

Superposition and expectation values

Introduction and background

In the following exercise, we will study the superposition of eigenstates and expectation values of operators in the harmonic oscillator potential

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

We can write a superposition of eigenstates $\psi_n(x)$ as

$$\Psi(x) = \sum_n c_n \psi_n(x). \tag{2}$$

The complex coefficient c_n tells us 'how much of the n -th energy eigenstate is present in the final superposition state $\Psi(x)$.

Recall also that the expectation value of an operator \hat{O} is calculated by

$$\langle \hat{O} \rangle = \langle \Psi | \hat{O} | \Psi \rangle = \int_{-\infty}^{\infty} \Psi^*(x) \hat{O} \Psi(x) dx. \tag{3}$$

In this case, \hat{O} could be, e.g., the position operator \hat{x} , the momentum operator \hat{p} or the Hamiltonian operator \hat{H} .

The flowfile

The *Potential* node has the following expression for a harmonic oscillator potential written inside of it: $0.5*a^2*x^2$, where the scalar a represents the harmonic frequency ω .

A superposition of $N_{\text{eigenstates}}$ eigenstates can be created using the *Linear Combination* node. The complex coefficients c_n in Equation (2) are entered in the different rows of the boxes listed in the node. The left and right columns in each row represent the real and imaginary parts of the coefficients, respectively. Upon opening the flowfile, the coefficients will all be zero except $c_1 = 1 + 0i$.

The *Position Plot* allows one to view the real and imaginary parts of the wavefunction by checking the boxes $\text{Re}(\psi)$ and $\text{Im}(\psi)$, in red and blue respectively. If you check the box labelled $|\psi|^2$, you will see the probability density of the wavefunction shown by the green line.

Note that with the *Energy Plot* can also show you the eigenstates of the system regardless of the linear combination represented in the *Position Plot*.

The exercise

First, let's consider the state $\Psi(x) = c_1 \psi_1(x)$, which is the state given in the *Linear Combination* node when you open the flowfile.

- Look at the real and imaginary parts of the wavefunction in the *Position Plot*. For the initial value of c_1 , why is $\text{Im}(\psi) = 0$ everywhere?
- Now look at the probability density of the wavefunction and set $c_1 = 0 + 1i$ by swapping the values in both columns of the first row. What happens to $|\psi|^2$? What about the real and imaginary parts of the wavefunction?
- Now try other values of c_1 (you should make sure the *Normalize output* option is checked in the *Linear Combination* node). What happens to $|\psi|^2$ and why?

- What are the expectation values $\langle \hat{x} \rangle$, $\langle \hat{p} \rangle$, and $\langle \hat{H} \rangle$. Do they depend on c_1 ?

Now consider the superposition state $\Psi(x) = c_1\psi_1(x) + c_2\psi_2(x)$. In the *Linear Combination* box, set $N_{\text{eigenstates}} = 2$ and a new row will appear at the bottom of the node where you can specify the coefficient c_2 .

- Create the state $\Psi(x) = \psi_1(x) + \psi_2(x)$. What are the expectation values $\langle \hat{x} \rangle$, $\langle \hat{p} \rangle$, and $\langle \hat{H} \rangle$?
- Create the state $\Psi(x) = \psi_1(x) - \psi_2(x)$. What are the expectation values $\langle \hat{x} \rangle$, $\langle \hat{p} \rangle$, and $\langle \hat{H} \rangle$?
- Argue for the observed behavior of $\Psi(x)$ and the expectation values when the sign was changed. (Hint: check how the individual eigenstates look in the *Energy Plot*.)
- Create $\Psi(x) = \psi_1(x) + i\psi_2(x)$. Look at $\langle \hat{x} \rangle$, $\langle \hat{p} \rangle$, and $\langle \hat{H} \rangle$ and use these to answer the following: Suppose $\Phi(x, t = 0) = \Psi(x)$, that is, the state $\Psi(x)$ represents the initial state of some time-dependent wavefunction $\Phi(x, t)$. What happens to $\langle \hat{x} \rangle$ after some small time δt ? Does it increase, decrease, or remain the same? Does your answer change if, instead, $\Psi(x) = \psi_1(x) - i\psi_2(x)$?
- Try increasing $N_{\text{eigenstates}}$ and play around with different superpositions. Challenge your neighbor to create the largest possible values of $\langle \hat{x} \rangle$, $\langle \hat{p} \rangle$, and $\langle \hat{H} \rangle$!

