Quantum dynamics exam

You will use the program **propagate.f90** that you have used during the QD tutorial.

Instead of propagating a gaussian wave packet, as you did in the tutorial, you will propagate a wave packet that is built with the eigenstates of the quantum harmonic oscillator. This means you have to modify the subroutine **initpsi**.

I remind you that a wave packet is a superposition of eigenstates of the time-independent Hamiltonian. Therefore, at $t = 0$ we have for the wave packet Ψ,

$$\Psi(x, t = 0) = \sum_{n=0}^{\infty} c_n \Phi_n(x) \tag{1}$$

For a harmonic potential the eigenstates $\Phi_n(x)$ are known:

$$\Phi_n(x) = \frac{1}{\sqrt{2^n n!}} \left(\frac{m\omega}{\pi}\right)^{1/4} e^{-m\omega x^2/2} H_n(x\sqrt{m\omega}) \qquad (n = 0, 1, 2, \cdots) \tag{2}$$

where $H_n(y)$ are Hermite polynomials:

$$H_n(y) = (-1)^n e^{y^2} \frac{d^n}{dy^n} \left(e^{-y^2}\right) \qquad (H_0(y) = 1, H_1(y) = 2y, \cdots) \tag{3}$$

which can also be obtained from the recursion relation

$$H_n(y) = 2yH_{n-1}(y) - 2(n-1)H_{n-2}(y) \tag{4}$$

I. EXERCISES

1. Add a subroutine (or function) to **propagate.f90** which calculates the recursion expression for the Hermite polynomials in Eq. (4). Try to make it as general as possible but at least calculate the Hermite polynomials up to $H_4(y)$. [**3 points**]
2. Add a subroutine to **propagate.f90** (or modify **initpsi**) which calculates the eigenstates in Eq. (2). Again, try to make it as general as possible but at least calculate the eigenstates up to $\Phi_4(y)$. [**2 points**]
3. Modify the subroutine **initpsi** such that it calculates the wave packet in Eq. (1) by truncating the sum at $n = 4$. Ideally, the coefficients are read from an input file but otherwise you can specify them inside the program. [**2 points**]
4. Make sure the wave packet is normalized. [**1 points**]
5. To debug the program, propagate wave packets for which $c_i = 1$ and $c_j = 0$ ($j \neq i$). When doing this test be sure to the set the initial position of the wave packet at the bottom of the potential. Explain in your report what should happen for these kind of wave packets, then verify if the code indeed produces the expected behaviour. [**1 points**]
6. Set the first 5 coefficients ($c_0, \cdots, c_4$) equal to 1 and all others equal to 0 and propagate the wave packet. Then set the first 3 even coefficients (c_0, c_2, c_4) equal to 1 and all others equal to 0 and propagate the wave packet. Finally, set the first 2 odd coefficients (c_1, c_3) equal to 1 and all others equal to 0 and propagate the wave packet. Discuss the symmetry of the wave packets and the periods T of the corresponding probability densities for the 3 cases. [**1 points**].

II. THINGS TO CHECK IN YOUR CODE AND IN YOUR REPORT

- Make sure your code compiles and runs without errors

- Make sure your code is commented, i.e., explain what is done at each step inside your code.
- In the report explain in detail how your code works and give a list and description of the input variables.
- For exercises 4,5, and 6, add figures to the report with snapshots of the time propagation