Exercise 06

PLEASE HAND IN YOUR SOLUTION BEFORE **THURSDAY, 08 DEC, 8.00 A.M.**

1 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:

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

The energy eigenvalues of this system are defined as:

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

a. 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 $L = 1000pm$.

b. Draw the energy levels. Which energy levels are degenerated?

c. 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? (This Task can also be solved with Pen and Paper)

2 Angular momentum 10 Points

a. Show that

$$\left[\hat{L}^2, \hat{L}_x\right] = \left[\hat{L}^2, \hat{L}_y\right] = \left[\hat{L}^2, \hat{L}_z\right] = 0$$

where

$$\hat{L}^2 = \hat{L}_x^2 + \hat{L}_y^2 + \hat{L}_z^2$$

b. Using the defintition of the angular momentum operators:

$$\hat{L}_x = y\hat{P}_z - z\hat{P}_y = -i\hbar\left(y\frac{\partial}{\partial z} - z\frac{\partial}{\partial y}\right)$$

$$\hat{L}_y = z\hat{P}_x - x\hat{P}_z = -i\hbar\left(z\frac{\partial}{\partial x} - x\frac{\partial}{\partial z}\right)$$

$$\hat{L}_z = x\hat{P}_y - y\hat{P}_x = -i\hbar\left(x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x}\right)$$

Convert the operators from Cartesian coordinates to spherical coordinates. To do this apply the chain rule

$$\frac{\partial}{\partial x}g(f(x)) = \frac{\partial}{\partial f}g(f)\frac{\partial}{\partial x}f(x)$$

where $g(f(x))$ is defined as $f(r(x,y,z), \Theta(x,y,z), \Phi(x,y,z))$.

Hint:

Your intermediate results should look like this:

$$\frac{\partial}{\partial x} = \sin(\Theta)\cos(\Phi)\frac{\partial}{\partial r} + \frac{1}{2}\cos(\Theta)\cos(\Phi)\frac{\partial}{\partial \Theta} - \frac{1}{2}\frac{\sin(\Phi)}{\sin(\Theta)}\frac{\partial}{\partial \Phi}$$

$$\frac{\partial}{\partial y} = \sin(\Theta)\sin(\Phi)\frac{\partial}{\partial r} + \frac{1}{2}\cos(\Theta)\sin(\Phi)\frac{\partial}{\partial \Theta} + \frac{1}{2}\frac{\cos(\Phi)}{\sin(\Theta)}\frac{\partial}{\partial \Phi}$$

$$\frac{\partial}{\partial z} = \cos(\Theta)\frac{\partial}{\partial r} - \frac{\sin(\Theta)}{r}\frac{\partial}{\partial \Theta}$$

3 Python Exercise **10 points**

a. Generate an array P of size $N \times 3$, with $N = 1000$ random numbers. Each row of the array represents the position of a point in 3D space.

b. Create a function that generates a symmetric matrix d of size $N \times N$, where each element d_{ij} is the euclidean distance between each pair of points (i, j) :

$d_{ij} = \sqrt{(x_i - x_j)^2 + (y_i - y_j)^2 + (z_i - z_j)^2}$

c. Calculate this distance matrix for P and measure the execution time.

d. Measure the execution time the scipy function `cdist` needs to calculate the same matrix.

e. Display the matrix as a matrix plot including a color bar legend.