7. Spherical Harmonics

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7.1 Angular momentum operator in spherical coordinates

Using vector calculus one can write the angular momentum operator in spherical coordinates. One first writes the gradient operator $\vec{\nabla}$ in components:

$$\vec{\nabla} = \frac{\partial}{\partial \vec{r}} = \vec{e}_r \frac{\partial}{\partial r} + \vec{e}_\phi \frac{1}{r sin(\theta)} \frac{\partial}{\partial \phi} + \vec{e}_\theta \frac{1}{r} \frac{\partial}{\partial \theta} \tag{1}$$

The three vectors $\vec{e}_r$, $\vec{e}_\phi$, $\vec{e}_\theta$, are unit vectors of the spherical coordinate system. All three vectors depend on the angles ϕ and θ. This needs to be taken into account when derivatives are taken. The angular momentum is now obtained from $\vec{L} = r\vec{e}_r \times (\hbar/i)\vec{\nabla}$ as:

$$\vec{L} = \frac{\hbar}{i} \left[r(\vec{e}_r \times \vec{e}_r) \frac{\partial}{\partial r} + (\vec{e}_r \times \vec{e}_\theta) \frac{\partial}{\partial \theta} + (\vec{e}_r \times \vec{e}_\phi) \frac{1}{sin(\theta)} \frac{\partial}{\partial \phi} \right] \tag{2}$$

Here, the first term is zero, $\vec{e}_r \times \vec{e}_\theta = \vec{e}_\phi$, and $\vec{e}_r \times \vec{e}_\phi = -\vec{e}_\theta$. This leads to

$$\vec{L} = \frac{\hbar}{i} \left[\vec{e}_\phi \frac{\partial}{\partial \theta} - \vec{e}_\theta \frac{1}{sin(\theta)} \frac{\partial}{\partial \phi} \right] \tag{3}$$

To extract from this equation the three components L_x, L_y, and L_z (in spherical coordinates), we have to express the unit vectors $\vec{e}_\phi$ and $\vec{e}_\theta$ in cartesian coordinates. This can be done as follows:

$$\begin{aligned} \vec{e}_\phi &= \frac{1}{r sin(\theta)} \frac{\partial}{\partial \phi} \vec{r} = (-sin(\phi), cos(\phi), 0) \\ \vec{e}_\theta &= \frac{1}{r} \frac{\partial}{\partial \theta} \vec{r} = (cos(\theta) cos(\phi), cos(\theta) sin(\phi), -sin(\theta)) \end{aligned} \tag{4}$$

Adding this into equ. 3 yields the final result:

$$\begin{aligned} L_x &= \frac{\hbar}{i} \left(-sin(\phi) \frac{\partial}{\partial \theta} - cos(\theta) cos(\phi) \frac{1}{sin(\theta)} \frac{1}{\partial \phi} \right) \\ L_y &= \frac{\hbar}{i} \left(cos(\phi) \frac{\partial}{\partial \theta} - cos(\theta) cos(\phi) \frac{1}{sin(\theta)} \frac{1}{\partial \phi} \right) \\ L_z &= \frac{\hbar}{i} \frac{\partial}{\partial \phi} \end{aligned} \tag{5}$$

7.2 Eigenvalues for L_z and L^2

The operator

$$L_z = \frac{\hbar}{i} \frac{\partial}{\partial \phi} \tag{6}$$

from previous equation equ. 5 has the eigenfunctions

$$\chi^m(\phi) = e^{im\phi} \tag{7}$$

with eigenvalues $\hbar m$. Since the functions should be unique, they must be 2π periodic in the angle ϕ. Hence, m must be an integer. One can in fact doubt this argument, because only the modulus is an observable. We see later below that this statement is almost correct.

