Exercise 04

SUBMIT YOUR FILES BEFORE NEXT FRIDAY AT 8.00 AM TO oliver.lemke@fu-berlin.de

1 Particle in a 1D-box

1.1 Theoretical basics (20 Points)

Consider a particle in a 1D-box with a potential:

$$V(x) = \begin{cases} 0 & 0 \leq x \leq L \\ \infty & \text{otherwise} \end{cases} \tag{1}$$

and the eigenfunctions:

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

1. Show that the eigenfunctions are orthonormal.
2. Use your result of 1. to calculate the normalization N.
3. Now consider that the initial state is defined as:

$$\psi(x, t=0) = \begin{cases} \frac{2}{\sqrt{L}} \sin(\frac{2\pi}{L}x) & 0 \leq x \leq \frac{L}{2} \\ 0 & \text{otherwise} \end{cases} \tag{3}$$

   and can be expressed as a linear combination of the eigenfunctions:

$$\psi(x, t=0) = \sum_{n=1}^{\infty} c_n(0)\phi_n(x) \tag{4}$$

   Show that the coefficients $c_n(0)$ are defined as:

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

4. Show that the average momentum of a particle in a 1D-box is zero:

$$\langle \hat{p_x} \rangle = \int_0^L \psi(x)^* \hat{p_x} \psi(x) dx = 0 \tag{6}$$

1.2 Time evolution of the probability density (20 Points)

Consider a time-dependency of the wave function:

$$\psi(x, t) = \sum_{n=1}^{\infty} c_n(0)\phi_n(x) \exp\left(-\frac{iE_n}{\hbar}t\right) \tag{7}$$

with energy eigenvalues:

$$E_n = \frac{\hbar^2}{2m}k^2 = \frac{\hbar^2}{2m}\frac{n^2\pi^2}{L^2} \tag{8}$$

1. Use the equations and your results from task 1.1 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.
2. Plot the initial probability density.
3. 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?
4. Compute and plot the expectation value of the position x for every time step.
5. Implement two methods to determine how long it takes until the initial probability density is reached again (Hint: Think about characteristics of the initial probability density).

2 Particle in a 2D-box (10 Points)

Consider a particle in a 2D-box with the dimensions L_x and L_y and a potential:

$$V(x) = \begin{cases} 0 & 0 \leq x \leq L_x \text{ and } 0 \leq y \leq L_y \\ \infty & \text{otherwise} \end{cases} \tag{9}$$

The energy eigenvalues of this system are defined as:

$$E_{n_x,n_y} = \frac{h^2}{8m}\left(\frac{n_x^2}{L_x^2} + \frac{n_y^2}{L_y^2}\right) \tag{10}$$

1. Now consider a molecule of metal porphyrin, which is planar and contains 18π-electrons. This molecule can be expressed as a particle in square box. Calculate the lowest energy absorption of the porphyrine molecule if the length of the molecule $L = 1000$ pm.
2. Draw the energy levels. Which energy levels are degenerated?
3. Write a *PYTHON* script that calculates the first 10 energy levels for a variation of the box lenghts. Plot the first 10 energy levels as a function of y for a box with $L_x = 1000$ pm and L_y varied from 800 pm to 1200 pm in steps of 50 pm. What does happen to the degenerated states. Why does it happen?