

Tutorial for PhET-Sim “Quantum Bound States”

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With this PhET-Sim, we will explore the properties of some prototypical quantum systems. This tutorial assumes that the particle in a box, tunneling, and the harmonic oscillator have been treated in class, or that this tutorial guides an in-class activity. The tutorial is meant for undergraduate and graduate level introductory quantum mechanics courses. Go to

http://phet.colorado.edu/simulations/sims.php?sim=Quantum_Bound_States.

Click on the Run Now! button. When the sim starts running, click pause and rewind to $t=0$.

1. Square well

We'll start with the square well, which is the default starting point in the sim. The potential energy function is displayed in the top panel as a full magenta line. The energy levels (energy eigenvalues) in the well are shown as thin green lines, and the energy level of the state currently displayed in the lower panel is highlighted as a red line.

1.1. Qualitative observations

- Click the double arrow symbol on the bottom of the well and drag it up and down. You will notice that the pattern of the energy eigenvalues moves with the well, but the spacing of the levels does not change. Why?
- Click on the double arrow symbol at the right hand side in the middle of the well and drag it left and right. Explain the behavior of the energy levels when you do this in your own words and with an equation.
- Click on the double arrow symbol at the right hand side of the top of the well and drag it up and down. Explain the behavior of the energy levels.
- On the right hand side of the sim, there is a sliding bar where you can vary the mass of the particle in the well. Explain the behavior of the energy levels when you do this in your own words and with an equation.

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- e. Push the “Reset All” button on the right hand side of the sim. Make sure that the bottom panel of the sim displays the probability density. Push the “Play” button, so that the timer starts to run. You can speed the sim up to “fast”. What happens to the probability density, and why? Do you expect to see the same behavior for the first excited state? Click on the green line representing the first excited state and check your prediction.
- f. Push the “Reset All” button again, then “Pause” and “Rewind” to set the time to $t = 0$. Click the radio button for “Wave Function” on the right hand side of the sim and check only the “real part” box. Set the sim speed to one level above “normal” and start the timer. What do you observe? You know from class that $\int_{-\infty}^{+\infty} \psi^* \psi dx$ must be 1 for a physically meaningful particle. Is this the case for all times for what is displayed? Now check the box “imaginary part” and repeat the experiment. Check both boxes and repeat. Explain your observations.

1.2. Quantitative experiments

Drag the “ \updownarrow ” symbol in the bottom of the potential well down until it is at -5.0 eV. Then, set the potential energy value outside the box to 0 eV dragging the “ \updownarrow ” symbol at the right of the well (this will then display “height 5.0 eV”). Drag the width controller symbol (“ \leftrightarrow ”) in the right hand wall of the potential well to adjust the width of the potential.

- a. Vary the width d of the potential well in steps of 0.1 nm up to 2.0 nm and write down the number of bound states for each width. Plot the number of bound states as a function of the width using a spreadsheet program. Also plot the number of bound states as a function of the minimum width that is needed to support that number of bound states and interpret the plot! (Hint: a linear fit of the second plot gives you some clues).
- b. Write down all energies of the eigenstates in the potential well for $d = 2.0$ nm and plot them as a function of the quantum number n (the lowest state has $n = 1$). Compare with the behavior of a particle in a box (i.e., infinitely high walls) of the same width and interpret! (Use the electron mass for the comparison, take into account that the bottom of the well is at -5 eV).
- c. Drag the “ \updownarrow ” symbol at the right of the well as high as it goes in the panel. The well is now 20.0 eV deep. Again, write down all energies of the eigenstates in the potential well for $d = 2.0$ nm and plot them as a function of the quantum number n (the lowest state has $n = 1$). Compare with the behavior of a particle in a box (i.e., infinitely high walls) of the same width and interpret! (Use the electron mass for the comparison, take into account that the well depth is at -5 eV).

- d. Push the “Reset All” button again, then “Pause” and “Rewind” to set the time to $t = 0$. Display the real part of the ground state wave function. It will be at its maximum value everywhere. Use the timer to measure the time until the real part comes to its maximum value again. How could you measure this time more accurately? Repeat this experiment with all the states currently displayed.
- e. Use the times you determined in part (d) to predict the energies of the states. Compare with the number that’s displayed when you hover the mouse above the green line representing each state.

2. Asymmetric well

The asymmetric well has properties similar to the square well, but it is ... well ... asymmetric! We will take a look at how that changes the behavior of the energies and states. Use the default setting of the well (click on “Reset All”, then select “Asymmetric” in the Potential Well pulldown menu).

2.1. Qualitative observations

- a. Take a look at the ground state probability density and the real part of the wave function. How is it different from that of the square well?
- b. Without doing the simulation, just think about the highest state in the asymmetric well, and try to predict the shape of the wave function and probability density. Will the wave function have any nodes? If so, how many? Where do think you are most likely to find the particle, on the shallow end of the well or in the deep region of the well? Why? Now do the experiment and describe the result. Does it fit with your expectations?

2.2. Quantitative experiments

Drag the “ \updownarrow ” symbol in the bottom of the potential well down until it is at -5.0 eV. Then, set the potential energy value outside the box to 0 eV dragging the “ \updownarrow ” symbol at the right of the well (this will then display “height 5.0 eV”). Drag the width controller symbol (“ \leftrightarrow ”) in the right hand wall of the potential well to adjust the width of the potential.