Next, we look for the eigenfunctions of L^2, which we call Y. These functions are defined by the equation

$$L^2 Y = \hbar^2 \lambda Y \tag{8}$$

where the eigenvalue of L^2 has been abbreviated as $\hbar^2\lambda$ ($\hbar$ has unit of angular momentum). Since L^2 and L_z commute, i.e. $[L^2, L_z] = 0$, Y is at the same time an eigenfunction of L_z. The functions Y only depend on the two angles of the spherical coordinate system, the polar and azimuthal angle, θ and ϕ, respectively. They are called spherical harmonics (Kugelfunktionen in German) and they are distinguished by two quantum numbers, l and m, where l still needs to be derived. They can be decomposed in a product of two functions:

$$Y_l^m(\theta, \phi) = \Omega_l^m(\theta)\chi^m(\phi) \tag{9}$$

where the first part is the polar and the second the azimuthal function. Y_l^m shall be normalized on the sphere of unit radius.

The goal is to derive that λ is given by $l(l+1)$ where l denotes the bounds for m given by the equation $-l \leq m \leq l$ with m an integer.

We have the following defining eigenvalue equations

$$L_z Y_l^m = \hbar m Y_l^m \tag{10}$$

and

$$L^2 Y_l^m = \hbar^2 \lambda Y_l^m \tag{11}$$

Next we write

$$(L_x^2 + L_y^2 + L_z^2) Y_l^m = \hbar^2 \lambda Y_l^m \tag{12}$$

and replace the L_z part with the respective eigenvalue leading to

$$(L_x^2 + L_y^2) Y_l^m = \hbar^2 (\lambda - m^2) Y_l^m \tag{13}$$

Since the expectation value for L_j^2 is larger than or equal zero, i.e. $(Y, L_j^2 Y) = (L_j Y, L_j Y) \geq 0 \ \forall j$, we also have $(Y, (L_x^2 + L_y^2) Y) \geq 0$ and therefore from equ. 13:

$$\lambda \geq m^2 \tag{14}$$

This equation says that $|m|$ is bound to some maximum value.

Next, we define new operators:

$$L_+ := L_x + iL_y \tag{15}$$

$$L_- := L_x - iL_y \tag{16}$$

Since $[L^2, L_j] = 0$, we also have

$$[L^2, L_\pm] = 0 \tag{17}$$

One can easily show that the following also holds:

$$[L_z, L_\pm] = \pm\hbar L_\pm \tag{18}$$

This follows simply by: $[L_z, L_x + iL_y] = [L_z, L_x] + i[L_z, L_y] = \hbar(iL_y + L_x) = \hbar L_+$. Now let us look at the following combination:

$$L^2(L_\pm Y_l^m) = L_\pm(L^2 Y_l^m) = \hbar^2 \lambda (L_\pm Y_l^m) \tag{19}$$

In other words, since L^2 and $L_\pm$ commute, the functions $L_\pm Y_l^m$ are also eigenfunctions of L^2. How do the functions $L_\pm Y_l^m$ behave, when L_z is acting upon them? We write:

$$\begin{aligned} L_z(L_\pm Y_l^m) &= ([L_z, L_\pm] + L_\pm L_z) Y_l^m \\ &= (\pm\hbar L_\pm + m\hbar L_\pm) Y_l^m \\ &= \hbar(m \pm 1)(L_\pm Y_l^m) \end{aligned} \tag{20}$$

and hence, $L_\pm Y_l^m$ is also eigenfunction of the operator L_z with the eigenvalue $m \pm 1$. The operators $L_\pm$ are therefore so called ladder operators that increase or decrease the index m by one. Up to normalization factors N, N' we have:

$$\begin{aligned} Y_l^{m+1} &= N(L_+ Y_l^m) \\ Y_l^{m-1} &= N'(L_- Y_l^m) \end{aligned} \tag{21}$$

