforms by presenting educational *Jupyter notebooks* for the study of a fundamental problem in quantum chemistry: the motion of a particle in 1D and 2D space. Although simple, this model offers the possibility to explore several important quantum chemistry concepts such as Heisenberg's uncertainty principle, confinement leading to quantization, tunneling effect, and even bonding and antibonding properties. We present four *Jupyter notebooks* that gradually walk the student from the properties of a free particle to the properties of a particle in a double potential well. Our experience gained from the implementation of the material in the undergraduate and graduate curriculum is discussed, including student feedback and examples of complementary homework to be used in the classroom.



KEYWORDS: *Quantum Chemistry, Computer-Based Learning, Upper-Division Undergraduate, Graduate Education/Research*

TEACHING QUANTUM CHEMISTRY INTERACTIVELY

With the development of new computational tools, the use of educational interactive platforms in the classroom has become increasingly accessible.[1−4] Interactive platforms can aid students not only as a powerful visualization tool but also to rationalize mathematical relations, solve complex equations, and explore analytical results with numerical calculations. Visualizing results for different problem parameters takes them beyond reading and trying to remember dry equations. In this work, we introduce a sequence of *Jupyter notebooks*[1] as an interactive platform to teach quantum chemistry. The choice of platform relies on its open-source nature and free availability, and it runs within a web browser interface; it allows inclusion of explanatory text, tables, images, and mathematical equations and includes powerful libraries. The *Jupyter notebook* can be implemented in a server version where the code is not visible to students, and the same capabilities offered in the *Jupyter* environment are available in an even user-friendlier interface.[6,7]

The main feature of the *Jupyter notebooks* is its modular form. Each module (cell) runs independently, leading to ease in debugging, and local errors do not propagate through the rest of the notebook. This cell structure permits their straightforward combination from multiple notebooks and its continuous update in a modular form. Currently, the popularity of *Jupyter* and the availability of a repository of notebooks is such that instead of developing any code from scratch, a "cut and paste" approach provides an easy introduction to preparing notebooks for multiple course applications.

SCOPE OF THIS WORK

In this work, we revisit a classical quantum chemistry textbook problem:[2−5] the particle in the box. To expand the reach of good educational papers devoted to this problem,[6−10] we show how teaching this fundamental topic interactively can enhance its understanding.[11]

The flexibility of *Jupyter notebooks* permits the implementation of the same interactive base material at different levels. In General Chemistry, the notebooks are used as closed packages (hidden code) to complement lectures devoted to the topic of quantization, absorption of electromagnetic radiation, and wave function interference to exemplify a rudimentary model for molecular bonding. In an undergraduate Physical Chemistry course, interactive exercises are shown during lecture time and numerical data is extracted to provide a better

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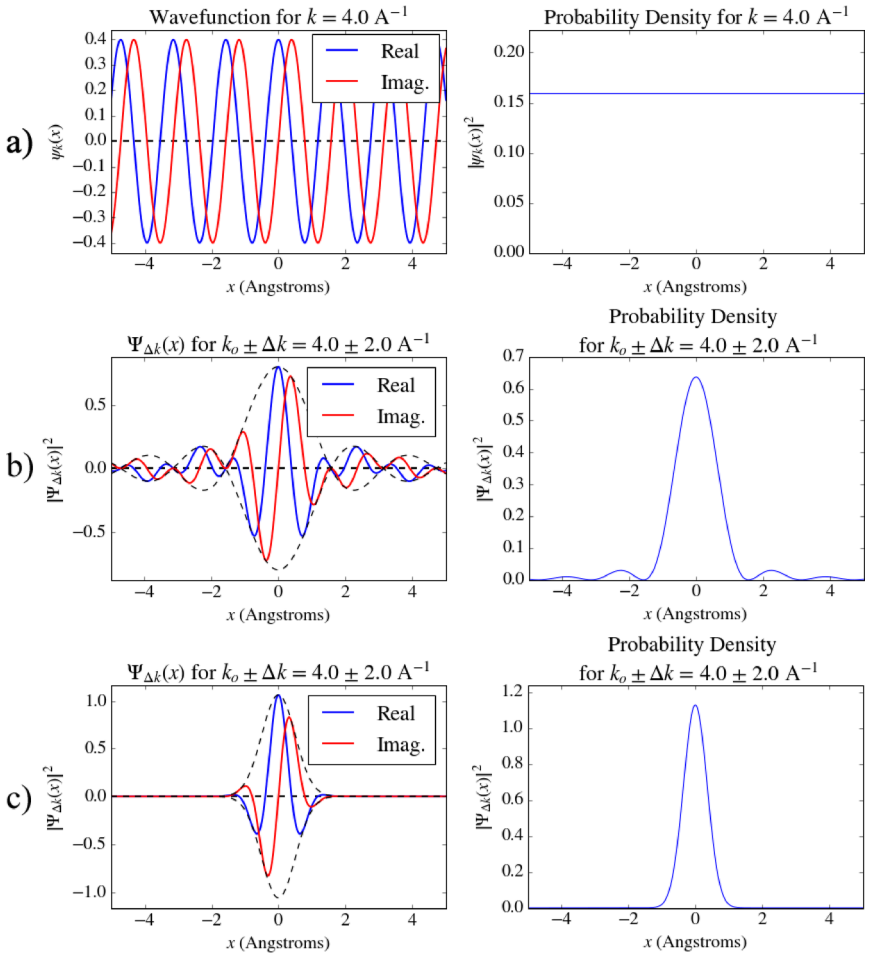

Figure 1. Wave functions and probability densities for (a) free particle and fully defined momentum, (b) free particle with an equally distributed momentum uncertainty, and (c) free particle with a Gaussian distributed momentum uncertainty.

understanding of the graphical representation of the concepts of wave function, probability density, boundary conditions, quantization, correspondence principle, 1D and 2D structures, and tunneling. At the graduate level, the notebooks are used to enhance lectures and are provided to students to be modified and expanded as they learn fundamental graphical and computational tools associated with quantum chemistry and its applications. At all levels, students use the interactive nature of the notebooks to extract data for homework problems (see Supporting Information).

The particle in one dimension is a good example to illustrate important quantum mechanics concepts such as allowed bounded energy levels, probability densities, tunneling, and wave-interference, and it can be used to show the differences between classical and quantum mechanics predictions. An interacting graphical representation of the analytical solutions provides a framework to visualize the equations and relate physical quantities to the variables of the equations.

The notebooks were implemented in three different classrooms, and students reported how the interactive components helped them to better understand the concepts discussed in class and facilitated their learning of the material. They did not find the use of the material difficult and used it multiple times over the course of the semester, including to solve homework problems. This is an example of pedagogical value and practicality, where student learning-enhancement is gained from the material presented in this paper.

The interactive approach was divided into four topics: free particle, particle in a box with an infinite potential, particle in a box within a finite potential, and particle in two boxes separated by a barrier. For each topic, we present an individual *notebook*, and each notebook links to the next one in a sequential manner. All notebooks are available for free in the Supporting Information and are accessible for use at http://kleimanteach.chem.ufl.edu:4000.

The paper is divided as follows: the first part focuses on the notebooks, describing the fundamental model, type of graphs, and information that can be extracted, and the second part describes the implementation of these notebooks at different levels of the chemistry curricula, adjusting the complexity of the presentation to the level of the course.

In the first part, we discuss the free particle problem and how a conceptual understanding of Heisenberg's uncertainty principle naturally arises from it. This is followed with a discussion of the particle in an infinite potential box, showing how confinement leads to quantization. This topic continues with a description of the particle in a finite box potential to introduce the concept of tunneling. Finally, we present results for a particle moving within two boxes defined by finite potentials and separated by a variable-height barrier. Using this simple model, we present bonding and antibonding behaviors in energy levels, wave functions, and probability densities.

