

Quantum Composer Exercises

Exercise 1

In this exercises we will introduce you to the work flow of Composer and you will see how easily you can find eigen energies and eigen states of an arbitrary potential.

Unzip the zip file and start composer by running 'composer.exe'.

Open the file 'Exercise 1 - eigenenergy and eigenstates.flow'. A block diagram with the following nodes appear:

- Spatial dimension: A definition of the x-axis, as well as the number of points ($n = 1024$).
- Potential: A definition of the potential.
- Hamiltonian: A definition of the Hamiltonian operator.
- Spectrum: Calculating the lowest eigen energies.
- Energy plot: A view of the wave functions and energies.

You can in principle build these charts yourself, but we have pre-made these for you so that you can spend your time on the physics.

1. Check that the current value of the eigen energies fit with the expected value. The program uses $m = \hbar = 1$.
2. Try a larger value / smaller value of $n = 1024$ in the definition of the x-axis - the precision of the calculations depends on this.
Note: The infinite potential well has 'steep wall' boundaries **that are** difficult to solve numerically, so $n = 1024$ is a good bid. For other potentials you may choose a lower value to reduce the calculation time.
3. Change the scalar 'a'. Does the eigen energy change as expected?
4. Which 'a', gives a ground state energy of 1?
5. Are the excited states as expected?
6. Replace the potential with the harmonic oscillator, e.g. $0.5 * a^2 * x^2$ (you may have to adjust the x axis). Check that the eigen energies fits as expected?
7. Try other potentials, eg. $0.5 * a^2 * \text{abs}(x)^q$, where q may be e.g. 1, 5, 10. Adjust 'a' so that the ground state energy becomes 1. How does the excited states distribution change for small and large values of q?

Quantum Composer Exercises

Exercise 2

In this exercise you will create a superposition and work with the position operator. Open the file 'Exercise 2 - probability density.flow' including the following nodes.

- Spatial dimension: A definition of an x-axis, as well as the number of points ($n = 1024$, can be adjusted as needed).
- Potential: A definition of a potential.
- Hamiltonian: A definition of the Hamiltonian operator.
- Spectrum: Calculating the 2 lowest eigen energies (can be changed to several by altering the value of $N_{eigenstate}$).
- Linear Combination: Here, c_1 and c_2 are defined and the linear combination $c_1 * \psi_1 + c_2 * \psi_2$ is calculated as output ψ .
- Position Plot: The calculated wave function is displayed with the mean position $\langle x \rangle \pm \sigma_x$

You can in principle build these charts yourself, but we have premade these for you so that you can spend your time on understanding the physics.

1. Try changing the coefficients c_1 and c_2 .
Does the norm-square change as you expect?
Look at the real-part and the imaginary part.
Investigate 'Normalize output' and 'Normalize coeff.'
2. Generalize to the 3 lower energy eigenvalues with the variables c_1 , c_2 and c_3 .
Try to form a linear combination positioned as far to the right as possible. What can you say about the spread σ_x now compared to the spread of the ground state.
Check if necessary, how the individual states looks at ex. $c_1 = 1$ and $c_2 = c_3 = 0$
3. You can also calculate the position $\langle x \rangle$ and the spread σ_x .
Try to find the x operator in the 'Operator' menu on the left. Its input must be connected to the selected x-axis (pull a wire between the yellow points).
Try to find the mean and scatter in the "State Analysis" menu on the left (the wave function ψ and the operator \hat{O} **must be connected**).
By combining and varying c_1 , c_2 and c_3 you can vary σ_x . Which combination gives the smallest/largest σ_x ? Formulate why.

Quantum Composer Exercises

Exercise 3

In this exercise you will investigate the time evolution of superposition in a harmonic potential.

Open the file 'Exercise 3 - probability density timeevolution.flow'. Then a node diagram appears with many of the same parts as in the previous exercises. There is also a field called 'Time evolution', which is just a 'pre-loop'. Inside this, you see the following:

- Time Evolution: The wave function is time-developed using the time-dependent Schrödinger equation.
- Position Plot: The current wave function is displayed.

Start the time development by clicking on the green play button at the top left. Observe the development of the wavefunction.