We have already seen before in equ. 14 that $|m|$ is bound to a maximum value. There exists therefore a maximum m and a minimum one, which we denote as m_{max} and m_{min}. In order for the ladder operators to terminate, we rquire

$$L_+ Y_l^{m_{max}} = 0 \quad \text{and} \quad L_- Y_l^{m_{min}} = 0 \tag{22}$$

Now we look at the product L_+L_- and L_-L_+: $L_+L_- = (L_x + iL_y)(L_x - iL_y) = L_x^2 - iL_xL_y + iL_yL_x + L_y^2 = L_x^2 + L_y^2 - i[L_x, L_y] = L_x^2 + L_y^2 + \hbar L_z = L^2 - L_z^2 + \hbar L_z$. And similarly, we obtain: $L_-L_+ = L^2 - L_z^2 - \hbar L_z$. Applying these two results to the wavefunctions Y_l^m yields:

$$\begin{aligned} (L_+L_-) Y_l^{m_{min}} &= \hbar^2(\lambda - m_{min}^2 + m_{min}) Y_l^{m_{min}} = 0 \\ (L_-L_+) Y_l^{m_{max}} &= \hbar^2(\lambda - m_{max}^2 - m_{max}) Y_l^{m_{max}} = 0 \end{aligned} \tag{23}$$

So we arrive at two algebraic equations:

$$\begin{aligned} m_{min}(m_{min} - 1) &= \lambda \\ m_{max}(m_{max} + 1) &= \lambda \end{aligned} \tag{24}$$

One can combine these two equations together and write

$$(m_{max} + m_{min})(m_{max} - m_{min} + 1) = 0 \tag{25}$$

Since $m_{max} \geq m_{min}$, the second term cannot be zero. Hence, the first term must be zero, i.e. $m_{max} + m_{min} = 0$, or equally

$$m_{min} = -m_{max} \tag{26}$$

Due to the sequential generation with the ladder operator, the difference $m_{max} - m_{min}$ must be an integer. As a consequence m_{max} is $\in \mathbb{N}/2$. We define $m_{max} = l$ and call l the angular momentum quantum number. l is either an integer or a half integer. [1] The latter is for example realized by the spin of an electron, proton or neutron who all have a 'self-momentum' of $l = 1/2$. We confine ourselves to integer momentum, since only these are realized in the orbital motion, and discuss spin later. We have arrived at the very important result:

$$m = -l, -l+1, \ldots l-1, l \quad l \in \mathbb{N} \tag{27}$$

Just be surprised. We have derived this result without even knowing the details of the functions Y_l^m. Taken equ. 24, we further obtain for the eigenvalue of $L^2/\hbar^2$:

$$\lambda = l(l+1) \tag{28}$$

The final result reads:

$$\begin{aligned} L_z Y_l^m &= \hbar m Y_l^m \quad m = -l, l+1, \ldots l-1, l \\ L^2 Y_l^m &= \hbar^2 l(l+1) Y_l^m \end{aligned} \tag{29}$$

For a given angular momentum quantum number l, there are $2l + 1$ different eigenfunctions which yield a definite momentum component L_z. The absolute value of the angular momentum, the length of the vector in a classical picture, is $\hbar\sqrt{l(l+1)}$. The L_z component is a multiple of $\hbar$. L_x and L_y are not defined, that is have not a defined value, because they do not commute with L_z. The maximum value of L_z is $l\hbar \leq \hbar\sqrt{(l(l+1)}$. This is a consequence of the uncertainty relation.

[1] We now see that the argument in the bgining that m should be an integer was not fully correct. m can also be a half integer.