In the second part, we describe the implementation of the *notebooks* in the classroom, including the use of homework

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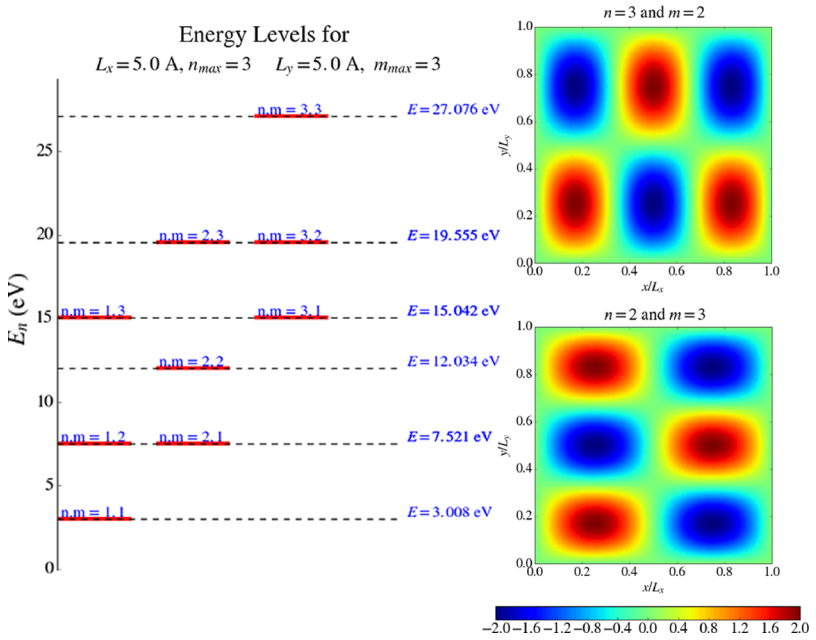

Figure 2. Energy level diagram for an electron inside a square 2D box of dimensions 5 Å × 5 Å. The energy degeneracy is observed, for example, for the states corresponding to $(n, m) = (3, 2)$ and $(2, 3)$ which have the same energy (19.555 eV). Their corresponding wave functions are plotted in the right side, showing a different distribution of nodes for each state described by a different wave function.

problems where students use the interactive features of the notebooks to construct their answer. Implementation of the interactive *Jupyter notebooks* in three different courses is presented in the last section. The notebook material allows the students to interactively generate independent graphs for wave functions, probability densities, and energy levels for different values of box sizes, particle mass, and potential wells, along with explanatory text. Additional details on the calculations, derivations, and graphics are also presented under the Supporting Information (SI).

THE NOTEBOOKS

Notebook 1: Free Particle

The first notebook, Free Particle, depicts a particle under a null potential. To introduce operators and wave functions properties, the notebook exemplifies how the solution wave function, $\psi_k(x) = \frac{1}{\sqrt{2\pi}} e^{ikx}$, which is found as an eigenfunction of the momentum operator $\hat{P} = -i\hbar\partial/\partial x$ ($P\hat{\psi}_k(x) = p\psi_k(x)$ where $p = \hbar k$), is also an eigenfunction of the Hamiltonian for the free particle, where $V(x) = 0$. This example is based on the use of commutator properties of quantum mechanical operators.

The notebook provides access to the graphical representation of wave functions where the momentum parameters can be easily varied. Figure 1a shows the real and imaginary components of the wave function and its probability density. The student can observe that the probability density is the same for every value of x and conclude that when the particle has a well-defined momentum ($p = \hbar k$), the probability of finding the particle is the same everywhere in this one-dimensional space. Using the notebook in class, students introduce different values of the wavenumber k and the length x and recalculate these graphs.

The concept of localization of a particle is introduced in the notebook by considering not just a single value of momentum, but a range of momenta. For example, it shows the superposition of waves with a range of momenta given by $p = p_0 \pm \Delta p$. Given that the momentum varies continuously, an integration is required to perform the superposition of waves. Two cases are presented. In the first case, each wave contributes equally to the overall superposition:

$$\psi_{\Delta k}(x) = N \int_{k_0-\Delta k}^{k_0+\Delta k} e^{ikx}\, dk = \frac{2N \sin(\Delta k x)}{x} e^{ik_0 x} \quad (1)$$

In the latter example, the distribution of momenta is modulated with a Gaussian function

$$\psi_{\Delta k}(x) = N \int_{-\infty}^{+\infty} e^{-(k-k_0)^2/2\Delta k^2} e^{ikx}\, dk = \sqrt{2\pi} N \Delta k e^{-1/2x^2\Delta k^2} e^{ik_0 x} \quad (2)$$

where N is a normalization constant.

Figure 1b shows the first wave function and its probability density. When $k_0 > \Delta k$, the $\cos(k_0 x)$ and $\sin(k_0 x)$ components oscillate with a higher frequency (k_0) and are modulated by a sinusoidal component with lower frequency (Δk). The student can test it with different parameters to generate plots where the probability density to find the particle is shown localized around $x = 0$. If Δk is very small, the particle will still be delocalized; as Δk increases, the particle becomes more localized in a specific region around $x = 0$. The observed incremental localization is used to introduce the concept of uncertainty, and how as the *uncertainty* in the momentum increases (larger Δk) the *uncertainty* in the position decreases, with the particle becoming more *localized*. This behavior is predicted by Heisenberg's uncertainty principle. The interactive graphical representation, with the possibility of varying Δk, allows students to grasp the concept and to understand the meaning of an equation seen in General Chemistry, which continues to puzzle even some advanced chemistry students.

The second example of superposition of waves (Figure 1c) is constructed such that each k-wave is modulated by a Gaussian distribution with the maximum contribution from k_0 and smaller contributions from waves with other k values. Once

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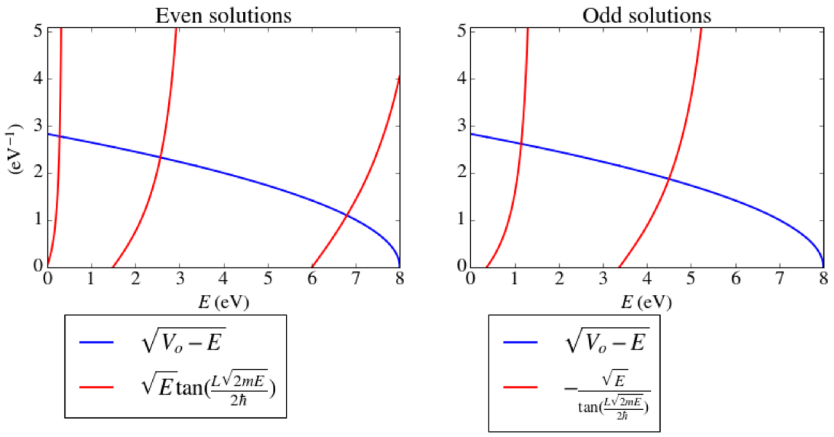

Figure 3. Allowed values of E found graphically for a particle in a finite box with V_o = 8 eV and L = 10 Å. The points of intersection of the two curves correspond to the E values for bound states. The reader may go to the *Jupyter notebook* to generate this figure for other values of V_o and L.

again, the probability density is localized around $x = 0$, showing that a decreasing value of Δk could yield a more precise value for the momentum, though still leading to delocalization in the position of the particle, as the reader is encouraged to check.

Notebook 2: Particle in a Box with Infinite Potential Walls

The next notebook presents the constrained motion of a particle, allowing it to move freely only within a certain region of a 1D space. The concept of Boundary Conditions ($\psi_n(0) = \psi_n(L) = 0$) is introduced, and the normalized wave functions and allowed energy values are presented. Students are introduced to quantization by highlighting the difference between the free particle results shown in notebook 1 and those in notebook 2, where not every energy value is allowed. The energies depend on the quantum number n, which is a direct consequence of the boundary conditions. Students are taught how the confinement of the particle between $x = 0$ and $x = L$ leads to quantization of its energy.

