

**Non-obvious controls:**

- You can select which wave function is shown in the bottom graph by moving your mouse over the corresponding energy level and clicking.
- The bottom graph will also show a highlight of the state that your mouse is over, so you can compare two states.
- Use the **Save/Load** feature in the **File** menu to save a configuration for lecture or homework.
- Be sure to try all the different tabs at the top of the simulation.
- You can **Pause** the sim and then use **Step** to incrementally analyze.
- **Restart** will return a wave packet to its initial configuration.
- You can change the configuration of the potential energy by dragging the lines on the graph, clicking or **Configure Potential**, or using the **Potential** menu.
- If you want to look at the time-independent real part of the wave function as it is shown in most textbooks, **Pause** and then press **Restart** to reset the phase.
- The **magnifying glass** is useful in the second two tabs to help distinguish closely spaced energy levels in bands.
- Use the **Colors** menu to change the color scheme.
- If you are doing a lecture demonstration, set your screen resolution to 1024x768 so the simulation will fill the screen and be seen easily.

**Important modeling notes / simplifications:**

- There is no option for an infinite square well potential, but you can approximate it by making the height of the finite square well potential very large.
- The wave function is not normalized, so you cannot directly compare the magnitude of one wave function to another.
- Because the speed of oscillation of the wave function depends on the energy, this speed will vary for different configurations. You can adjust the speed with the slider at the bottom. Superposition states of closely spaced energies are particularly slow.
- The simulation solves the 1D Schrodinger equation numerically in real time. The mass is set to the electron mass, so you can use this mass to do calculations.
- In **1D Coulomb** mode, we solve the 1D Schrodinger equation for  $V(x) = -ke^2/|x|$ . Because of the discontinuity at  $x = 0$ , odd solutions are unstable<sup>1</sup>, so only even solutions are shown. These even solutions have the same energies as in a 3D Coulomb well.
- In **3D Coulomb** mode, we solve the radial part of the 3D Schrodinger equation for  $V(r) = -ke^2/r$  and  $L = 0$ . The “probability density” shown in **3D Coulomb** mode is  $|\psi(r)|^2$ . Technically the probability density is given by  $r^2|\psi(r)|^2$ , which is equivalent to the probability density  $|\psi(x)|^2$  shown in **1D Coulomb** mode.
- We often teach that in double well systems, the energy levels split but do not shift. This is true for square wells, but for other wells the behavior is much more complicated, as you can see by selecting **1D Coulomb** potential in the **Two Wells** or **Many Wells** tabs.
- In the **Many Wells** tab, if you choose **Average probability density of band**, it will show  $|\psi_1|^2 + |\psi_2|^2 + |\psi_3|^2 + \dots$ , including each state in the band. This feature, taken from the

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<sup>1</sup> There is a vast literature debating the existence and properties of the odd solutions of the 1D Coulomb potential: Loudon, *Am. J. Phys.* **27**, 649 (1959); M. Andrews, *Am. J. Phys.* **34**, 1194 (1966); L. K. Haines and D. H. Roberts, *Am. J. Phys.* **37**, 1145 (1969); M. Andrews, *Am. J. Phys.* **44**, 1064 (1976); J. F. Gomes and A. H. Zimmerman, *Am. J. Phys.* **48**, 579 (1980); C. L. Hammer and T.A. Weber, *Am. J. Phys.* **56**, 181 (1981); L. S. Davtyan et al., *J. Phys. A* **20**, 2765 (1987); M. Andrews, *Am. J. Phys.* **56**, 776 (1988).

Consortium for Upper Level Physics Software (CUPS) program `latce1d2`, allows students to get a sense of the overall distribution of electrons in a band.

**Insights into student use / thinking:**

- Students may ask why there is a clock, since nothing is changing in time in the default setting. The clock is there to emphasize that the probability densities of energy eigenstates do not change in time, and to contrast this with the probability densities of superposition states and the wave functions of all states.
- Students often have difficulty understanding the meaning of complex wave functions. This can perhaps best be illustrated by the observation that students frequently ask, “What is the physical meaning of the imaginary part of the wave function?” (Students never ask about the physical meaning of the real part!) Using both the real part and the imaginary part in the simulation can help students understand how the two are related and see that they are both equally important.
- The simulation includes additional representations of the wave function which show the **magnitude** as a black curve and the **phase** as a color included within the magnitude curve. In interviews, we found that *none* of the students were able to make sense of this representation without significant help from the interviewer, including one student who had taken a class where the representation was used extensively. We note that this “phase color” representation is the *only* representation used in most quantum mechanics simulations, both commercial and free. Please use this representation with caution!

**Suggestions for sim use (NOT an exhaustive list!):**

- For tips on using PhET sims with your students see: [Guidelines for Inquiry Contributions](#) and [Using PhET Sims](#)
- The simulations have been used successfully with homework, lectures, in-class activities, or lab activities. Use them for introduction to concepts, learning new concepts, reinforcement of concepts, as visual aids for interactive demonstrations, or with in-class clicker questions. To read more, see [Teaching Physics using PhET Simulations](#)
- For activities and lesson plans written by the PhET team and other teachers, see: [Teacher Ideas & Activities](#)
- Ask students to use the simulation to determine general rules for the effects of changing width, depth and offset of a potential well, and the *reasons* for these rules.
- Use the **Two Wells** panel to illustrate energy splitting and symmetric and antisymmetric wave functions.
- Use the **Many Wells** panel to help students to build up a model of an electron in a wire as a finite square well by gradually adding more wells.
- If your goal is to help students understand the phase color representation, it is helpful to superimpose the real and imaginary parts on top of it. You can then point out that the color is always red at the peaks of the real part and always yellowish green at the peaks of the imaginary part. Thus, the color is a measure of where you are in the cycle of real and imaginary.

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<sup>2</sup> J. R. Hiller, I. D. Johnston, and D. F. Styer, “Quantum mechanics simulations : the Consortium for Upper-Level Physics Software,” New York: Wiley (1995).