SECTION 1: GENERAL PROPERTIES OF ANGULAR MOMENTUM IN QUANTUM MECHANICS

(From Cohen-Tannoudji et al., Volume I, Chapter VI)

Overview:

- General theory
- Application to orbital angular momentum
- Angular momentum and rotations

A. INTRODUCTION: THE IMPORTANCE OF ANGULAR MOMENTUM

Quantum theory of angular momentum, which will be developed here, is important in many areas of physics, for example:

- atomic, molecular and nuclear physics: classification of spectra;
- particle and high energy physics: spin of elementary particles;
- condensed matter physics: magnetism;
- quantum gravity in 2+1 dimensions, and many more.

The angular momentum plays a very important role in mechanics: classically, the total angular momentum of an isolated physical system is a constant of motion:

$$\frac{\mathrm{d}}{\mathrm{d}t}\vec{\mathcal{L}} = \vec{0}$$

and this is true also when a particle moves in a central potential. This last fact will become relevant in development of quantum theory of the hydrogen atom.

Notation for angular momentum operators:

- *orbital angular momentum* operators, $\hat{\vec{L}} = \{\hat{L}_x, \hat{L}_y, \hat{L}_z\}$, which will be obtained from the corresponding classical quantities by taking the appropriate operators;

- *spin angular momentum* operators , $\hat{\vec{S}} = \{\hat{S}_x, \hat{S}_y, \hat{S}_z\}$, which will represent intrinsic angular momentum of a particle; as it has no analog in classical mechanics, it will be defined more generally through algebra of their commutation relations;

- *general/total angular momentum* operators, $\hat{\vec{J}} = \{\hat{J}_x, \hat{J}_y, \hat{J}_z\}$, which will result from addition of both orbital and spin angular momenta of a particle.

B. COMMUTATION RELATIONS CHARACTERISTIC OF ANGULAR MOMENTUM

1. Orbital angular momentum

The component of the classical angular momentum are given as $\vec{r} \times \vec{p}$:

$$
\begin{aligned}
\mathcal{L}_x &= y p_z - z p_y \\
\mathcal{L}_y &= z p_x - x p_z \\
\mathcal{L}_z &= x p_y - y p_x
\end{aligned}
$$

The corresponding quantum operator is obtained by **canonical quantization**, that is substituting position and momentum observables for the corresponding classical quantities

$$
\begin{aligned}
\hat{L}_x &= \hat{Y}\hat{P}_z - \hat{Z}\hat{P}_y \\
\hat{L}_y &= \hat{Z}\hat{P}_x - \hat{X}\hat{P}_z \\
\hat{L}_z &= \hat{X}\hat{P}_y - \hat{Y}\hat{P}_x
\end{aligned}
$$

The components of the orbital angular momentum satisfy important commutation relations. To find these, we first note that the angular momentum operators are expressed using the position and momentum operators which satisfy the **canonical commutation relations**:

$$[\hat{X},\hat{P}_x]=[\hat{Y},\hat{P}_y]=[\hat{Z},\hat{P}_z]=i\hbar$$

All the other possible commutation relations between the operators of various components of the position and momentum are zero. The desired commutation relations for the angular momentum operators are then calculated as follows:

$$\begin{aligned}
\left[\hat{L}_x,\hat{L}_y\right] &= \left[\hat{Y}\hat{P}_z-\hat{Z}\hat{P}_y,\hat{Z}\hat{P}_x-\hat{X}\hat{P}_z\right] \\
&= \left[\hat{Y}\hat{P}_z,\hat{Z}\hat{P}_x\right]+\left[\hat{Z}\hat{P}_y,\hat{X}\hat{P}_z\right] \\
&= \hat{Y}\left[\hat{P}_z,\hat{Z}\right]\hat{P}_x+\hat{X}\left[\hat{Z},\hat{P}_z\right]\hat{P}_y \\
&= -i\hbar\hat{Y}\hat{P}_x+i\hbar\hat{X}\hat{P}_y \\
&= i\hbar\hat{L}_z
\end{aligned}$$

Similar calculations can be performed (do it as a homework!) to obtain all the commutation relations between the components of the orbital angular momentum:

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

which can be shortened using the antisymmetric tensor ϵ_{ijk} as follows

$$\left[\hat{L}_i, \hat{L}_j\right] = \epsilon_{ijk} i\hbar\hat{L}_k$$

For the system of N particles, the total angular momentum is a sum of the angular momenta of the individual particles

$$\hat{\vec{L}} = \sum_{i=1}^{N} \hat{\vec{L}}_i$$

where $\hat{\vec{L}}_i$ is given as follows:

$$\hat{\vec{L}}_i = \hat{\vec{R}}_i \times \hat{\vec{P}}_i$$

1. Generalization: definition of an angular momentum

We will now define an angular momentum $\hat{\vec{J}}$ as any set of observables $\hat{J}_x$, $\hat{J}_y$ and $\hat{J}_z$ which satisfy

$$\boxed{\begin{aligned} \left[\hat{J}_x, \hat{J}_y\right] &= i\hbar \hat{J}_z \\ \left[\hat{J}_y, \hat{J}_z\right] &= i\hbar \hat{J}_x \\ \left[\hat{J}_z, \hat{J}_x\right] &= i\hbar \hat{J}_y \end{aligned}}$$