By making use of the interactive platform, the instructor can present several insightful graphs. These graphs clearly depict the spacing between energy levels (increasing linearly with increasing n), a dependency that is highlighted in class and utilized in homework problems (Supporting Information). The graphical representation is used to introduce the nodes of a wave function and to count them for different values of n to establish the "$n - 1$ rule". The interactive plotting of this figure for different parameters is used to show how the characteristics of the wave functions (boundary condition, shape, number of maxima, minima, and nodes) remain the same for a given quantum number. The provided notebook encourages the student to compare the characteristics of wave functions, probability densities, and energy levels for boxes of different size and particles of different mass.

Notebook 2 also includes a brief discussion of a particle in a two-dimensional box. The introduction of a second dimension (and therefore a second quantum number) opens the possibility of different states with the same energy and allows the teacher to introduce the concept of degeneracy and its existence in multidimensional systems. The difference between an energy level and a state is examined with the help of a heat plot for the wave functions and an energy diagram. Figure 2 shows how the state described by the wave function $\psi_{3,2}(x, y)$ has a different spatial distribution than the state described by the wave function $\psi_{2,3}(x, y)$, even though the energy levels for $n, m = 2, 3$ and for $n, m = 3, 2$ have the same energy. Students can graphically generate the wave function for different combinations of quantum numbers (n, m) and evaluate degeneracy as observed in Figure 2. More details are presented in the Supporting Information where a homework example is also presented.

Notebook 3: Particle in a Box with Finite Potential Walls

In order to understand the effect of the height of the box wall, notebook 3 considers a particle moving freely within the walls of a box defined by *finite* potentials. The box has length L, and V_o is the depth of its potential. In this notebook we choose to move the center of the box to $x = 0$ yielding a symmetric potential $V(-x) = V(x)$. This is an important point to call to the attention of students, since a common mistake of undergraduate students is to assume absolute properties for the position of the box. As students interacted with these notebooks in the classroom, we observed that, by plotting the wave function or probability density for boxes centered at different values of x, students better captured the relative nature of the axes of motion.

The notebook describes the Schrödinger equation in the different regions and finds a general solution for the region inside the box, $\psi(x) = q_1 \cos(kx) + q_2 \sin(kx)$, and for the region outside the box, $\psi(x) = q_1 e^{\alpha_o x} + q_2 e^{-\alpha_o x}$, where q_1 and q_2 are coefficients defined by the boundary conditions and $\alpha_o^2 = \frac{2m(V_o - E)}{\hbar^2} > 0$.

The classroom presentation of this notebook emphasizes the Postulates of Quantum Mechanics, indicating that the wave function must remain finite as $x \to \pm\infty$, leading to $q_1 = 0$ if $x \to +\infty$ and $q_2 = 0$ if $x \to -\infty$. The finite-wave function postulate defines the constraints for a unique set of solutions. The notebook highlights the importance of Boundary Conditions and how they must be obeyed to fully describe a specific system: the wave function must have the same value at $x = \pm L/2$ whether this position is reached from the outside or from the inside of the box.

For even potentials there are two families of solutions with $\psi(-x) = \psi(x)$ or $\psi(-x) = -\psi(x)$ (details in Supporting Information). In both cases, the boundary conditions impose constraints on the α_o parameter, associated with the energy.

As the notebook shows, it is not possible to obtain an analytical expression for the unknown values of E. When analytical solutions cannot be found, graphical or numerical

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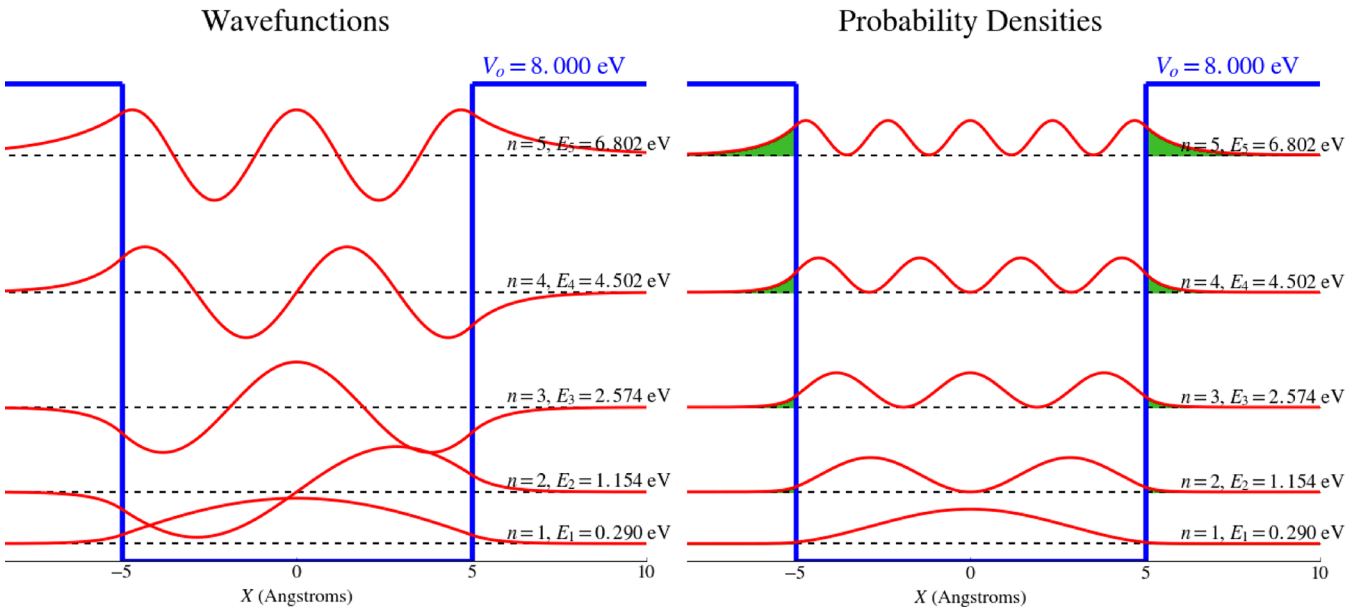

Figure 4. Wave functions (left) and probability densities (right) for an electron in a finite box with V_o = 8 eV and L = 10 Å. The areas shaded in green correspond to the tunneling probability. The reader may go to the *Jupyter notebook* to generate these figures for other values of V_o and L.