7.3 Eigenvalues for L_z and L^2

We have already derived L_x, L_y and L_z in spherical coordinates, see equ. 5. We obtain from these equations:

$$L_+ = e^{i\phi}\left(\frac{\partial}{\partial\theta} + icot(\theta)\frac{\partial}{\partial\phi}\right) L_- = e^{-i\phi}\left(\frac{\partial}{\partial\theta} - icot(\theta)\frac{\partial}{\partial\phi}\right) \tag{30}$$

Since the ladder has to terminate at $m = -l$, we have $L_- Y_l^{-l} = 0$. This can be expressed in the following differential equation:

$$\frac{\partial Y_l^{-l}}{\partial\theta} = lcot(\theta)Y_l^{-l} . \tag{31}$$

This equation has the solution

$$Y_l^{-l}(\theta,\phi) = C(sin(\theta))^l e^{-il\phi} , \tag{32}$$

where C is the normalization constant. This constant is obtained by requiring:

$$\int\int Y_l^{-l}(\theta,\phi)sin(\theta)d\theta d\phi = 1 . \tag{33}$$

One obtains

$$C = \sqrt{\frac{(2l+1)!}{4\pi}}\frac{1}{l!\,2^l} . \tag{34}$$

Now, we are in the position to generate all spherical waves starting with Y_l^{-l} and sequentially applying the raising operator L_+. Each time L_+ is used the obtained functions needs to be normalized, i.e. L_+ does not protect the normalization. Using operator algebra, one can derive the respective normalization factor. This then yields:

$$Y_l^{m+1} = \frac{1}{\hbar\sqrt{(l-m)(l+m-1)}} L_+ Y_l^m . \tag{35}$$

The spherical functions can be found in many books. They are written in terms of so called associated Legendre functions $P_l^m(cos(\theta))$, which are obtained from the so called Lengendre polynomials:

$$P_l(x) = \frac{1}{2^l\,l!}\left(\frac{d}{dx}\right)^l (x^2-1)^l . \tag{36}$$

The first five polynomials are

$$\begin{aligned} P_0(x) &= 1 \\ P_1(x) &= x \\ P_2(x) &= \frac{1}{2}(3x^2-1) \\ P_3(x) &= \frac{1}{2}(5x^3-3x) \\ P_4(x) &= \frac{1}{8}(35x^4-30x^2+3) \end{aligned} \tag{37}$$

The associates Legendre functions are then obtained as:

$$P_l^m(x) = (1-x^2)^{|m|/2}\left(\frac{d}{dx}\right)^{|m|} P_l(x) . \tag{38}$$

Obviously the function P_l^m is even in the index m, i.e. $P_l^m = P_l^{-m}$. Again, we give a few examples:

$$\begin{aligned} P_2^0(x) &= \frac{1}{3}(3x^2-1) \\ P_2^1(x) &= 3x\sqrt{1-x^2} \\ P_2^2(x) &= 3(1-x^2) \end{aligned} \tag{39}$$

Finally, the spherical harmonics are given by

$$Y_l^m(\theta,\phi) = \epsilon\sqrt{\frac{2l+1}{4\pi}\cdot\frac{(l-|m|)!}{(l+|m|)!}}\, e^{im\phi}\, P_l^m(\cos(\theta)). \tag{40}$$

The factor $\epsilon = (-1)^m$ for $m > 1$ and $\epsilon = 1$ otherwise. For us, this factor is pure convention. We will not make use of it.

It is best to visualize these functions on a sphere. It is a good idea to once google the term 'spherical harmonics' and look at the different representations! Here, some examples:

$$\begin{aligned}
Y_0^0(\theta,\phi) &= \frac{1}{4\pi} \\
Y_1^0(\theta,\phi) &= \sqrt{\frac{3}{4\pi}}cos(\theta) \\
Y_1^{\pm 1}(\theta,\phi) &= \mp\sqrt{\frac{3}{8\pi}}sin(\theta)e^{\pm i\phi} \\
Y_2^0(\theta,\phi) &= \sqrt{\frac{5}{16\pi}}(3cos^2(\theta)-1) \\
Y_2^{\pm 1}(\theta,\phi) &= \mp\sqrt{\frac{15}{8\pi}}sin(\theta)cos(\theta)e^{\pm i\phi} \\
Y_2^{\pm 2}(\theta,\phi) &= \sqrt{\frac{15}{32\pi}}sin^2(\theta)e^{\pm 2i\phi}
\end{aligned} \tag{41}$$