1. How does evolution change if the sign of the coefficient is change or we add an imaginary coefficient ?
2. Maintain the wave function as an equal linear combination of the two lower energy eigenvalues. If you change the angular frequency of the potential (here called 'a') what happens to the wave function? the magnitude of the fluctuation of $\langle x \rangle$? and the time dynamics?
Explain your observations?
3. Try to include more states in your linear combination. Can you get $\langle x \rangle$ to be static even if the wave function develops in time?
4. Try to include eg. the 5 lowest eigenstates c_n , with $n = 0, 1, 2, 3, 4$. Select the coefficients as $c_n = \lambda n / \sqrt{n!}$, Where $\lambda = 0.5$ is a suitable value. Is there anything special about the resulting wave function?
Note, composer itself ensures that the coefficients are normalized - the above $|c_n|^2$ corresponds (after correct normalization) to a Poisson distribution, and the wave function is in practice what is called a coherent state.
What happens if λ doubles?
5. You can also get Composer to calculate the integral over $|\psi(x, t)|^2$. Open the file 'Exercise 3 - probability integral timeevolution.flow' and run the program. Try to include more coefficients in the linear combinations and see if you have a good intuition about the dynamics.

Quantum Composer Exercises

Exercise 4

In this exercises you will investigate Open the file 'Exercise 4 - mean values timeevolution.flow'. Then a node diagram appears, much like it from exercise 3. In addition to a 'Position Plot' which shows the wave function for the current time, there are also calculations of the mean values $\langle x \rangle$ and $\langle p \rangle$.

Start the time development by clicking on the green play button at the top left. Note the initial wave function, which is defined as a linear combination of stationary states in the node 'Linear combination'.

1. How does the dynamics of $\langle x \rangle$ and $\langle p \rangle$ look like?
2. How does the image change if the sign is changed on one of the coefficients?
3. What happens if the angular frequency (here called 'a') doubles or halves?
4. What is the relationship between $\langle x \rangle$ and $\langle p \rangle$ from the graphs in Composer? How should they be connected theoretically?
5. Try to change the potential of $0.5 * a^2 * x^4$ and repeat the above question. Can you get more 'wildness' into the time development for $\langle x \rangle$ and $\langle p \rangle$? If so, why? What is special about the harmonic oscillator?
6. To shine a little more light on the above quirks of the harmonic oscillator, consider how $\langle x \rangle$ behaves as a function of time for an arbitrary linear combination of stationary states. Which modes plays a role in the sandwich formula when the x or p operator is expressed through the raising and lowering operators?
7. Try the following start conditions for the harmonic oscillator (remember to return the potential to $0.5 * a^2 * x^2$): $c_0 = 0.74$, $c_1 = 0.60$, $c_2 = 0.01$, $c_3 = -0.27$, $c_4 = -0.16$. Get 'Position Plot' to show $\langle x \rangle \pm \sigma_x$ as well. What happens to the spread as a function of time?
The condition is called 'amplitude-squeezed', since σ_x is small when the amplitude $\langle x \rangle$ is large. On the other hand, one must live with a large σ_x when $\langle x \rangle$ is small !!!
8. Plot σ_x, σ_p and even their product to check whether Heisenberg's uncertainty relationship is met. What are the values of these spreads and their product for the ground state?

Quantum Composer Exercises

Exercise 5

In this task we will try to illustrate what happens if many individual finite wells are connected together. The idea is that the results should reflect the difference between a single finite well and many finite wells representing one atoms to many atoms.

Open the file 'Exercise 5 - towards solids.flow'. (Note: If you have had problems with just a black screen, zoom out a lot and the chart will appear). Then a node diagram appears with the following content:

- 'Spatial dimension' - definition of x-axis.
- 'Number of wells - a packed structure that defines a series of final wells (each with width 2) and with a distance between them defined by the number "separation". The five outputs correspond to 1, 2, 3, 4 or 5 wells. You can unpack the structure by clicking on the small arrow at the bottom of the field.
- Two 'energy plots'. The upper one is programmed to display the energy levels in a single well, the bottom of five wells. You can move the '**connecting wires**' if you want to see the example of 2, 3 or 4 wells.

Try answering the following questions:

1. How many bound states are there for a single well? How many are there for the five wells? This is most easily seen by changing ' $N_{eigenstates}$ ' in 'Energy plot'. Start with value 1 and then gradually increase the value.
2. Note that the energies 'come in groups' for the five wells. How many solutions are there in each group?
3. What conditions are met when energies bundles into a single group?
4. You can also look at the individual wave functions by clicking on $\{\psi_n\}$ in the 'Energy plot'. How do the wave functions next to the five wells compare to the case of a single well?
5. What happens to the wave functions and energies of the individual groups if the distance between the wells change? You can adjust the distance to the left in the diagram by changing the 'Separation between wells'.
6. Discuss what happens if there are not five wells, but a very large number - just as there are many atoms in a solid. If you have heard about about energy band gaps in solids, discuss the relation with them.