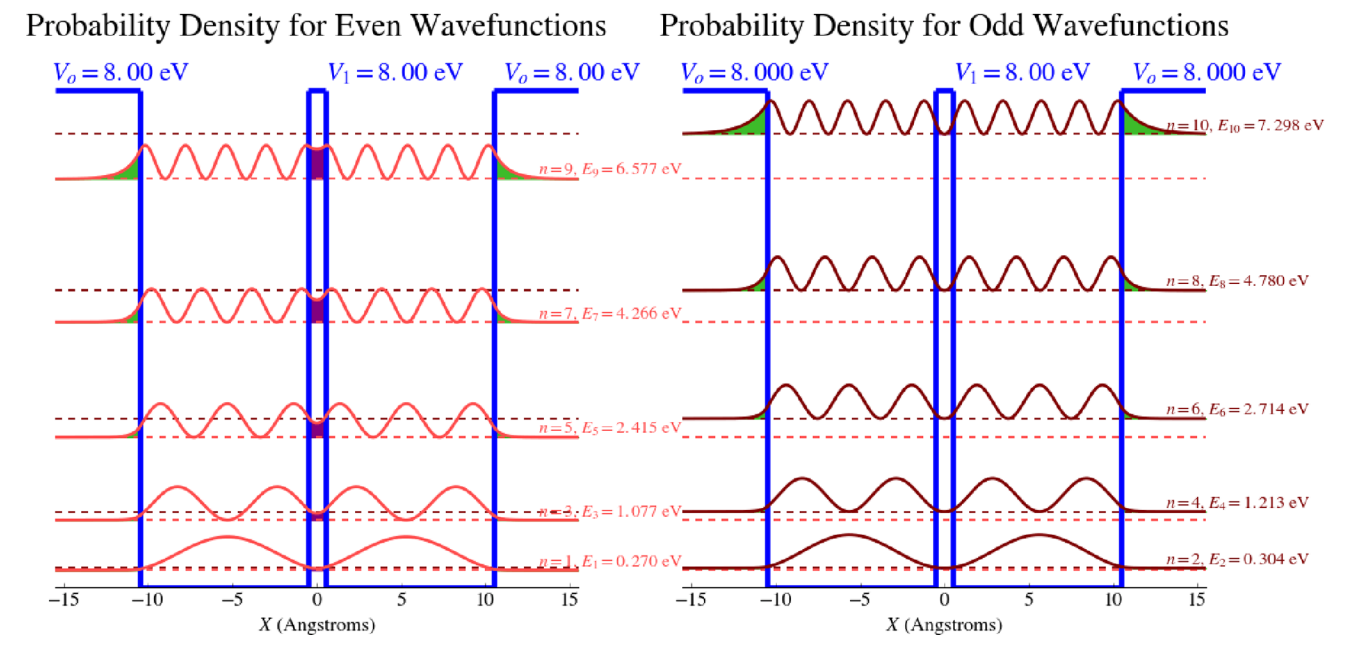

Figure 5. Probability densities for an electron in a two finite boxes potential with V_o = V_1= 8 eV, L = 10 Å, and d = 1 Å. The areas shaded in green correspond to the tunneling probability, and the area shaded in purple corresponds to the probability of finding the particle between the boxes.

methods are commonly used, and this notebook exemplifies one such case (Figure 3). It provides a simple example to teach advance undergraduate and graduate students the techniques for finding nonanalytical solutions. Students learn by visualization that the lowest allowed energy corresponds to an even solution.

Although possible, it is hard to read a precise numerical value from a plot; thus, the interactive platform is used to numerically find the (more) accurate allowed values of E. The *Jupyter notebook* provides the answers and creates a figure showing all the states with energies lower than the wall potential V_o; thus, the student can see the number of bound states, their energies, and the energy spacing between them.

Once the energies are obtained, students can plot the bound wave functions and their probability densities for given values of V_o and L superimposed on a graph of the corresponding energy levels (Figure 4).

Comparison of results from this notebook and notebook 2 are used to teach the effect that walls of finite height have on the energy of bound states, on the wave functions, and on the probability density to find the particle in a given position in space. In the presence of a finite potential, the energy of the ground state increases and the number of bound states also increases as the potential increases. Students are encouraged to recalculate the notebook for several values of V_o, to graphically verify what may be difficult for them to grasp from the written form of the equations: As the potential increases they see the

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number of bound states increasing toward infinite, and for finite potentials, the lowest energy state always has a lower energy compared to a particle confined by an infinite potential. A simple proof of this property together with an example of a homework problem are presented as Supporting Information.

The peculiarities of the wave function (and the probability density) are more striking and might be hard for students to comprehend. Figure 4 (right side) illustrates the nonzero probability to find the particle outside the box (green shaded areas in the probability density plot). This graph is used to introduce the purely quantum mechanical tunneling effect with its probability also calculated in the notebook. Students can observe how the tunneling probability increases for states with higher energies, where it becomes easier for the particle to tunnel through.

The ground state energy and tunneling probability obtained with the *Jupyter notebook* match with results published elsewhere,[12] and a homework problem based on this notebook exemplifies the tunneling effect (Supporting Information).

Notebook 4: Particle in Two Boxes with Finite Potential Walls

Notebook 4 includes calculations to consider a particle found within the potentials of two nearby boxes where d is the width of the barrier between the boxes with height V_1, and L is the size of each individual box with outside walls V_o. This notebook focuses on the solutions and what can be learned from their graphical representations and numerical evaluation. The problem is divided into 5 different regions, and in each case the boundary conditions provide the constraints needed to obtain unique solutions of the Schrödinger equation. After imposing the boundary conditions, further relationships are extracted for the wave function parameters α_o, α_1, d, and L. The complex form of the equations shown in the notebook underlines the limitation of not finding an analytical expression for the allowed values of E. The interactive platform provides the graphical and numerical evaluation of those allowed energies.

Once the bound energies are found, the wave functions and probability density functions can be generated. Figure 5 shows the probability densities for one electron in a double well. The interactive component of the *Jupyter notebook* provides an opportunity to vary the parameters (V_o, V_1, L, and d) and visualize the changes in those bound states.

A comparison of these results with a single finite box shows the consequence of the coupling between the boxes as they become close to each other. The energy levels of a single finite box split into two in the 2-box potential: one higher in energy (odd wave function solutions, even quantum numbers) and one lower in energy (even wave function solutions, odd quantum numbers). The graphical representation of the wave functions (Figure S1) shows that the odd solutions have an additional node at the center of the barrier.

The representation of the two-well potential with a variable barrier is proposed as the simplest model to describe wave functions and energies of diatomic systems using constructive and destructive interference of waves. As the distance between the wells is reduced, we can observe interference between the wave functions. The constructive interference leads to the even solutions, with increased probability to find the electron between the two nuclei (bonding states), and the odd solutions correspond to destructive interference, with a node between the two nuclei and increased energy (antibonding states).[11]

Students are encouraged to repeat the evaluation for large interbox distances, $d \gg L$, where they will observe that even and odd solutions become equal (degenerate energies and equal probability densities), and as expected, the results match those of independent single finite boxes of length L. When $d = 0$, the barrier disappears, and the results correspond to those of the particle in a single finite box with $L' = 2L$.

Even more interesting is the possibility to use the notebook to explore the effect of the height of the potential between the boxes. In the limit of $V_1 \gg V_o$, the wave function between the boxes goes to zero (Figure S2). This is not due to interference of the two wave functions. Instead, the potential in the barrier is so high that tunneling into the barrier becomes negligible, and the two boxes behave independently: The splitting on the energy levels disappears, and the even and the odd states become degenerate, with equal probability densities on either side of the barrier.

IMPLEMENTATION IN THE CLASSROOM

The easiest use of these notebooks in the classroom is to provide students access through a code-hidden server version as shown in http://kleimanteach.chem.ufl.edu:4000. Each notebook is written with a description of the work, followed by the interactive modules that include all the graphic and input parameters. Throughout each notebook, some simple questions help the student test her/his understanding of the material, e.g., what is being plotted? What can be learned from the plot?

The *Jupyter notebook* material provided with this paper has been tested using different levels of detail and complexity in classrooms with undergraduate students of "One-Semester Intensive General Chemistry" (~50 students), "Quantum Chemistry and Spectroscopy" (20−40 students), and first-semester graduate students taking "Chemical Bonding and Spectroscopy" (10 students) at the University of Florida.

An important issue to consider when implementing interactive material is the different levels of (un)familiarity that students might have with programming languages. The notebooks presented here do not require any previous knowledge on any programming language. Moreover, the *Jupyter notebooks* are implemented at two different levels. The first echelon of classroom implementation is designed for students who might be dazed by seeing any code, but for whom the interactive component is critical (most undergraduate students). No software, language, or app is installed in their device. The notebook is accessed through a link to a public server where the student can run all the cells, modify any input value, and recreate all the graphics. The student does not see the code, nor can she/he change any component of the notebook other than input parameters. The second echelon is aimed at students who want to take full advantage of the web-based *Jupyter* environment. They have access to the code, and they can use the individual modules to expand the notebooks and create their own applications. At the graduate level, after access to this prepared notebook, students are encouraged to create their own notebooks with applications to spectroscopy or their area of research.

