Exploring the infinite and finite square well

Introduction and Background

This exercise will explore the similarities and differences between the finite and infinite square wells.

The infinite square well potential is given by

$$V_{\text{infinite}}(x) = \begin{cases} 0, & \text{if} \quad -\frac{L}{2} \leq x \leq \frac{L}{2} \\ \infty, & \text{otherwise.} \end{cases} \tag{1}$$

The finite square well is similar, but the potential does not go to infinity at the edges. Rather, the finite square well looks like

$$V_{\text{finite}}(x) = \begin{cases} 0, & \text{if} \quad -\frac{L}{2} \leq x \leq \frac{L}{2} \\ a, & \text{otherwise.} \end{cases} \tag{2}$$

Thus, the two systems behave similarly, but there are some important differences between them. We will explore this in the following exercise.

The flowfile

Initially the potential in this flowfile takes the form of an infinite square well, as the expression in the *Potential* node reads `infinite(0,a)`. This expression represents a well of width a centered around the position $x = a/2$. The *Energy Plot* shows the potential (black line) with the $N_{\text{eigenstates}} = 5$ first eigenenergies and eigenstates shown in red and blue, respectively. Each eigenstate is offset on the y-axis by its eigenenergy.

To change the infinite square well to a finite square well of depth h, change the expression in the *Potential* node to `h*finite(0,a)`.

1 The infinite square well

In this exercise, you will explore the infinite square well.

1. Change the width of the well to $a = 2$. What are the new values of the three lowest eigenenergies E_1, E_2, and E_3?
2. What are the values of these eigenenergies if the width is set to $a = 4$? Play around with the different values of a and observe what happens to the energy eigenstates. What changes?[1] What stays the same? In your own words, briefly describe the behavior you observe.
3. Argue why the eigenstates change in this way. You may use your intuition about physics and/or mathematical expressions.

2 The finite square well

To study the finite square well, you must change the potential as described in the **Flowfile** section above. The height is initially set to $h = 1 \times 10^9$.

1. If you entered the expression correctly, nothing will have changed. Why?

[1] The eigensttes may sometimes change sign, causing them to 'flip around'. This is because the eigenstates are only unique up to an overall phase $e^{i\phi}$. The program only ensures that the eigenstates are real, so $\phi = 0$ or π, corresponding to an overall factor of $e^{i\phi} = \pm 1$ multiplying the eigenstates.

2. Change the height to $h = 15$. What happened to the eigenvalues and eigenstates? (Note that you can move the *Energy Plot* around interactively by clicking and dragging, and you can zoom by scrolling while hovering over the plot. The *Reset view* button re-focuses on the boundaries specified in the *Spatial Dimension* and the values of y_{min} and y_{max} that you specify in the *Energy Plot* node.)

3. Argue which of the eigenstates looks the most classical and which looks the least classical. Hint: can a classical state go into a wall?

4. Change the height to $h = 4$ and set $y_{\text{max}} = 8$. Classify each eigenstate as either a bound state or a scattering state.

5. Change the height to $h = 15$ and the width of the well to $a = 1.5$- Set $y_{\text{max}} = 35$ and $N_{\text{eigenstates}} = 15$. Uncheck the ψ_n box to hide the eigenstates, but keep the E_n box checked so the eigenenergies are still shown. You will notice a clear difference in the energy level spacing of the bound and scattering states. Can you give a qualitative explanation for this behavior? (Hint, you may find the study of the free particle ($V(x) = 0$) useful.)