- a. Write down all energies of the eigenstates in the potential well for $d = 2.0$ nm and plot them as a function of the quantum number n (the lowest state has $n = 1$). Compare with the behavior of a particle in a box (i.e., infinitely high walls) of the same width and interpret! (Use the electron mass for the comparison, take into account that the bottom of the well is at -5 eV).
- b. Drag the “ \updownarrow ” symbol at the right of the well as high as it goes in the panel. The well is now 20.0 eV deep. Again, write down all energies of the eigenstates in the potential well for $d = 2.0$ nm and plot them as a function of the quantum number n (the lowest state has $n = 1$). Compare with the behavior

of a particle in a box (i.e., infinitely high walls) of the same width and interpret! (Use the electron mass for the comparison, take into account that the bottom of the well is at -5 eV).

3. Harmonic Oscillator

Use the default setting of the well (click on “Reset All”, then select “Harmonic Oscillator” in the Potential Well pulldown menu).

- Click on the double arrow symbol at the left hand side of the potential curve and drag it left and right. Explain the behavior of the energy levels when you do this in your own words and with an equation.
- On the right hand side of the sim, there is a sliding bar where you can vary the mass of the particle in the well. Describe your observations. Why does the level spacing not change in this sim?
- Push the “Reset All” button on the right hand side of the sim and choose the Harmonic Oscillator again. Try to remember the curvature of the potential and slide the mass all the way to the left. Then use the double arrow symbol to recreate the potential curve to the same curvature it had before you changed the mass. How did the energy levels change? Explain the behavior of the energy levels when you do this in your own words and with an equation.

4. 3D Coulomb Potential

This part of the sim displays a radial cut through the potential energy function of a H-atom for s-states. Use the default setting of the well (click on “Reset All”, then select “3D Coulomb (L=0)” in the Potential Well pulldown menu).

- Display the real part of the ground state wave function. Is it differentiable at $x = 0$? Why or why not?
- Now click on the radio button “Probability Density”. What do you see the radial probability density? How can you tell?
- In the Particle in a Well and in the Harmonic Oscillator, the wave function symmetry alternates between even and odd as you increase the quantum number in steps of 1. Without doing the experiment, do you expect the same to happen here? After you have decided what to expect, check whether you expected the right thing. If the wave function does not behave according to your expectations, try to find the reason why.

Note that the 1D Coulomb potential (which you can also find in this sim) displays anomalous behavior and is mathematically rather advanced. You can check it out and read up on it if you like. It turns out that the

discontinuity for $x = 0$ results in the Hamiltonian for this potential not being Hermitian, unless certain tricks are used. It does not belong into the standard class of QM systems, so we will not treat it further in this Tutorial.

5. Superposition States in a Harmonic Oscillator

Choose the Harmonic Oscillator for this example. Similar ideas work with the other potentials as well.

- a. Consider the first excited state (don't display it yet). Since this system is the QM version of the Harmonic Oscillator, do you expect the probability density to oscillate as time passes? After you have decided, click on the first excited state, and display the probability density. Push the "Play button" and explain your observation. Pause the sim after you have finished your observation.
- b. Display the ground state and display the probability density. Click the "Superposition State" field in the upper right corner of the sim. In the window that appears, you can prepare a wave function as a linear combination of eigenfunctions. All you need to do is to choose the relative weight, i.e., the coefficients c_v for each eigenstate $|v\rangle$. Start by setting both c_0 and c_1 to 1. Hit the "Normalize" button, followed by "Apply" and "Close". Switch between the wave function and probability density displays and explain the shape of the wave function and probability density.
- c. Now hit "Play" and let the timer run until it shows at least 10 fs. Describe your observations.
- d. Reset the timer. Measure the time it takes for the shape of the probability density to regain its initial shape. Now move the mouse pointer over the double arrow on the left hand side of the potential curve and note what is displayed there. Make the connection between the time you measured and the displayed quantity. Check your interpretation by making the potential curve tighter by dragging the double arrow in to double the initially displayed value, then measuring the time for "reshaping" again.
- e. Now prepare a superposition state of the ground state and the 2nd excited state. Repeat part (d). Do the same for each excited state up to $v = 10$. Enter the quantum numbers of the excited states you used together with the times you measured into a spreadsheet and plot the time as a function of the quantum number. Interpret your result.
- f. Try to back up your interpretation from part (e) mathematically by writing down the probability density function for a superposition state of two eigenfunctions belonging to energies E_1 and E_2 . Simplify the equation to extract the time dependence. What do you predict for the time needed to "reshape", if you prepare a superposition for $v = 5$ and $v = 6$? Test your prediction.

6. Two Wells

Choose the “Two Wells” tab at the top of the sim.

- a. Display the real part of the ground state wave function. Describe the pattern of levels that you see.
- b. Try to find a rule for the symmetry behavior of each pair of states.
- c. Vary the width of the wells. Describe the behavior of the splitting between states within a pair and between pairs as the width changes.
- d. Vary the well depth. Describe the behavior of the splitting between states within a pair and between pairs as the width changes.
- e. Vary the well separation. Describe the behavior of the splitting between states within a pair and between pairs as the width changes. Also describe the behavior of the ground state wave function.
- f. Prepare a superposition state of the ground and first excited states. Set the sim speed to the third setting (one below “fast”). Hit “Play” and describe your observations.
- g. Measure the oscillation period of the superposition state as prepared. Make a spreadsheet with the separation between the wells (you can read that by placing the pointer over the double arrow above the barrier between the wells) and the oscillation period. Vary the separation in steps of 0.01 nm from 0.05 nm to 0.1 nm and measure the oscillation period for each separation (you may have to vary the sim speed). Then continue in steps of 0.02 nm to 0.2 nm separation and in steps of 0.03 nm to 0.29 nm. Plot the oscillation period as a function of separation and interpret. Can you find a fit function that describes the dependence? Which phenomenon is at play here?

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