We now introduce the operator

$$\hat{J}^2 \quad = \quad \hat{J}_x^2 + \hat{J}_y^2 + \hat{J}_z^2$$

that represents the scalar square of the angular momentum. It has two notable properties:

- it is a self-adjoint operator, and thus an observable, and

- it commutes with the components of the angular momentum:

$$\boxed{\left[\hat{J}^2, \hat{\vec{J}}\right] = \vec{0}}$$

$$
\begin{aligned}
\left[\hat{J}^2, \hat{J}_x\right] &= \left[\hat{J}_x^2 + \hat{J}_y^2 + \hat{J}_z^2, \hat{J}_x\right] \\
&= \left[\hat{J}_y^2, \hat{J}_x\right] + \left[\hat{J}_z^2, \hat{J}_x\right] = 0
\end{aligned}
$$

$$
\begin{aligned}
\left[\hat{J}_y^2, \hat{J}_x\right] &= \hat{J}_y^2 \hat{J}_x - \hat{J}_y \hat{J}_x \hat{J}_y + \hat{J}_y \hat{J}_x \hat{J}_y - \hat{J}_x \hat{J}_y^2 \\
&= \hat{J}_y \left[\hat{J}_y, \hat{J}_x\right] + \left[\hat{J}_y, \hat{J}_x\right] \hat{J}_y \\
&= -i\hbar \hat{J}_y \hat{J}_z - i\hbar \hat{J}_z \hat{J}_y \\
\left[\hat{J}_z^2, \hat{J}_x\right] &= \hat{J}_z \left[\hat{J}_z, \hat{J}_x\right] + \left[\hat{J}_z, \hat{J}_x\right] \hat{J}_z \\
&= i\hbar \hat{J}_z \hat{J}_y + i\hbar \hat{J}_y \hat{J}_z
\end{aligned}
$$

Complete set of commuting observables (C.S.C.O.) relevant to the quantum theory of angular momentum is given by the operators $\hat{J}^2$ and $\hat{J}_z$.

C. GENERAL THEORY OF ANGULAR MOMENTUM

1. Definitions and notations

a. THE J_+ AND J_- OPERATORS

$$\boxed{\begin{aligned}\hat{J}_+ &= \hat{J}_x + i\hat{J}_y \\ \hat{J}_- &= \hat{J}_x - i\hat{J}_y\end{aligned}}$$

which satisfy the following commutation relations

$$\begin{aligned}
\left[\hat{J}_z, \hat{J}_+\right] &= \hbar\hat{J}_+ \\
\left[\hat{J}_z, \hat{J}_-\right] &= -\hbar\hat{J}_- \\
\left[\hat{J}_+, \hat{J}_-\right] &= 2\hbar\hat{J}_z \\
\left[\hat{J}^2, \hat{J}_+\right] &= \left[\hat{J}^2, \hat{J}_-\right] = \left[\hat{J}^2, \hat{J}_z\right] = 0
\end{aligned}$$

They also satisfy the following useful relations:

$$\begin{aligned}
\hat{J}_+\hat{J}_- &= \left(\hat{J}_x + i\hat{J}_y\right)\left(\hat{J}_x - i\hat{J}_y\right) \\
&= \hat{J}_x^2 + \hat{J}_y^2 - i\left[\hat{J}_x, \hat{J}_y\right] \\
&= \hat{J}_x^2 + \hat{J}_y^2 + \hbar J_z \\
&= \hat{J}^2 - \hat{J}_z^2 + \hbar J_z \\
\hat{J}_-\hat{J}_+ &= \left(\hat{J}_x - i\hat{J}_y\right)\left(\hat{J}_x + i\hat{J}_y\right) \\
&= \hat{J}_x^2 + \hat{J}_y^2 + i\left[\hat{J}_x, \hat{J}_y\right] \\
&= \hat{J}_x^2 + \hat{J}_y^2 - \hbar J_z \\
&= \hat{J}^2 - \hat{J}_z^2 - \hbar J_z \\
\hat{J}^2 &= \frac{1}{2}\left(\hat{J}_+\hat{J}_- + \hat{J}_-\hat{J}_+\right) + \hat{J}_z^2
\end{aligned}$$

b. NOTATION FOR THE EIGENVALUES OF J^2 AND J_Z

$\hat{J}^2$ is the sum of the squares of three self-adjoint operators, i.e. for any ket $|\psi\rangle$, the matrix element $\langle\psi|\hat{J}^2|\psi\rangle$ is non-negative:

$$\begin{aligned}\langle\psi|\hat{J}^2|\psi\rangle &= \langle\psi|\hat{J}_x^2|\psi\rangle + \langle\psi|\hat{J}_y^2|\psi\rangle + \langle\psi|\hat{J}_z^2|\psi\rangle \\ &= \left\|\hat{J}_x|\psi\rangle\right\|^2 + \left\|\hat{J}_y|\psi\rangle\right\|^2 + \left\|\hat{J}_z|\psi\rangle\right\|^2 \geq 0\end{aligned}$$

That is all the eigenvalues of $\hat{J}^2$ are positive or zero.

