Exercise 04

1 Particle in a box (15 points)

Consider a particle in a box with potential:

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

and eigenfunctions:

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

Suppose that at time $t = 0$, the particle is in the state:

$$\psi(x,0) = \begin{cases} A \sin\left(\frac{2\pi x}{L}\right) & 0 \leq x \leq \frac{L}{2} \\ 0 & otherwise \end{cases}$$

1. Find the normalization constant A.
2. Now consider the initial state expressed as linear combination of the eigenfunctions:

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

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

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

3. Now consider the time-dependent wave function:

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

   Write a MATLAB 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:

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

2 Particle in a box (two-dimensional case) (20 points)

1. Derive the wave function for a particle in a rectangle ($L_x \neq L_y$) with potential:

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

   Hint: use the separation of the variables.
   Find the energy eigenvalues:

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

2. Consider a molecule of metal porphyrin. This molecule is planar and contains 18π electrons that can be considered like particles in a square box. If the length of the molecule ($L_x = L_y$) is 1000 pm, then what is the predicted lowest energy absorption of the porphyrin molecule?

3. Draw the energy levels. Which energy levels are degenerate?

4. Let $L_x = 1000$ pm constant and L_y vary from 800 pm to 1200 pm with a step of 50 pm. Using MATLAB, plot the first 10 Energy levels as a function of y. What does it happen to the degenerate states?

For the parts where you do not need MATLAB you can write a report by hand and deliver it at the office 35.17. For the MATLAB parts, send the .m script by email to luca.donati@fu-berlin.de before next Wednesday at noon.