Implementation in General Chemistry

The One-Semester General Chemistry course is populated with students with previous IB or AP Chemistry background. These students already have familiarity with electronic configurations (atomic), s and p orbitals, and ionic or covalent

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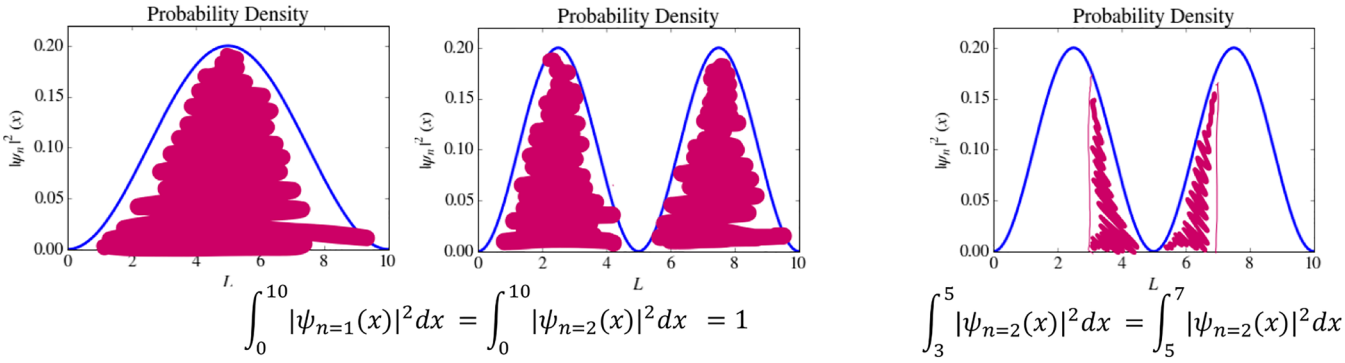

Figure 6. Snapshot of figures used in the One-Semester General Chemistry course. Graphical tools are used to exemplify the properties of different n states as they are generated live during lecture time.

bonds based on electronegativity tables. In most cases, their skills are based on repetitive problem solving; i.e., students might know that H has a $1s^1$ electronic configuration but have no understanding of quantization, what is an orbital, what is a probability density, degeneracy, etc.

For this class, notebook 2 (Particle in an infinite potential box) is used interactively in the lecture. Students are prompted to access the *Jupyter notebook* in their own mobile devices, and they plot the figures for different parameters during the course of the lecture. For example, to answer the question "What is normalization?", the instructor presents graphs of probability densities for different values of n with shaded areas (Figure 6) explaining that the areas are equal. In order to answer "What is the probability of finding the electron between x_a and x_b? How does this probability compare with the probability to find the electron between x_c and x_d?", Figure 6 shows how shaded areas are used for the graphical representation of the integrals.

Other interactive features include comparison of 1D boxes with different lengths or comparison of energy levels for particles with different masses. Individual students are asked to run the notebook for different box lengths and/or masses, after which the whole class compares their results. These explorations are used to introduce the correspondence principle. In addition, a quick overview of a two-dimensional box is shown to teach the concept of degeneracy and to identify states by counting nodes. Outside the classroom, two homework problems (see Supporting Information) make use of the notebook to generate the required data or graphs.

Implementation in Undergraduate Physical Chemistry

In Physical Chemistry courses, students are generally introduced to fundamental quantum mechanics models followed by fundamental spectroscopic topics. The mathematical preparation of students is such that operators, postulates, Schrödinger equations, and some basic linear algebra can be introduced during the course of the semester. In our course, students are presented with the corresponding Schrödinger equations, and solutions are provided by the instructor. The notebooks, presented in their totality using the hidden-code feature, are used to expand the application of these models. For example, notebook 1 (free particle) is used to explore the properties of wave functions, imaginary and real contributions, normalization and the properties of operators, commutators, hermiticity, and eigenfunctions; notebook 2 (particle in infinite potential walls) is presented to understand the intricacies of the a 1D and 2D boxes, boundary conditions, graphical representations, degeneracy, and the correspondence principle; notebook 3 (finite potential) explores concepts of tunneling and introduces numerical and graphical solutions for problems with no analytical solutions; finally, notebook 4 (two wells with a variable barrier) displays the application of the learned concepts into a very simple system, illustrating the addition of wave functions leading to constructive and destructive interference and its effect in the probability density within the barrier. This *Jupyter notebook* allows for the introduction of a simplistic picture of bonding and antibonding wave functions and the introduction of covalent bonding with calculations of probability densities for barriers of different widths.

Implementation in a Quantum Chemistry Graduate Course

For graduate students, we present an introductory lecture on *Jupyter*. This level of classroom implementation takes advantage of the full capabilities of the notebook and allows students to explore their own questions, add variables, and see how the equations and graphs were coded. To run and modify the notebook, students install *Jupyter* in their own computers (Supporting Information). The notebooks are interactively run for different parameters to engage students in questions and answers associated with the models. For example, "For a finite potential box with a 8.0 eV wall, and given n quantum numbers, which state function will have a higher tunneling probability?" Once students answer the question, the graphical representation calculated in notebook 3 can be shown to emphasize the probability density as a function of energy, or as the following: "In the simplest model of 1 electron in a 2-well potential, how do the state energies change as a function of the distance between the center of the wells?" Running notebook 4 for different parameters shows how the energies converge to the independent single box energies when the wells are separated at increasingly large distances. More important is to provide students with time outside the classroom to "tinker" with parameters. Students see the code that generates the numerical answers and graphical outputs, and they can implement some of the cells in their own *Jupyter notebooks* as they create them during the rest of the semester.

Student Feedback

At the end of the undergraduate Physical Chemistry and graduate Quantum Chemistry courses, we executed a very short survey to get student feedback. Detailed results from these surveys are presented in the Supporting Information. The overall response was very positive in both courses, with approximate 80−90% of students finding the notebook "Very Helpful" or "Helpful" to understand the specific topic. The

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graduate level implementation needed more participation from students, and they were required to create their own *Jupyter notebook* for other topics. For the graduate students, as expected, the results were tainted by their experiences trying to write their own notebooks. As a follow-up to this survey we created the server version, which removes any visible code and allows them to focus *only* on the quantum mechanics. This is quite reasonable for an undergraduate level course, although at the graduate level we will continue to provide the full code of the *Jupyter notebooks*. In today's academic environment, every graduate student needs to learn at least a little bit of a programming language, and *Jupyter* has become tremendously useful for physical chemists.

In our experience, using this material enabled students to better understand concepts like plotting and representing wave functions and probability densities, localization and delocalization of wave functions, boundary conditions, tunneling probabilities, degeneracy, and difference between even and odd solutions, among others. This conclusion is based on the type of questions students asked during office hours, the quality of the plots they presented to answer homework questions, and the fact that, during lectures of other topics, students referred back to the plots encountered in these notebooks to try to understand the new subjects.

For example, during lecture, when the instructor introduced the harmonic oscillator and its zero point energy in the undergraduate Physical Chemistry course, students referred to the particle in the box energy diagrams and the energy dependence on "*n*" observed in the second notebook; when the instructor talked about bonding and antibonding MOs in H_2^+ and introduced a linear combination of atomic orbitals to form an MO, students recalled the two boxes separated by a barrier they had seen at the beginning of the semester and asked whether the LCAO was in any way related to the sum of waves they had seen in the last notebook. These types of questions and connections between concepts had not been observed in previous semesters, where no interactive graphical platform had been used.

We note that these notebooks are meant to complement a lecture, not to replace it.

CONCLUSIONS

In this work, we showed how the quantum mechanical description of a particle in simple model potentials can be explored and taught interactively in the classroom with the use of the *Jupyter notebook* platform. While the concepts are well-developed in standard textbooks, our students reported an enhanced learning experience from the use of this material which allowed them to better grasp the concepts and mathematical equations presented in class.

We hope this paper will encourage students and educators to develop new educational interactive platforms, in the area of quantum chemistry.

ASSOCIATED CONTENT

Supporting Information

The Supporting Information is available on the ACS Publications website at DOI: 10.1021/acs.jchemed.9b00195.

