Quantum Mechanics

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Sheet 8 Due: 28/05 at 12:00

1 Properties of angular momentum operators (2 P)

Let $J = (J_x, J_y, J_z)$ be angular momentum operators. Thus, it holds $[J_x, J_y] = iJ_z$ and cyclic permutations thereof. We define the associated *ladder operators* as $J_\pm = J_x \pm iJ_y$. The following properties can be derived from the commutation relations and will be used in the lecture. Show that:

a) (2/3 P)

$$[J_z, J_\pm] = \pm J_\pm$$

b) (2/3 P)

$$J_- J_+ = J^2 - J_z^2 - J_z$$

c) (2/3 P)

$$[J^2, J_z] = 0.$$

2 Orbital angular momentum in spherical coordinates (2 P + 2 bonus points)

We will see that the orbital angular momentum of a particle with Hilbert space $L^2(\mathbb{R}^3)$ is associated with the following angular momentum operators:

$$L_x = -i\left(y\frac{\partial}{\partial z} - z\frac{\partial}{\partial y}\right), \tag{1}$$

$$L_y = -i\left(z\frac{\partial}{\partial x} - x\frac{\partial}{\partial z}\right), \tag{2}$$

$$L_z = -i\left(x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x}\right). \tag{3}$$

We claim that these operators have the following form in spherical coordinates:

$$L_x = i\left(\sin\varphi\frac{\partial}{\partial\theta} + \frac{\cos\varphi}{\tan\theta}\frac{\partial}{\partial\varphi}\right), \tag{4}$$

$$L_y = i\left(-\cos\varphi\frac{\partial}{\partial\theta} + \frac{\sin\varphi}{\tan\theta}\frac{\partial}{\partial\varphi}\right), \tag{5}$$

$$L_z = -i\frac{\partial}{\partial\varphi}. \tag{6}$$

a) Prove the claim for L_z. **(2 P)**

b) Bonus: Do an analogous computation for L_x, L_y. **(2 bonus points)**

Hint: You should have encountered similar computations in the mathematical methods lecture. While the computation might be a bit lengthy, it is not difficult by itself.

3 p-orbitals (6 P)

We are using the orbital angular momentum operators L_x, L_y, L_z in spherical coordinates from exercise **2**. Here, we want to visualise certain eigenstates of the orbital angular momentum operators L_z, L^2.

The joint eigenvectors of L_z, L^2 are the so-called *spherical harmonics* $Y_{l,m}(\theta, \phi)$. Some of these are given by

$$Y_{1,1}(\theta,\varphi) = -\sqrt{\frac{3}{8\pi}} \sin\theta e^{+i\varphi}, \quad Y_{1,-1}(\theta,\varphi) = \sqrt{\frac{3}{8\pi}} \sin\theta e^{-i\varphi}, \quad Y_{1,0}(\theta,\varphi) = \sqrt{\frac{3}{4\pi}} \cos\theta.$$

We will see that these functions are an orthonormal basis in the space of functions with $l = 1$. However, we want the construct a different basis for this space which is better suited for the construction of wave functions in molecules. (The connection of this basis to the H_2O molecule will be explained in the exercise class.)

a) (1.5 P) First, we will check that at least $Y_{1,1}$ is indeed a joint eigenfunction. Show directly that $Y_{1,1}$ is an eigenvector of L_z with eigenvalue $m = 1$. Afterwards, show that $L_+ Y_{1,1} = 0$ and deduce from this that $Y_{1,1}$ is an eigenvector of L^2 with eigenvalue $l = 1$.

Hint: Use the angular momentum operators in spherical coordinates and the formula $L^2 = L_- L_+ + L_z^2 + L_z$ from exercise **1**.

b) (1.5 P) We define $p_z(\theta,\varphi) = Y_{1,0}(\theta,\varphi)$. (Here, the symbol p does not represent a probability but is referring to the common name *p-orbitals* for wave functions with $l = 1$). Sketch the angular dependence of p_z in the plane $x = 0$ (i.e. $\varphi = \pi/2$). To do so, draw the modulus of $p_z(\theta, \pi/2)$ for any angle θ. In other words: draw the points with polar coordinates $r = |p_z(\theta, \pi/2)|$ and $\theta \in [0, \pi]$. Sketch an analogous three-dimensional figure for all values of θ, φ.

c) (1 P) Consider the function

$$p_x(\theta,\varphi) = -\frac{1}{\sqrt{2}}(Y_{1,1}(\theta,\varphi) - Y_{1,-1}(\theta,\varphi)).$$

Sketch p_x as you did in **2b**.

d) (2 P) Show that p_x is normalised an orthogonal to p_z (use that the functions $Y_{m,l}$ are orthonormal – there is no need to compute any integrals!). Up to a phase factor, there is exactly one vector p_y in the $l = 1$ space which is normalised an orthogonal to both p_x and p_z. Write down this function and show that it indeed fulfills the desired properties. Choose the phase such that $p_y(\theta, \varphi)$ is real. Sketch as you did before.