QUANTIZATION OF ANGULAR MOMENTUM

[Ø 11.2, H 8.1–8.2, G 4.3]

Angular momentum operators

Our starting point is that we define an angular momentum operator: $\vec{J}$ by requiring that the cartesian components J_x, J_y and J_z are Hermitian operators satisfying the commutation relations

$$\left.\begin{aligned} [J_x, J_y] &= i\hbar J_z \\ [J_y, J_z] &= i\hbar J_x \\ [J_z, J_x] &= i\hbar J_y \end{aligned}\right\} \quad [J_i, J_j] = \sum_k i\hbar\, \varepsilon_{ijk} J_k ,$$

with ε_{ijk} the completely antisymmetric Levi-Cevita symbol, with $\varepsilon_{xyz} = 1$.

This might seem strange. Why can't/don't the operators commute? This is related to the fact that in 3D, rotations do not commute: If you rotate something first around the x-axis, and then around the y-axis, this gives a different result compared to first rotating around the y-axis and then around the x-axis!

[The angular momentum operators are the <u>generators</u> of rotation, and must therefore also not commute]

For the operator for the orbital angular momentum, $\vec{L} = \vec{r} \times \vec{p}$, the commutation relations can be shown explicitly.

We can also define the operator $\vec{J}^2 = J_x^2 + J_y^2 + J_z^2$, which commutes with each of the components of $\vec{J}$:

$$[\vec{J}^2, J_k] = 0, \qquad k = x, y, z.$$

<u>Proof:</u>

$$[\vec{J}^2, J_j] = \sum_i [J_i^2, J_j] = \sum_i \{[J_i, J_j] J_i + J_i [J_i, J_j]\}$$
$$= \sum_i \sum_k i\hbar \, \varepsilon_{ijk} (J_k J_i + J_i J_k)$$

Since we sum over both k and i, we can relabel $k \Leftrightarrow i$ in the last term:

$$[\vec{J}^2, J_j] = \sum_{i,k} i\hbar (\varepsilon_{ijk} + \varepsilon_{ikj}) J_k J_i = 0,$$

since $\varepsilon_{ijk} = -\varepsilon_{ikj}$.

Since $\vec{J}^2$ commutes with the components, we can choose one of the components, e.g. J_z, and find <u>simultaneous eigenvectors</u> of $\vec{J}^2$ and J_z. We will write these as $|a, b\rangle$, with the property

$$\vec{J}^2 |a, b\rangle = a |a, b\rangle$$
$$J_z |a, b\rangle = b |a, b\rangle,$$

where a and b are the eigenvalues of the eigenvalues of the two operators. So far we now nothing about what they actually are.

Eigenvalues

To find the eigenvalues, we will use operator methods similar to what we used for the harmonic oscillator. We define ladder operators

$$J_+ = J_x + iJ_y$$
$$J_- = J_x - iJ_y$$

where $J_+^\dagger = J_-$, meaning they are not Hermitian. We will need the commutators with the other operators:

$$[\vec{J}^2, J_\pm] = 0,$$

since both J_x and J_y commute with $\vec{J}^2$.

$$[J_z, J_\pm] = [J_z, J_x] \pm i[J_z, J_y]$$
$$= i\hbar J_y \pm i(-i\hbar J_x) = \pm\hbar J_\pm.$$

We now follow a similar procedure as for the Harmonic oscillator, and take a closer look at the vectors $J_\pm |a,b\rangle$:

$$\vec{J}^2 J_\pm |a,b\rangle = J_\pm \vec{J}^2 |a,b\rangle = J_\pm a |a,b\rangle = a J_\pm |a,b\rangle.$$

Hence $J_\pm |a,b\rangle$ are eigenvector of $\vec{J}^2$ with the same eigenvalue as $|a,b\rangle$.

Similarily, we calculate:

$$J_z J_\pm |a,b\rangle = (J_\pm J_z \pm \hbar J_\pm)|a,b\rangle$$
$$= J_\pm (J_z \pm \hbar)|a,b\rangle = (b \pm \hbar) J_\pm |a,b\rangle.$$

$J_\pm |a,b\rangle$ are eigenvectors of J_z with eigenvalues $b \pm \hbar$, granted that $J_\pm |a,b\rangle \neq 0$. Since J_+ increases the eigenvalue by $\hbar$, and J_- decreases the eigenvalue by $\hbar$, they are called raising and lowering operators, respectively.

Can we raise or lower the eigenvalue indefinitely? Intuitively we should expect that the eigenvalue $|b|$ should be smaller than $\sqrt{a}$, since J_z is a component of $\vec{J}$.

To show this, we can again use the requirement that the norm of a vector should be positive. We calculate the norm of $J_\pm |a,b\rangle$:

$$\langle a,b|(J_\pm)^\dagger J_\pm|a,b\rangle = \langle a,b|J_\mp J_\pm|a,b\rangle \geq 0.$$

We need an expression for J_+J_-:

$$J_\mp J_\pm = (J_x \mp iJ_y)(J_x \pm iJ_y)$$

$$= J_x^2 + J_y^2 \pm i\underbrace{(J_xJ_y - J_yJ_x)}_{i\hbar J_z} + J_z^2 - J_z^2$$

$$= \vec{J}^2 - J_z^2 \mp \hbar J_z.$$

Inserted into the expression for the norm, we get

$$\langle a,b|\vec{J}^2 - J_z^2 \mp \hbar J_z|a,b\rangle$$

$$= \langle a,b|a - b^2 \mp \hbar b|a,b\rangle$$

$$= a - b^2 \mp \hbar b = a - b(b \pm \hbar) \geq 0,$$

can be violated for both positive and negative b!