Homework problems (PDF, DOCX)
Student survey information (PDF, DOCX)
Proofs and additional plots (PDF, DOCX)
Instructions for using *Jupyter Notebooks* (PDF, DOCX)
Jupyter notebook files (ZIP)

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Notes

The authors declare no competing financial interest.

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Supporting Information for " Implementing new educational platforms in the classroom: an interactive approach to the Particle in a Box problem "

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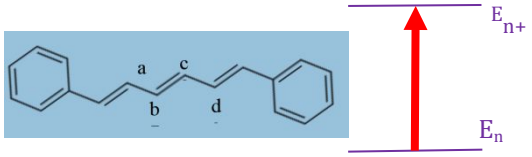
HOMEWORK PROBLEMS ASSOCIATED WITH JUPYTER NOTEBOOKS

One-Semester General Chemistry

1. Exploring a particle in a 2-Dimensional box. Use the link http://kleimanteach.chem.ufl.edu:4000/02_particle_in_an_infinite_potential_box.html to further explore the model of a particle in 1D and in a 2D box. For a particle in a 8.72 Å square box.
   a. How many degenerate states are possible for Energies below 13 eV? (Hint: use a value of *n* or *m* larger than 4)
   b. For each energy level that has degenerate states, list all the groups of degenerate wavefunctions, labeling them according to their n_x and n_y quantum numbers.
2. Consider the molecule 1,6-diphenyl-1,3,5-hexatriene. The region of the linear polyene (excluding the phenyl rings) can be modeled using a 1D box of length L.



   a. For 1,6-diphenyl-1,3,5-hexatriene, the transition is observed at approximately λ =358 nm corresponding to n_i =3 → n_f =4.What is the apparent length of the π-network?
   b. Use the link http://kleimanteach.chem.ufl.edu:4000/02_particle_in_an_infinite_potential_box.html to plot the wavefunction ($\psi(x)$), and the probability density ($|\psi(x)|^2$) for *n=3*, where the size of the model 1-D box correspond to the length of the π-conjugated network.
   c. If we consider the length to be the box size, what is the most likely and the least likely position for one electron in the n=3 state?
   d. What is the probability of finding the electron between the C_a and C_b? How does that compare with the probability to find the electron between C_c and C_d?
   e. In the graph constructed in part b, shade the area that represents the probability to find the particle between C_b and C_d.

The following problems are solved using the *Jupyter notebo*oks introduced in class to obtain the required data,

1. Use the *Jupyter notebook* to evaluate the energy levels of 1 electron in a box 1 Angstrom wide.
    a. Use those values to construct a graph with 4 plots:
        i. Plot the energy of each level as a function of quantum number.
        ii. Plot the energy separation between levels as a function of quantum number.
        iii. Plot together these two quantities.
        iv. Plot the ratio of ΔE/E.
    b. What can you conclude about the behavior of the system as the quantum number increases (at a fix and given T)? (Hint: Bohr's correspondence principle)

    This problem can also be tried using H_2 molecules, $m(H_2) = 2x1836m_e$, in a 1D box of length 500 pm.

2. Show that the function $\Psi_{n_x,n_y}(x,y) = A\sin\left(\frac{n_x\pi}{a}x\right)\sin\left(\frac{n_y\pi}{b}y\right)$ is an eigenfunction of the Hamiltonian of a particle in a 2D box of lengths *a* x *b.*
    a. Given a 5 Å x 5 Å square box, are there any degenerate states at or below E=19.6 eV? If so, write the complete eigenfunction for each state (assume mass =mass of 1 electron, which is what the notebooks uses).
    b. Sketch the the plot for the probability density for each state found in part a. and compare it to the graphs obtained from the notebook.
    c. How many nodes are there in each direction? Can you predict the number of nodes without performing the plot of the 2D wavefunction?

3. Let's look at the behavior of particles confined within finite-size potentials.
    a. What is the major difference in the Probability Densities for a particle constrained within a box of infinite-height potentials versus a particle confined in a finite-height potential?
    b. Consider a particle within a potential box of 1 nm and confined within a V=15 eV potential. What is the state with largest tunneling probability? What is the probability of tunneling outside the classically allowed region?
4. Consider a particle in a 2-well of V_0=6 eV, L= 5 Å and barrier V_1=8 eV. For n =3, plot the Probability density of finding the particle in the classically forbidden region as a function of distance between the wells (work with distance between 0 and 5 Å. If you are looking for the maximum probability to find the particle within the barrier, what would be the optimal distance between wells?

Graduate Level Chemical Bonding

After students had access to the *Jupyter notebooks*, they are required to build their own notebooks. For this assignment, students may modify the notebooks provided and create their own components.

1. A rough treatment of π-electrons in a conjugated molecule regards these electrons as particles moving in a "particle in the box potential", where the length of the box is somewhat longer than the conjugated chain. The Pauli exclusion principle allows no more than 2 electrons in each energy level. For butadiene CH_2=CHCH=CH_2, taking the box to be 7.0 Å, estimate the λ of the light absorbed when a π -electron is excited from the highest occupied level to the lowest unoccupied level. Compare the results with the experimental value of λ= 217 nm and draw some conclusions on the limitations of the model.

2. Consider a square box of length 1 Å x 1 Å . Use *Jupyter Notebooks* to:
    a. Draw the contour plot for the wavefunction and the probability density of an electron in a 2D box with (n_x , n_y)= (1,2) and (2,1).
    b. In a graph, show that for a constant value of x , the functions look like a 1-D particle in a box with $n_y - 1$ nodes.
    c. Write a short script to evaluate the probability of finding the particle in the region between (0.2, 0.7) and (0.2 + Δx, 0.7 + Δy) Å.
    d. Compare that probability with the probability of finding the particle in the region between (0.8, 0.3) and (0.8 - Δx, 0.3 - Δy) Å. For this comparison, a graphical representation is good: Plot the Probability Density as a function of position and use shaded areas to show the integrated values.

3. Consider the simplistic description of H_2^+ as a 1D box of length 95 pm. Use Jupyter Notebooks to evaluate the energies of the eigenstates of a particle within that box.
    a. Graph 3 plots: in the first one, plot the Energy of each level as a function of quantum number; on the second one: plot the Energy separation between levels as a function of quantum number, and on the last one, plot the ratio of ΔE/E.
    b. Compare these plots with kT (for a given T), what can you say about the behavior of the molecule as the quantum number increases? (Hint: Bohr's correspondence principle)

Supporting Information for " Implementing new educational platforms in the classroom: an interactive approach to the Particle in a Box problem "

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STUDENT SURVEY

Some responses from survey of students who used the *Jupyter notebooks*.

Undergraduate Physical Chemistry students

The course had 16 students, with 9 of them answering the anonymous survey. Overall, students were satisfied with the notebooks they used. The implementation in the undergraduate course was as a single interactive notebook in a public server. Students could change parameters but did not see the code nor they had access to modify it.

	The Free Particle	The infinite potential:		The finite potential box	Tunneling
		1D box	2D box		
Did you find the notebook helpful to understand...?	% Very helpful (Helpful)	% Very helpful (Helpful)		% Very helpful (Helpful)	
	55.6 (44.4)	44.4 (44.4)	22.2 (66.7)	66.7 (22.2)	77.8 (11.1)
Did you run the notebook multiple times using different parameters?	% Yes	% Yes		% Yes	
	66.7	88.9	75.0	100	77.8
Students were asked about concepts they felt they understood by using the *Jupyter notebooks*, written in their own words	• Visualizing uncertainty between momentum and position in the free particle • How energy, of a particle, is related to its space of confinement • The graphs helped in visualizing the wave functions. Since we were able to change the values it was easy to see what the results would be for a given set of conditions. • Tunneling effect when a box has finite-sized walls	• Effect of box length on the 2-Box wavefunction • Degenerate energy levels of different coordinates in the 2D box •How the boundaries of the box allow only certain energy levels		• The cause of tunneling, the effect of energy on tunneling probability, • Probability can be found outside of a finite-sized wall • How the size of the barrier affects the tunneling effect.	

