Exercise 03

Wave packet

Please hand in your solution before **Thursday, 17 Nov, 8.00 a.m.**

1.1 Python exercises (10 P)

- Create a 4x4 matrix M with random values between 0 and 1 drawn from a uniform distribution.
- Replace all elements of the 2nd row with 1. Then, change all elements of the 3rd column to 0.
- Count the number of values larger than 0.5 using a double for loop.
- Check your result using numpy array indexing.
- Create two arrays A and B of 20 elements each, with random integer values between 0 and 10
- Create a function that takes an array x with N elements as input and returns an array y of the same size. The elements of y are $y_i = \sum_{j=0}^{i} x_j, \quad \forall i = 0, ..., N$

  E.g.: $y[0] = x[0]; \quad y[1] = x[0] + x[1]; \quad y[2] = x[0] + x[1] + x[2]; \quad ...$
- Use this function to calculate the arrays S and T respectively using the arrays A and B.
- Plot S and T as lines of different colors. Add a legend to show which color belongs to A and B, respectively.

1.2 Time evolution of the probability density (20 Points)

Consider a time-dependent wave function for a particle in a 1D box:

$$\psi(x,t) = \sum_{n=1}^{\infty} c_n(0)\phi_n(x) \exp\left(-\frac{iE_n}{\hbar}t\right) \tag{1}$$

with eigenfuctions:

$$\phi_n(x) = N \sin\left(\frac{n\pi}{L}x\right) \tag{2}$$

and energy eigenvalues:

$$E_n = \frac{\hbar^2}{2m}k^2 = \frac{\hbar^2}{2m}\frac{n^2\pi^2}{L^2} \tag{3}$$

For this kind of system the coefficents $c_n(0)$ are defined as:

$$c_n(0) = \begin{cases} \frac{1}{\sqrt{2}} & n = 2 \\ 0 & n = 4, 6, 8, ... \\ \frac{4\sqrt{2}(-1)^{\frac{n+1}{2}}}{(n-2)(n+2)\pi} & n = 1, 3, 5 \end{cases} \tag{4}$$

a. Use these informations to write a *PYTHON* script that simulates the time evolution of the probability density $|\psi(x,t)|^2$ for a superposition of the first 100 energy eigenfunctions. Use the following parameters:

   $$x_0 = 0; \qquad \Delta x = 0.01; \qquad L = 10; \qquad \hbar = 1; \qquad m = 1$$

   and describe what happens.

b. Plot the initial probability density.

c. Compute the integral $|\psi(x,t)|^2$. What happens if the number of used energy eigenfunctions is reduced to 2/increased to 150. Explain why. How many eigenfunctions are needed to obtain a probability density of at least 0.99?

d. Compute and plot the expectation value of the position x for every time step.

e. Implement one method to determine how long it takes until the initial probability density is reached again (Hint: Think about characteristics of the initial probability density).