Universitat de Barcelona
Facultat de Física

Quantum Composer

In this Computer Session, we will employ the software `Quantum Composer`, available in

quatomic.com/composer/

This software is developed at Aarhus University (Denmark) as a teaching tool for Quantum Mechanics.

`Quantum Composer` is an interactive tool for visualizing and simulating quantum mechanical ideas. It uses a graphical user interface and drag-and-drop panels to solve quantum mechanics problems visually. The Composer is formed by `Nodes`, small boxes with inputs and outputs. These are then connected easily. You can save the solution in so-called `Flow Files`.

Installation

`Quantum Composer` is a standalone program that does not require installation privileges. You should first download `Quantum Composer`, by accessing the website quatomic.com/composer/ and clicking on the "Download" icon of the banner on top. Within the Downloads website, you will find the Windows version of the code, which can be downloaded as a compressed zip file. It's probably best to save this on your Desktop, or any other accessible folder in your computer.

Unzip the file and enter the `Composer` folder. There, you should start `Quantum Composer` by executing the file `Composer.exe`.

The problems below are inspired by original `Quantum Composer` material originally written by Jesper Hasseriis Mohr Jensen (Aarhus University) in 2018.

Submission details

This work is not assessed in terms of marks, but it is compulsory. To submit your results, take a screenshot of your `Quantum Composer` workspace at the end of Problem 3, showing evidence that you have ran a full time evolution of a coherent state. Submit the screenshot and your brief text, as a single file, in the Campus Virtual. Otherwise, send an email with the screenshot and a brief discussion of the time evolution to `arnau.rios@fqa.ub.edu`.

Universitat de Barcelona
Facultat de Física

Computer Session 1

The aim of this session is to build flow files that solve the Harmonic Oscillator (HO) in real space; provide coherent states in a static formulation; and time-evolve the corresponding coherent states.

Harmonic oscillator

The first exercise aims at finding the first 3 eigenstates of a given Hamiltonian. We start with an HO of frequency ω, which has

$$\hat{H} = \frac{1}{2}\frac{\partial^2}{\partial x^2} + \frac{1}{2}\omega^2 x^2. \tag{1}$$

The corresponding eigenenergies are

$$E_n = \left(\frac{1}{2} + n\right)\omega. \tag{2}$$

To get the eigenstates of the HO, you can follow the following steps in `Quantum Composer`:

1. Create a `Spatial Dimension` node and a `Potential` node. Make sure you connect them.
2. The default potential is already $0.5ax^2$. To represent the frequency value a, use a `Scalar` node and attach it to the a input of the `Potential` node. Set it to a sensible value, e.g. 1.
3. Create a `Hamiltonian` node and connect the `Potential`.
4. Create an `Energy Plot` node and connect the `Hamiltonian` and `Potential`. You may have to tick some of the option boxes in the right of the node to display the states and energies.
5. To get numerical values for the energies, use a `Spectrum` node and connect the `Hamiltonian`. Create 3 `Get Eigenvalue` nodes and attach each of them to the output of the `Spectrum`, each with a different value of `n` specified inside.
6. Compare the analytical results of Eq. (2) stated above to the numerical values found in Composer. Do they agree? Try adjusting the parameters in your simulation, e.g. x_{min}, x_{max}.

By now, you should have created HO eigenstates. Your plot should show the eigenstates and the corresponding eigenvalues. If you have time, you may want to check the overlap between your numerically generated eigenstates and the analytical ones given by the equation

Extra challenge: Consider now the quartic potential $V = ax^4$. This potential does not have exact analytical solutions, but we can still calculate it numerically with the `Quantum Composer`. How does the energies roughly scale with n? Is E_n linear, sub-linear, super-linear, or something else in n?

Coherent states: statics

Now that you have already solved the HO, we will look into the more challenging case of building a coherent state. In this exercise, we will build this by displacing the center of the HO well by a distance x_c. The ground state wavefunction in this case is simply a displaced gaussian,

$$\psi_0(x) = \mathcal{N} \exp\left(-\frac{\omega\,(x - x_c)^2}{2}\right), \tag{3}$$

with $\mathcal{N}$ a normalization constant.