First semester graduate students

In this course, 11 students answered the survey. Students were provided the notebooks and had full access to modify the code. Part of their learning included *Jupyter* components; HW problems took advantage of this, and students were asked to create their own small notebooks, in which the notebooks provided could be used as the starting point.

	The free particle	The infinite potential:		The finite potential box
		1D box	2D box	
Did you find the notebook helpful to understand...?	% Very useful (Useful) 9.1 (81.8)	% Very helpful	(Helpful)	% Very helpful (Helpful) 27.3 (63.6)
		10.0 (90.0)	9.1 (63.6)	
Did you run the Notebook multiple times using different parameters?	% YES 54.5	% YES		% YES 81.8
		63.6	63.6	
Students were asked about concepts they felt they understood by using the *Jupyter notebooks*, written in their own words	• Standing wave representation, *Jupyter* plots representation, and user input format • Generating formulas and graphs in python, superposition, probability distributions • Real contribution of wavefunction, imaginary contribution of wavefunction, probability density • Plotting graphs, Understanding the trends by using for different parameters • Uncertainty principle, localization and delocalization, feeling for gaussian function	• Degeneracies of eigenstates of 2-D, 3-D operator, 2-D contour plots in *Jupyter*, background image loading • Finding odd and even solutions in *Jupyter*, offsetting graphical results in python, tunneling probabilities • Wavefunction and probability depending on box size / depending on the magnitude / and the energy level differences • Plotting the wavefunction and probability density varying the parameters, Energy level diagram and Contour plots • Better understanding of what is a wavefunction • 2D representation of wavefunctions, 2D probability densities, 2D degeneracies • Boundary condition, superposition of eigenfunctions, contribution of coefficient and box sizes		• Bound and unbound wavefunctions, effect of potential barrier, tunneling • Even and odd solutions depending on box size and Vo, finding bound state, wavefunction changes • Numerical solutions to the finite potential box. • Plotting wave function, Probability density & energy level diagram • Tunneling probabilities • How it is different from infinite box

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PROOF: WAVEFUNCTIONS CAN BE EVEN OR ODD WHEN THE POTENTIAL IS EVEN

For even potentials there are two families of solutions with : $\psi(-x)=\psi(x)$ or $\psi(-x)=-\psi(x)$. Here we show the proof. Let's assume the potential is even, that is, that $V(-x)=V(x)$. The time-independent Schrödinger equation is:

$$-\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2}+V(x)\psi(x)=E\psi(x) \quad (1)$$

We can now write the equation for $x\to -x$:

$$-\frac{\hbar^2}{2m}\frac{d^2\psi(-x)}{dx^2}+V(-x)\psi(-x)=E\psi(-x) \quad (2)$$

As $V(-x)=V(x)$, we see that $\psi(x)$ and $\psi(-x)$ obey exactly the same equation. For this reason, $\psi(x)$ and $\psi(-x)$ must be equivalent solutions except for a multiplicative constant, that is:

$$\psi(-x)=a\psi(x) \quad (3)$$

Because $\psi(x)$ and $\psi(-x)$ must have the same norm, we have that $|a|=1$. This leads then to two possibilities: $a=1$ (even wavefunction) and $a=-1$ (odd wavefunction).

It is important to mention that it is possible to make linear combinations of $\psi(x)$ and $\psi(-x)$ in such a way that it would still be a solution but with undefined parities.

PROOF: WHY THE ENERGY LEVELS SHIFT DOWN FOR THE FINETE BOX

Let's consider the following potential:

$$V(x,\lambda)=\begin{cases} 0 & \text{for} \quad -L/2 < x < L/2 \\ V_o+\lambda(V_2-V_o) & \text{for} \quad \text{other values} \end{cases} \tag{4}$$

We see that for $\lambda=0$ we have a particle in a finite box potential with a potential depth equal to V_o, and for $\lambda=1$ the potential depth is equal to V_2. Let's assume that $V_2>V_o$, therefore $V(x,\lambda)$ increases with λ. We have that:

$$\frac{\partial V(x,\lambda)}{\partial\lambda}=\begin{cases} 0 & \text{for} \quad -L/2 < x < L/2 \\ V_2-V_o & \text{for} \quad \text{other values} \end{cases} \tag{12}$$

Therefore, as $V_2>V_o$, we have $\frac{\partial V(x,\lambda)}{\partial\lambda}\geq 0$.

According to the Hellmann-Feynman theorem, we have that:

$$\frac{dE_{n,\lambda}}{d\lambda}=\int_{-\infty}^{+\infty}\psi_{n,\lambda}^{*}\frac{d\hat{H}_{\lambda}}{d\lambda}\psi_{n,\lambda}\,dx \tag{13}$$

As the kinetic energy operator does not depend on λ, we have that:

$$\frac{dE_{n,\lambda}}{d\lambda}=\int_{-\infty}^{+\infty}\psi_{n,\lambda}^{*}\frac{\partial V(x,\lambda)}{\partial\lambda}\psi_{n,\lambda}\,dx\geq 0 \tag{14}$$

Therefore, as $\frac{dE_{n,\lambda}}{d\lambda}\geq 0$, the higher the value of λ, the higher the value of the energy level is (or the energy value remains the same if $\frac{dE_{n,\lambda}}{d\lambda}=0$). So we can conclude: E_n for $V_2\geq E_n$ for V_o. This conclusion is still true on the limit in which $V_2\to+\infty$, and explains why the energy levels for the finite box shift down in comparison to the infinite box levels.

PARTICLE IN TWO BOXES WITH FINITE-POTENTIAL WALLS

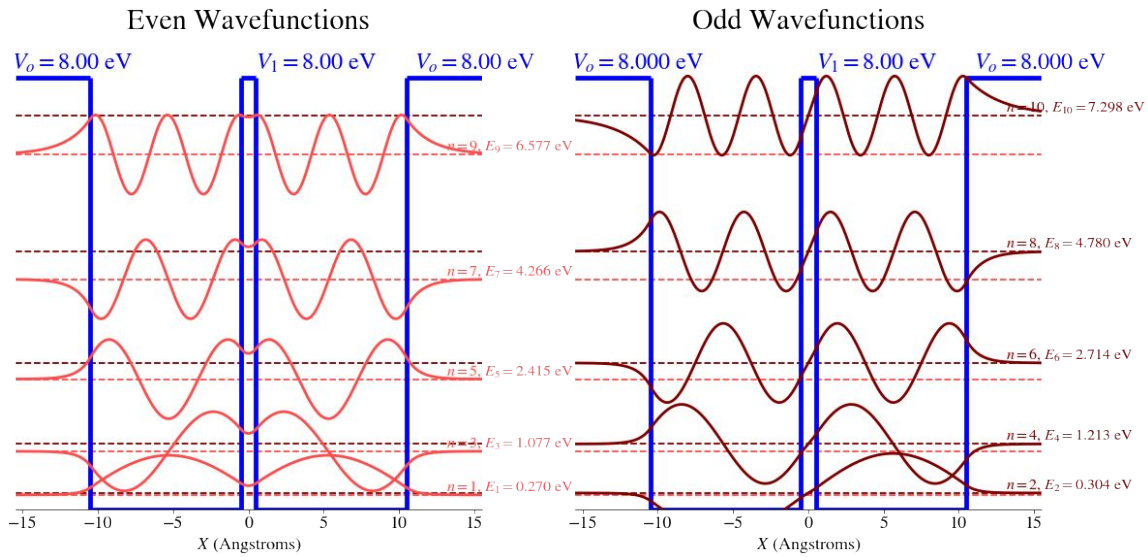

Figure S1. Wavefunction solutions for $V_o = V_1 = 8$ eV, $L = 10$ Å, and $d = 1$ Å. Even wavefunctions maintain the numbers of nodes as in the corresponding separate box, while the odd solutions have an additional node at the center of the barrier.

