

# Probability density, expectation values, and superposition

## Introduction and background

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

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

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

$$\Psi(x) = \sum_n c_n \psi_n(x). \quad (2)$$

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

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

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

Note that these operators can be time-dependent, that is,  $\hat{O} = \hat{O}(t)$ , so in this exercise, we are going to explore how these quantities change under time evolution. Remember the Heisenberg equation of motion

$$\frac{d\hat{O}}{dt} = \frac{i}{\hbar} [H, \hat{O}] + \frac{\partial \hat{O}}{\partial t}. \quad (4)$$

If we take the expectation value everything in this equation, we arrive at Ehrenfest's theorem,

$$\frac{d\langle \hat{O} \rangle}{dt} = \frac{i}{\hbar} \langle [H, \hat{O}] \rangle + \left\langle \frac{\partial \hat{O}}{\partial t} \right\rangle. \quad (5)$$

In this way, we can mathematically describe how operators and their expectation values evolve in time. Finally, the spread in the values that an operator can take is represented by the *variance*

$$\sigma_O^2 = \langle \hat{O}^2 \rangle - \langle \hat{O} \rangle^2. \quad (6)$$

The square root of the variance is known as the *standard deviation*.

## The first flowfile

There are two flowfiles in this exercise, and you will use the first of them for Exercise 1 below. This flowfile titled:

expectation\_values\_and\_time\_dependence\_1.flow, and it is described below.

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  $\omega$ .

A superposition of  $N_{\text{eigenstates}} = 5$  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 be set so that  $c_1 = c_2 = 1 + 0i$ . If you click *Normalize output*, the wavefunction will automatically be normalized, so you don't have to worry about those pesky square roots of 2.

Inside the *Time evolution* loop, there is a *Time Evolution* block that solves the Schrödinger equation and a *Position Plot* that displays how the wavefunction evolves in time. 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. If you click the box labeled  $\langle x \rangle \pm \sigma_x$ , you can see how the expectation value of the position  $\hat{x}$  and the standard deviation  $\sigma_x$  change in time.

## Exercise 1

1. First, let's consider the initial superposition state  $\Psi(x, t = 0) = (\psi_1(x) + \psi_2(x))/\sqrt{2}$ , which is the state given in the *Linear Combination* node when you open the flowfile. Click the green *Play* button at the top left of your screen. Observe how the wavefunction evolves in time. What changes if we change the sign of  $c_1$  or  $c_2$ ?
2. What happens if we make  $c_1$  or  $c_2 = i$ ? What if they are both equal to  $i$ ?
3. What happens to the time dynamics you change the *frequency*  $\omega$  of the trapping potential (denoted in Composer as a *scalar* labelled *omega*)? How does the behavior of  $\langle \hat{x} \rangle$  and  $\omega_x$  change as you change  $\omega$ ? Can you explain what you see?
4. Here, we will make what is known as a *coherent state*. In order to do this, for the first 5 eigenstates,  $n = 1, \dots, 5$ , set  $c_n = \lambda(n - 1)/\sqrt{(n - 1)!}$  where  $\lambda = 0.5$ . This distribution is known as a *Poisson distribution*. Observe the time dynamics. Is anything special about how this wavefunction evolves in time?
5. What happens if you double  $\lambda$ ?

## The second flowfile

Now open the second flowfile, titled:

`expectation_values_and_time_dependence_2.flow`, described below.

Here, you see the same *Potential* node and *Linear Combination* nodes leading to the same *Time Evolution* loop. However, this *Time Evolution* loop has two additional *Scalar Time Trace Plots* that plot  $\langle \hat{x}(t) \rangle$  and  $\langle \hat{p}(t) \rangle$ , or how the expectation values of the position and momentum vary in time, respectively, as described by Equation 5.

In the following exercise, we will explore these dynamics in some more detail.

## Exercise 2

1. First, let's consider the initial superposition state  $\Psi(x, t = 0) = (\psi_1(x) + \psi_2(x))/\sqrt{2}$ , which is the state given in the *Linear Combination* node when you open the flowfile. Click the green *Play* button at the top left of your screen. Observe how the expectation values of  $\hat{x}$  and  $\hat{p}$  evolve in time. As in Exercise 1, what changes if we change the sign of  $c_1$  or  $c_2$ ?
2. What happens if we make  $c_1$  or  $c_2 = i$ ? What if they are both equal to  $i$ ?
3. How do these expectation values evolve in time if we change the value of  $\omega$ ?
4. How do the values of  $\langle \hat{x}(t) \rangle$  and  $\langle \hat{p}(t) \rangle$  relate to one another at any given time? Given what you know about Heisenberg's uncertainty principle, how should they be connected theoretically?
5. Change the potential to  $0.5 * \omega * x^4$  and repeat the above questions. We call this potential an *anharmonic oscillator*. What changes? How is the harmonic oscillator different?
6. Now go back to the typical harmonic oscillator by changing the potential back to where it was when you loaded the flowfile. Try to include more states in your *Linear Combination*. Can you get  $\langle \hat{x} \rangle$  to be static, even though the wavefunction changes in time?

7. How does the addition or subtraction of different states change how  $\langle \hat{x}(t) \rangle$  and  $\langle \hat{p}(t) \rangle$  evolve?
8. Try to link your last answer to theory by writing  $\hat{x}$  and  $\hat{p}$  as combinations of the raising and lowering operators, then understanding how different states link together when you calculate  $\langle \hat{x} \rangle$  and  $\langle \hat{p} \rangle$ .
9. Now we will build what we call an *amplitude-squeezed* state. Set  $c_1 = 0.74$ ,  $c_2 = 0.60$ ,  $c_3 = 0.01$ ,  $c_4 = -0.27$ , and  $c_5 = -0.16$ . Change the position plot so that it shows  $\langle \hat{x} \rangle \pm \sigma_x$  as in Exercise 1. What happens to  $\langle \hat{x} \rangle$  and  $\sigma_x$  as a function of time? For this state,  $\sigma_x$  is small when  $\langle \hat{x} \rangle$  is large. How is this different from the coherent state you made in Exercise 1?

