Lecture Tutorial: The Infinite Square Well

In this tutorial you will solve the time independent Schrodinger Equation (TISE) for the infinite square well (also called the particle in a box), one of the simplest possible quantum systems. Although this system seems trivial and completely unrealistic, we can actually model some real physical systems using this potential. Additionally, the infinite well and its solutions will serve as a "testbed" for many interesting and complex ideas in quantum mechanics like collapse of the wave function, superposition of states, etc.

Learning objectives: After you have completed this tutorial, you should be able to

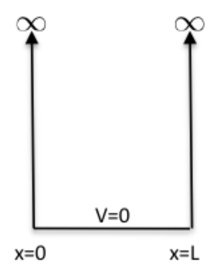
1. Solve the 1D time independent Schrodinger Equation for the infinite square well potential.
2. Draw and visualize solutions to the Schrodinger Equation for this system.
3. Demonstrate that energy quantization arises as a result of boundary conditions.
4. Utilize properties of the energy eigenstates of this system such as orthonormality and completeness.

Let's begin:

Consider a particle moving in 1D and trapped between two hard walls. The potential is

$$V(x) = \begin{cases} 0, & 0 \leq x \leq L \\ \infty, & \text{otherwise.} \end{cases}$$

We call this a particle in a box or a particle in an infinite well.



1. We know that the particle cannot exist outside of the hard walls (because it's energy would have to be infinite). So what is the solution $\psi(x)$ for the time independent Schrodinger Equation in the regions $x < 0$ and $x > L$?

2. Write down the TISE for the region between the walls.

3. Inside the well ($0 < x < L$), is the energy of the particle positive or negative? Why?

4. Show that $\psi(x) = A\sin(kx) + B\cos(kx)$, where $k \equiv \sqrt{2mE}/\hbar$ is a solution to the TISE between the walls.

5. Since the Schrodinger Eq. is a 2nd order ODE, in order for it to make sense the derivatives of $\psi(x)$ must exist. In general, for a function to be differentiable it must be continuous (exceptions exist of course ...). Therefore our first condition on $\psi(x)$ is that it is continuous.

   What must be the value of $\psi(0)$? Why? What about $\psi(L)$?

6. Use the conditions given above to find the value of B.

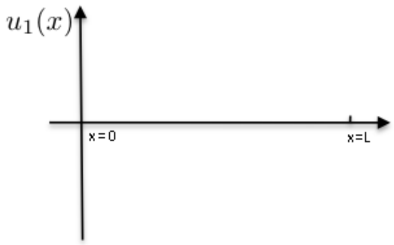
7. Use the conditions given above to find the possible values for k.

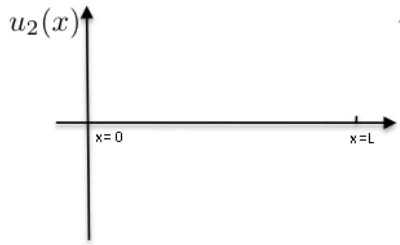
8. Explain why we cannot allow $k = 0$ in our solution.

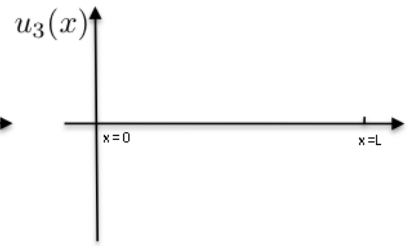
9. Use the definition of k to find a formula for the energy eigenvalues E_n.

10. Normalize your solution. Definition: $u_n(x)$ is defined to be the normalized solution corresponding to the positive integer n. We call these functions energy eigenstates, since they are solutions of the Schrodinger Equation (which is just an eigenvalue-eigenfunction equation) with definite energy. Write out the first three $u_n(x)$.

11. On the axes provided below plot both $u_n(x)$ for n =1, 2, and 3.. Using a dashed lined or a different color superimpose $|u_n(x)|^2$ for n = 1, 2, and 3 as well.



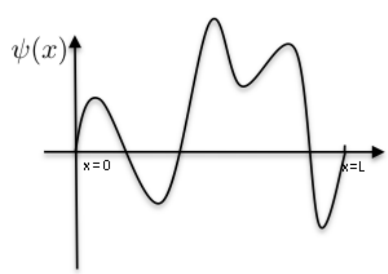




12. For n =1, 2, and 3 what is the most likely position of the particle? Where is there zero probability of finding the particle? Do you see anything weird in the $n = 2$ case?

13. Is du_n/dx continuous at $x = 0$ and $x = L$? Is this OK? Why or why not? Hint: No need to take derivatives - look at your plots of $u_n(x)$ on the previous page.

14. It is important to note that the states $u_n(x)$ are solutions to the Schrodinger Equation and hence eigenstates of the Hamiltonian. However, a particle inside an infinite well need not be in a pure state $u_n(x)$. For example, is the state shown below a valid wave function for a particle in an infinite well? Why or why not?



What is the energy of the state above? Does it have a definite energy?

15. **Orthonormality and Completeness:** The solutions $u_n(x)$ are a set of orthonormal functions. What this means is that the functions are normalized and that they are also orthogonal to each other. What this means practically is that we can use the energy eigenstates $u_n(x)$ as basis functions - any wave function for the particle in a box system can be written as a linear combination of the functions $u_n(x)$.

    Look up the definition of orthogonality for functions and show that $u_2(x)$ and $u_3(x)$ are orthogonal.

16. Write a general wave function $\psi(x)$ for a particle in this one dimensional infinite well in terms of the energy eigenstates $u_n(x)$. If one were given $\psi(x)$, how would one actually calculate this expansion?

Name: ______________________________

Infinite Square Well Tutorial Self-Assessment

Please rate yourself on the learning objectives of the tutorial using the scale provided. Be honest and identify areas in which you are still struggling!

Objective (Students will be able to ...)	Did not Meet Objective	Need more help to meet objective	Met Objective
1. Solve the 1D time independent Schrodinger Equation for the infinite square well potential.			
2. Draw and visualize solutions to the Schrodinger Equation for this system.			
3. Demonstrate that energy quantization arises as a result of boundary conditions.			
4. Utilize properties of the energy eigenstates of this system such as orthonormality and completeness.			

1. After completing the tutorial, where are you still struggling? What are you still confused about and what questions do you have?

2. Any suggestions for improving this tutorial?

3. Quick assessment question: Suppose a particle in a box of size L has the following wave function:

$$\psi(x) = \sqrt{\frac{2}{L}}\left(\sqrt{\frac{1}{3}}\sin(\pi x/L) + \sqrt{\frac{2}{3}}\sin(3\pi x/L)\right).$$

Now suppose we measure the energy of the particle. What possible values of the energy would we obtain and what are the probabilities of obtaining these measurements?