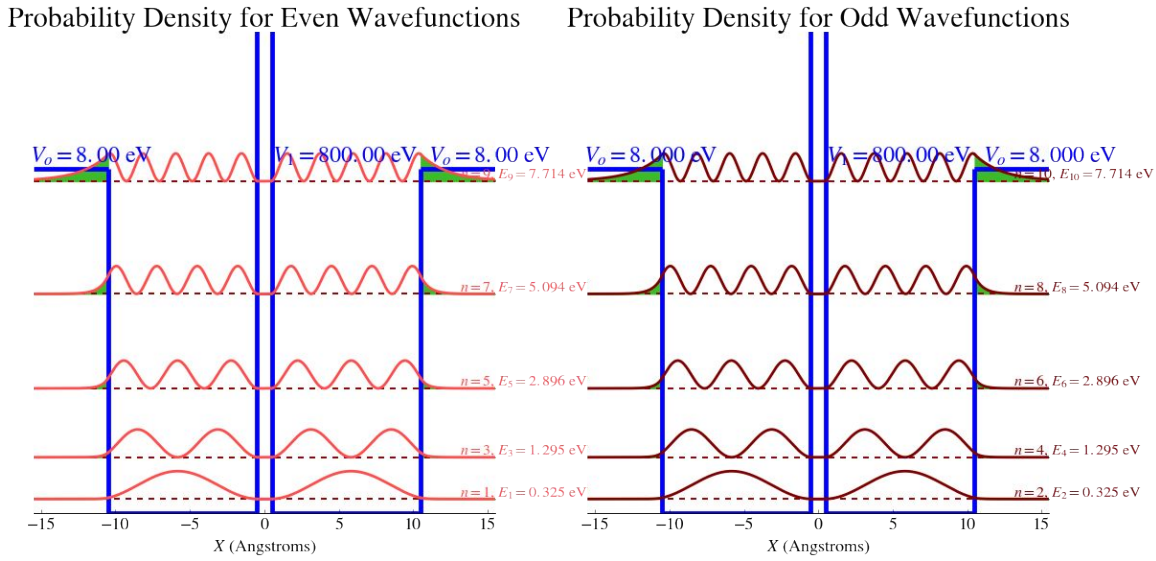

Figure S2. Probability densities for an electron in a two finite-potential boxes with V_o =8 eV, V_1 = 800eV L = 10 Å, and d = 1 Å. The areas shaded in green correspond to the tunneling probability and the area shaded in purple corresponds to the probability of finding the particle between the boxes.

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INSTRUCTIONS FOR RUNNING THE NOTEBOOKS IN A WEB SERVER

To make it convenient for instructors to use the notebook without having to ask students to install and learn the Jupyter environment, we converted the notebook into a webpage where the student could use the notebook with full functionality purely inside a browser. The webpage is hosted at http://kleimanteach.chem.ufl.edu:4000/.
Students only need to type numbers into the form and click "Show" button to see the result.
The webpage has a server-client architecture where the inputs of students are sent to a server, the server draws the figures and return it back to students to display in the browser. The source code for the server is hosted on GitHub at: https://github.com/zasdfgbnm/a_quantum_particle_moving_in_space-server
Instructors could modify the code on their own and build their own server. The server runs inside Docker, which makes building the server as simple as a single command:
"docker build".

INSTRUCTIONS FOR INSTALLING AND RUNNING *JUPYTER NOTEBOOK* AND ALL THE NECESSARY LIBRARIES

The host website for *Jupyter* can be found here: https://jupyter.org/

There are several ways of installing *Jupyter notebook* (like through pre-packaged distributions as Anaconda, available for several operational systems: https://www.anaconda.com/distribution). Hereafter, we provide step-by-step instructions on how to install *Jupyter notebook* and all necessary libraries on Windows, Linux and Mac OS.

Installation instructions for Windows

1) Download the latest version of Anaconda for Python 3 from: https://www.anaconda.com/distribution/. You will get a *.exe file.

2) Install the *.exe file following its instructions. After installation, you should see a new application called "Anaconda Navigator" added to your start menu.
3) Extract the supporting information ZIP file downloaded from the *J. Chem. Educ.* website and copy its content (*Jupyter notebook* files in format *.ipynb, and figures in format *.png) somewhere in your home directory, for example, C:\Users*YourUserName* . Avoid directories that contain special characters if you run into problems.
4) Open "Anaconda Navigator", and open "Notebook" from Anaconda Navigator. A browser window should be opened automatically.
5) Navigate to the directory where you put these *.ipynb files, and open the file you want.

Installation instructions for Linux

The following instructions were tested on an Ubuntu machine.

1) Download the latest version of Anaconda for Python 3 from: https://www.anaconda.com/distribution/. You will get a *.sh file.
2) Open a terminal window.
3) From the same folder where the *.sh file is, execute the following command:
```
$ bash Anaconda3-*.sh
```
4) Follow the on-screen prompts to complete your installation. When asked about the initialization of Anaconda in your $HOME/.bashrc file, enter: yes. Once the installation is complete, execute:
```
$ source ~/.bashrc
```
5) Extract the supporting information ZIP file downloaded from the *J. Chem. Educ.* website and copy its content (*Jupyter notebook* files in format *.ipynb, and figures in format *.png) into the same directory of your terminal window.
6) In your terminal window execute *Jupyter notebook* with the following command:
```
$ jupyter notebook
```
7) A tab should open in your web browser. Among the files and subfolders listed, click on any *.ipynb file to launch that given *Jupyter notebook*, which will open in a new tab in the browser.

Installation instructions for Mac OS

Although Python is a default package in Mac OS, we are going to perform a new installation based on Anaconda to make sure that all the libraries necessary to run all the *Jupyter notebook* programs provided in this paper are going to run properly.

1) Download the latest version of the Anaconda installation file for Mac OS (*.pkg) from https://www.anaconda.com/distribution. Make sure you download the Python 3 version of anaconda.

2) Execute the *.pkg file by double clicking on it and follow all instructions on the screen.
3) Open a terminal window.
4) Extract the supporting information ZIP file downloaded from the *J. Chem. Educ.* website and copy its content (*Jupyter notebook* files in format *.ipynb, and figures in format *.png) into the same directory of your terminal window.
5) In the terminal execute *Jupyter notebook* with the following command:

```
$ jupyter notebook
```

6) A tab should open in your web browser. Among the files and subfolders listed, click on any *.ipynb file to launch that given *Jupyter notebook*, which will open in a new tab in the browser.

How to run the *Jupyter notebook* program

If the reader is getting started with *Jupyter notebooks*, introductory lectures written by J. R. Johansson are an excellent starting point and are available at: https://github.com/jrjohansson/scientific-python-lectures . Information about *Jupyter notebook* can also be gathered from *Jupyter's* website: https://jupyter-notebook.readthedocs.io/en/stable/

A *Jupyter notebook* is structured as a sequence of cells. Roughly speaking, there are two main types of cells: code cells (that contain Python code) and markdown cells (to display text, including in LaTeX format). Our *Jupyter notebook* programs were written in such a way that the code cells have to be executed in consecutive order. Each code cell can be individually executed by pressing *Shift+Enter* with the cell selected. A useful way to speed up executing cells in the correct order is to select the cell of interest and then click on "Run All Above" at the tab "Cell" at the toolbar on the upper part of the page.

NOTE: there are some code cell that require the user to enter information before executing. The desired information can be entered in the boxes that appears on the screen right after the cell.

NOTE: A message saying that the notebook has been converted from an older format (v3) to a new format (v4) may appear on the screen when the *Jupyter notebook* files are open. This is not an issue. The programs will execute normally. The notebook files were written in an older version because newer versions are able to read it, however if the files were written in a newer version users using older versions may not able to open the files.