Exercise 08

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

1 Angular momentum

1. Show that

$$\left[\hat{L}^2, \hat{L}_x\right] = \left[\hat{L}^2, \hat{L}_y\right] = \left[\hat{L}^2, \hat{L}_z\right] = 0 \tag{1}$$

where

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

2. Using the defintition of the angular momentum operators:

$$\hat{L}_x = y\hat{P}_z - z\hat{P}_y = -i\hbar\left(y\frac{\partial}{\partial z} - z\frac{\partial}{\partial y}\right) \tag{3}$$

$$\hat{L}_y = z\hat{P}_x - x\hat{P}_z = -i\hbar\left(z\frac{\partial}{\partial x} - x\frac{\partial}{\partial z}\right) \tag{4}$$

$$\hat{L}_z = x\hat{P}_y - y\hat{P}_x = -i\hbar\left(x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x}\right) \tag{5}$$

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

$$\frac{\partial}{\partial x}g(f(x)) = \frac{\partial}{\partial f}g(f)\frac{\partial}{\partial x}f(x) \tag{6}$$

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:

$$\frac{\partial}{\partial x} = \sin(\Theta)\cos(\Phi)\frac{\partial}{\partial r} + \frac{1}{2}\cos(\Theta)\cos(\Phi)\frac{\partial}{\partial \Theta} - \frac{1}{2}\frac{\sin(\Phi)}{\sin(\Theta)}\frac{\partial}{\partial \Phi} \tag{7}$$

$$\frac{\partial}{\partial y} = \sin(\Theta)\sin(\Phi)\frac{\partial}{\partial r} + \frac{1}{2}\cos(\Theta)\sin(\Phi)\frac{\partial}{\partial \Theta} + \frac{1}{2}\frac{\cos(\Phi)}{\sin(\Theta)}\frac{\partial}{\partial \Phi} \tag{8}$$

$$\frac{\partial}{\partial z} = \cos(\Theta)\frac{\partial}{\partial r} - \frac{\sin(\Theta)}{r}\frac{\partial}{\partial \Theta} \tag{9}$$

2 Rotational dynamics

Let's consider a IBr molecule with a rotational constant $B = 0.05683\ \text{cm}^{-1}$. Write a *Python* script that propagates the rotational dynamics using an overlap of the rotational states $l = 1, m_l = 0$ and $l = 2, m_l = 0$ and the rotational wavefunction

$$\Psi(\Theta, \Phi, t) = N \sum_{l=1}^{2} c_l(t = 0) \exp\left(-\frac{iE_l t}{\hbar}\right) Y_{l,m_l}(\Theta, \Phi) \tag{10}$$

with $c_1 = 1$ and $c_2 = 1$ and do the following tasks

1. Normalize the function numerically within your *Python* script
2. Calculate the period
3. Propagate $|\Psi(\Theta, \Phi, t)|^2$ for one period (Use at least 100 time steps)
4. Analyze the propagation. Therefore, plot first the density in dependency of Θ and second the density as a polar plot with respect to Θ. To do this add to your *Python* script a part that simulates the propagation of the density or take snap shots of the density at significant time steps.

Hints:

- for more informations on rotational spectroscopy look at:

  https://de.wikipedia.org/wiki/Mikrowellenspektroskopie
- Be careful with the units (Use SI-Units)