Energy Spectra in Quantum Mechanics

Background

It is common for beginning students of quantum physics to study (among other things) two basic potentials that approximate many real physical systems. The first of these is the infinite square well potential

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

where, for a particle of mass m, the energy of the n-th state is given by

$$E_n = \frac{n^2\pi^2\hbar^2}{2mL^2}. \tag{2}$$

The simple harmonic oscillator potential with frequency ω

$$V_{\text{SHO}}(x) = \frac{1}{2}m\omega^2x^2 \tag{3}$$

admits eigenstates with energies given by

$$E_n = \hbar\omega(n + 1/2). \tag{4}$$

The energy scaling of the eigenstates with increasing n is extremely interesting. For the infinite square well, the energy scaling is quadratic in n, whereas for the simple harmonic oscillator, the energy scales linearly in n.

This exercise will take you through the construction of these scenarios in Composer. After the aforementioned behavior has been verified, you will move on to two other potentials that are not analytically solvable. Herein lies one of the powerful things about Composer, as it easily solves problems that are difficult to tackle analytically. However, by studying these potentials, you will gain some intuition about how the structure of the potential influences the resulting energy spectrum of the system.

The flowfile

We have already made flowfiles that contain flowscenes that you can use to answer the questions below. However, we encourage you to try to build the flowscenes yourself in Composer in order to get a better understanding of the problem. The problem statements will take you through some of the steps necessary to build the flowscenes.

Note that in the provided flowfiles, we have hidden a lot of the background functionality in collapsible elements called scopes. You can use scopes as needed to clean up your code.

When verifying your numbers, remember that in Composer (and most sensible numerical code for simulating quantum mechanics problems), $\hbar = 1$.

1 Problem 1

First, set up a scene that calculates the first 5 eigenstates and eigenenergies of $H = T + V_{\text{SHO}}$.

1. First, you have to define space. Create a *Spatial Dimension* node and a *Potential* node. Connect them with wires.
2. The default potential in Composer is already set to `0.5*a*x^2`. To define the frequency value ω, use a *Scalar* node and attach it to the *a* input on the *Potential* node. Set this to a sensible value, e.g. 1.

3. Create a *Hamiltonian* node and connect the *Potential* node to it.
4. Create an *Energy Plot* node and connect the *Hamiltonian* and *Potential* nodes to it. You may have to tick some of the boxes on the right of the plot to display the different states and energies. This is a great way to visualize the eigensolutions of the system.
5. To get numerical values for the energies, create a *Spectrum* node and connect the *Hamiltonian* node to it. Create 5 *Get Eigenvalue* nodes to the output of the *Spectrum* node. By specifying the *n* values corresponding to different states (remember that the ground state is at $n = 0$), you can get numerical values for the energies.
6. Compare the analytical results that you can calculate using Eq. (4) to the results in Composer. How do these change as you change the values in the *Spatial Dimension* node? What is the minimum value for $x_{\min}$ and $x_{\max}$ that give you accurate results?

2 Problem 2

Do the same as in Problem 1, but change the potential to $V_{\text{well}}(x)$. You can copy the same flowscene as you used in Problem 1, but you need to change the text in the *Potential* node to `infinite(-a/2, a/2)` to create an infinite well potential centered around zero with width a. You will probably experience less accurate results for this potential than you did with the harmonic oscillator potential. Why do you think this is? (Hint: Zoom in on the plots by scrolling with your mouse wheel, and try looking at the wave function near the boundaries of the wall.)

3 Problem 3

Now consider the quartic potential $V_{\text{quartic}}(x) = ax^4$. This potential does not have an exact analytical solution, but we can still use Composer to calculate it numerically. How do the energies roughly scale with n. That is, if $E_n \propto n^k$, what is the value of k (roughly). Is the scaling linear ($k = 1$), sub-linear ($k < 1$), super-linear ($k > 1$) or something else?

4 Problem 4

Do the same as in Problem 3, but for the absolute value potential $V_{\text{abs}}(x) = a|x|$. This can be written in Composer as `a*abs(x)`.

5 Problem 5

Briefly comment qualitatively on the relative energy scaling of the four potentials you explored here. Refer to the shape of the potential. How does the potential shape effect the energy scaling? Do you now better understand the scaling of the potentials you explored in Problems 3 and 4?