Exercise 07

1 Angular momentum (12 points)

The three components of the quantum-mechanical operators are:

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

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

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

Exercise

1. Convert the operators $\hat{L}_x$, $\hat{L}_y$, $\hat{L}_z$ from Cartesian coordinates to spherical coordinates:

$$\hat{L}_x = -i\hbar\left(-\sin\phi\frac{\partial}{\partial\theta} - \cot\theta\cos\phi\frac{\partial}{\partial\phi}\right)$$

$$\hat{L}_y = -i\hbar\left(\cos\phi\frac{\partial}{\partial\theta} - \cot\theta\sin\phi\frac{\partial}{\partial\phi}\right)$$

$$\hat{L}_z = -i\hbar\frac{\partial}{\partial\phi}$$

Hints:

- At the center of this exercise are derivatives of this kind

$$\frac{\partial}{\partial x}f(r(x,y,z),\theta(x,y,z),\phi(x,y,z))\,.$$

To solve convert these derivatives with respect to Cartesian coordinates into derivatives with respect to r, θ, and ϕ, one need to apply the chain rule

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

- Intermediate result

$$\begin{aligned}
\frac{\partial}{\partial x} &= \sin\theta\cos\phi\frac{\partial}{\partial r} + \frac{1}{2}\cos\theta\cos\phi\frac{\partial}{\partial\theta} - \frac{1}{2}\frac{\sin\phi}{\sin\theta}\frac{\partial}{\partial\phi} \\
\frac{\partial}{\partial y} &= \sin\theta\sin\phi\frac{\partial}{\partial r} + \frac{1}{2}\cos\theta\sin\phi\frac{\partial}{\partial\theta} + \frac{1}{2}\frac{\cos\phi}{\sin\theta}\frac{\partial}{\partial\phi} \\
\frac{\partial}{\partial z} &= \cos\theta\frac{\partial}{\partial r} - \frac{\sin\theta}{r}\frac{\partial}{\partial\theta}
\end{aligned}$$

2 Uncertainty in the angular momentum components (15 points)

Because of the commutators,

$$\begin{aligned}[\hat{L}_x, \hat{L}_y] &= i\hbar \hat{L}_z \\ [\hat{L}_y, \hat{L}_z] &= i\hbar \hat{L}_x \\ [\hat{L}_z, \hat{L}_x] &= i\hbar \hat{L}_y \end{aligned} \tag{1}$$

only one component of the quantum mechanical angular momentum can be measured with arbitrary precision. Conventionally, this component is chosen to be the z-component. The other two components are subject to the Heisenberg uncertainty principle.

$$\Delta L_x \Delta L_y \geq \frac{1}{2} \left| \left\langle \Psi \middle| [\hat{L}_x, \hat{L}_y] \middle| \Psi \right\rangle \right| . \tag{2}$$

In this exercise, you will calculate the uncertainties of the x- and y-component of the angular momentum for the 2p hydrogen atomic wavefunctions

$$\begin{aligned}\Psi_{210}(r,\theta,\phi) &= \frac{1}{\sqrt{32\pi}} \left(\frac{1}{a_0}\right)^{5/2} r \exp\left(-\frac{r}{2\alpha_0}\right) \cos\theta \\ \Psi_{21\pm1}(r,\theta,\phi) &= \frac{1}{\sqrt{32\pi}} \left(\frac{1}{a_0}\right)^{5/2} r \exp\left(-\frac{r}{2\alpha_0}\right) \sin\theta \, e^{\pm i\phi} \end{aligned} \tag{3}$$

The uncertainty is given as

$$\Delta L_x = \Delta L_y = \sqrt{\left\langle \hat{L}_y^2 \right\rangle - \left\langle \hat{L}_y \right\rangle^2} . \tag{4}$$

Exercise

1. Calculate the product of the uncertainties $\Delta L_x \Delta L_y$ for the hydrogen atomic wave functions Ψ_{210} and $\Psi_{21\pm1}$. Are you surprised by the results? Why / why not?
2. In which special case is it possible to know exactly all three components of the angular momentum without violating the Heisenberg uncertainty principle? (Hint: have a look at the list of the hydrogen atomic wave functions and their quantum numbers.)
3. Calculate $\langle L_x \rangle$ and $\langle L_y \rangle$ for Ψ_{210}.
4. Calculate $\langle L_x \rangle$ and $\langle L_y \rangle$ for $\Psi_{21\pm1}$. (Hint: $\int_0^\pi \sin x \cos x \, dx = 0$)
5. Calculate $\langle L_x \rangle^2$ and $\langle L_y \rangle^2$ for Ψ_{210} and $\Psi_{21\pm1}$. (Hint: $\hat{\mathbf{L}}^2 = \hat{L}_x^2 + \hat{L}_y^2 + \hat{L}_z^2$ and $\left\langle L_x^2 \right\rangle = \left\langle L_y^2 \right\rangle$).
6. What is ΔL_x and ΔL_y for Ψ_{210} and $\Psi_{21\pm1}$?
7. Assuming that $\langle L_x \rangle = \langle L_y \rangle = 0$ for all hydrogen atomic wave functions, give a general expression for ΔL_x and ΔL_y.
8. For which magnetic quantum number m is the uncertainty the smallest?
9. Does the relative uncertainty $\Delta L_x / \sqrt{\langle L^2 \rangle}$ increase or decrease with increasing l? (Formulate $\Delta L_x / \sqrt{\langle L^2 \rangle}$ using the magnetic quantum number m which yields the smallest uncertainty.)

Solve with pen and paper and report all important intermediate steps of your calculations. Hand in the report at the office 35.17 before next Wednesday at noon.