We therefore require that there exists a b_{max} and b_{min} such that

$$J_+|a, b_{max}\rangle = 0$$

$$J_-|a, b_{min}\rangle = 0,$$

where b_{max} and b_{min} must satisfy

$$a = b_{max}(b_{max} + \hbar),$$

$$a = b_{min}(b_{min} - \hbar),$$

meaning that $b_{max} = b_{min} - \hbar$ or $b_{max} = -b_{min}$. The first option would mean that $b_{max} < b_{min}$, which by assumption is not true. Hence, we conclude that $b_{min} = -b_{max}$.

We have also seen that we can apply ladder operators to change the eigenvalue b of J_z in steps of $\hbar$, and we should be able to move between the state with b_{max} and the state with b_{min} by applying ladder operators n times, meaning:

$$b_{max} = b_{min} + n\hbar, \qquad n = 0, 1, 2, 3 \ldots$$

$$\Rightarrow b_{max} = \frac{n\hbar}{2}.$$

Inserted back into the equation relating a and b_{max}, we get

$$a = \frac{\hbar^2}{4} n(n+2),$$

the eigenvalue of $\vec{J}^2$.

Notice that

$$a = \frac{\hbar^2}{4} n(n+2) > b^2_{\substack{max \\ min}} = \frac{\hbar^2 n^2}{4},$$

the eigenvalue of J_z^2 is <u>always</u> smaller than that of $\vec{J}^2$, meaning that the length of J_z is always smaller than the total length of $\vec{J}$.

This is related to the fact that since J_x, J_y, J_z don't commute, we cannot know all simultaneously.

To switch to the standard notation, we define $j = \frac{n}{2}$, and $m = \frac{b}{\hbar}$, resulting in the eigenvalue equations

$$\vec{J}^2 |j, m\rangle = \hbar^2 j(j+1) |j, m\rangle$$
$$J_z |j, m\rangle = \hbar m |j, m\rangle$$

with

$$m = -j, -j+1, \ldots, j-2, j-1, j$$

and

$$j = 0, \frac{1}{2}, 1, \frac{3}{2}, \ldots$$

We can move to a state with eigenvalue $m \pm 1$ using the ladder operators:

$$J_\pm |j, m\rangle = \hbar \sqrt{j(j+1) - m(m \pm 1)}\, |j, m \pm 1\rangle.$$

This is very similar to the solutions we would find for the orbital angular momentum operator $\vec{L} = \vec{r} \times \vec{p}$. However, in that case, j could only take the values $0, 1, 2, \ldots$, i.e. non-negative integers.

The half-integer values of j can not be explained by $\vec{L}$, and means that such states cannot be described by the position representation of QM.
One very important example of such a state is the spin of the electron, which has $j = \frac{1}{2}$.

ORBITAL ANGULAR MOMENTUM

From classical expression, we have
$$\vec{L} = \hat{\vec{r}} \times \hat{\vec{p}},$$
and can find simultaneous eigenvectors of $\vec{L}^2$ and L_z:
$$\vec{L}^2 |\ell, m\rangle = \hbar^2 \ell(\ell+1) |\ell, m\rangle$$
$$L_z |\ell, m\rangle = \hbar m |\ell, m\rangle.$$

To get the eigenfunctions in position representation, we can project $|\ell, m\rangle$ onto position eigenvectors $|\vec{r}\rangle \equiv |r, \theta, \varphi\rangle$ in spherical coordinates:
$$\psi_{\ell m}(r, \theta, \varphi) = \langle r, \theta, \varphi | \ell, m\rangle = \underbrace{R(r)}_{\text{radial part}} Y_{\ell m}(\theta, \varphi)$$

$Y_{\ell m}(\theta, \varphi)$ are the <u>spherical harmonics</u>, with $Y_{\ell m}(\theta, \varphi) \propto e^{im\varphi}$.

The wavefunction should be single-valued, i.e. we should have
$$\psi_{\ell m}(r, \theta, \varphi + 2\pi) = \psi_{\ell m}(r, \theta, \varphi)$$
$$\rightarrow e^{im(\varphi + 2\pi)} = e^{im\varphi} \Rightarrow \underline{e^{im2\pi} = 1.}$$

For this to hold, <u>m must be an integer</u>. Hence, for orbital angular momentum, m, and therefore ℓ, must be integers.

EXAMPLE — Hydrogen atom
(Only short recap).

The Coulomb potential is spherically symmetric, allowing us to write the Hamiltonian in spherical coordinates as

$$\hat{H} = -\frac{\hbar^2 \nabla^2}{2m} + V(r)$$

$$= \left[-\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial r^2} + \frac{2}{r}\frac{\partial}{\partial r}\right) - \frac{e^2}{4\pi\epsilon_0}\frac{1}{r} + \frac{\vec{L}^2}{2mr^2}\right]$$

This commutes with both $\vec{L}^2$ and L_z, meaning that we can find simultaneous eigenstates of $\hat{H}$, $\vec{L}^2$ and L_z. Solving the Schrödinger equation gives

$$\psi_{\ell m n}(r,\theta,\phi) = R_{n\ell}(r)\, Y_{\ell m}(\theta,\phi)$$

with eigenvalues

$\hat{H}$: $\quad E_n = -\frac{13.6\,\text{eV}}{n^2}, \quad n = 1,2,3,\ldots$

$\vec{L}^2$: $\quad \hbar^2 \ell(\ell+1), \quad 0 \leq \ell < n,$

L_z: $\quad \hbar m, \quad m = -\ell, -\ell+1, \ldots, \ell-1, \ell.$

See plots in lecture slides.