1. Setup a scene employing the same structure as in the previous exercise, with an HO centered at 0.To this aim, create and connect a `Spatial Dimension`, a `Potential`, a `Scalar` and a `Hamiltonian` node.

2. Just as before, find a few of the lowest eigenvalues of this Hamiltonian employing a `Spectrum` node and a few `Get Eigenvalue` nodes.

3. To find the ground state wavefunction, attach a `Linear Combination` node to the `Spectrum` output. By choosing, for instance, 2 eigenstates in this node and $c_0 = 1$ and $c_1 = 0$, you have access to the wavefunction. This can be used as input in an `Energy Plot`.

4. Repeat Step 1 above, but now create a HO centered on x_c, that is $V(x; xc) = 0.5\,(x - x_c)^2$. x_c should ideally be a parameter changed in a `Scalar` node.

5. Repeat Steps 2 and 3 above with the new potential. You should have access to a few ground state wavefunctions, $\phi_n^{\mathrm{num}}(x)$.

6. To check that the obtained result is correct, create an `Analytic wave function` and enter the expression of Eq. (3) above. If you tick off the `Normalize output` box, the wave function is automatically normalized. You can now compare them by looking at the overlap, $o_0 = \langle \psi_0 | \phi_0^{\mathrm{num}} \rangle$, which should ideally be 1.

7. You can also compute the projection of the coherent state into Fock states by computing the overlaps $o_n^2 = |\langle \psi_0 | \phi_n^{\mathrm{num}} \rangle|^2$. How do these compare to the expansion coefficients of a coherent state into Fock states,

$$P_z(m) = |\langle z | m \rangle|^2 = e^{-|z|^2} \frac{|z|^{2m}}{m!}? \tag{4}$$

Coherent states: dynamics

Finally, you are now asked to simulate the dynamics of the coherent state obtained in the previous exercise. This will exploit the full time evolution capabilities of the `Quantum Composer`. You should start from the results of the previous exercise.

1. The `Time Evolution` node takes a single step in time of a given Hamiltonian. We want to take many such steps in succession. To do this, create a `For Loop` scope from the `Misc` category. Put `Time Evolution` inside the `For Loop`, and create boundary nodes of the `Hamiltonian`, the initial wave function, ϕ_0^{num}, and the `Potential`

2. Create three `Scalar` nodes and attach them to the special `For Loop` boundary node. These three scalars define the loop conditions (from, to and increment). Also, create a separate boundary `Scalar` node representing the increment in time. You can rename this boundary node to dt, if you like. Connect all these required parts to the `Time Evolution` node.

3. Create a `Position Plot`, and attach to it the `Potential` and the output wavefunction of the `Time Evolution`. Now you can press the `Play` button (green arrow, top left corner), and the for loop will start running. How does the wavefunction change over time?

4. To visualize the time evolution differently, we now look into the average position of the wavefunction, $\langle \hat{x} \rangle$, as a function of time. To this end, you first need to create the position `Operator`, $\hat{x}$. You can compute the `Expectation Value` employing the corresponding node in the `State Analysis` dropdown menu. The input wavefunction to this node should be the time-evolved estate. When you click play, you should see the number changing over time.

5. You can now create a time evolution plot, a so-called `Scalar Time Trace Plot`. To make this work, you need to connect it to the time in the `For Loop` and the `Expectation Value` as the plotting variable. Make sure the plotting limits, x_{min}, x_{max}, y_{min} and x_{max} make sense. What kind of time evolution do you observe? How does this compare to the expectations for a single coherent state?

6. Finally, employing the corresponding operators and state analysis tools, compute the dispersions in position, Δx^2, and momentum, Δp^2, as a function of time. Check that the product $\Delta x^2 \Delta p^2$ has the correct value.

Extra challenge: Can you code in a "momentum kick" employing the `Quantum Composer`? If so, prepare the a coherent state of the shape

$$\psi_z(x) = \frac{1}{\pi^{1/4}} e^{-i\frac{p_0 x_0}{2}} e^{ip_0 x} e^{-\frac{(x-x_0)^2}{2}} \tag{5}$$

and find its time evolution.