Let $|\psi\rangle$ be an eigenvector of $\hat{J}^2$, then

$$\langle\psi|\hat{J}^2|\psi\rangle \quad = \quad \lambda\langle\psi|\psi\rangle \geq 0$$

We shall write the eigenvalues of $\hat{J}^2$ in the form

$$j\,(j+1)\,\hbar^2 \quad = \quad \lambda$$

with the convention that

$$j \quad \geq \quad 0$$

The eigenvalues of $\hat{J}_z$ are traditionally written as

$$m\hbar$$

where m is a dimensionless number.

c. EIGENVALUE EQUATIONS FOR J^2 AND J_z

We can now summarize the eigenvalue equations for both operators relevant to quantum theory of angular momentum $\hat{J}^2$ and $\hat{J}_z$:

$$\begin{aligned}\hat{J}^2|k, j, m\rangle &= j\,(j+1)\,\hbar^2|k, j, m\rangle \\ \hat{J}_z|k, j, m\rangle &= m\hbar|k, j, m\rangle\end{aligned}$$

where k is included for completeness to represent an additional commuting observables from C.S.C.O.

2. Eigenvalues of J^2 and J_z

a. LEMMAS

α. Lemma I (Properties of the eigenvalues of $\hat{J}^2$ and $\hat{J}_z$)

If $j(j+1)\hbar^2$ and $m\hbar$ are the eigenvalues of $\hat{J}^2$ and $\hat{J}_z$ associated with the same eigenvector $|k, j, m\rangle$, then j and m satisfy the inequality

$$-j \leq \quad m \quad \leq j$$

Proof: consider the vectors $\hat{J}_{+}|k, j, m\rangle$ and $\hat{J}_{-}|k, j, m\rangle$ and note that the square of their norms is positive or zero

$$\begin{aligned}
\left\|\hat{J}_{+}|k, j, m\rangle\right\|^{2} = \langle k, j, m|\hat{J}_{-}\hat{J}_{+}|k, j, m\rangle &\geq 0 \\
\left\|\hat{J}_{-}|k, j, m\rangle\right\|^{2} = \langle k, j, m|\hat{J}_{+}\hat{J}_{-}|k, j, m\rangle &\geq 0
\end{aligned}$$

We assume that $|k, j, m\rangle$ is normalized and use the formulas developed in the context of rising and lowering operators

$$\begin{aligned}
\langle k, j, m|\hat{J}_{-}\hat{J}_{+}|k, j, m\rangle &= \langle k, j, m|\left(\hat{J}^{2} - \hat{J}_{z}^{2} - \hbar\hat{J}_{z}\right)|k, j, m\rangle \\
&= j\,(j+1)\,\hbar^{2} - m^{2}\hbar^{2} - m\hbar^{2} \\
\langle k, j, m|\hat{J}_{+}\hat{J}_{-}|k, j, m\rangle &= \langle k, j, m|\left(\hat{J}^{2} - \hat{J}_{z}^{2} + \hbar\hat{J}_{z}\right)|k, j, m\rangle \\
&= j\,(j+1)\,\hbar^{2} - m^{2}\hbar^{2} + m\hbar^{2}
\end{aligned}$$

Substituting these expressions to the inequalities above we get

$$
\begin{aligned}
j(j+1) - m(m+1) = (j-m)(j+m+1) &\geq 0 \\
j(j+1) - m(m-1) = (j-m+1)(j+m) &\geq 0
\end{aligned}
$$

and consequently

$$
\begin{aligned}
-(j+1) \leq \; & m \; \leq j \\
-j \leq \; & m \; \leq j+1
\end{aligned}
$$

β. Lemma II (Properties of the vector $J_{-}|k, j, m\rangle$)

Let $|k, j, m\rangle$ be an eigenvector of $\hat{J}^2$ and $\hat{J}_z$ with the eigenvalues $j\,(j+1)\,\hbar^2$ and $m\hbar$

1. If $m = -j$, $\hat{J}_{-}|k, j, -j\rangle = 0$.

2. If $m > -j$, $\hat{J}_{-}|k, j, m\rangle$ is a non-null eigenvector of $\hat{J}^2$ and $\hat{J}_z$, with the eigenvalues $j\,(j+1)\,\hbar^2$ and $(m-1)\hbar$.

Proof: (1) the square norm of $\hat{J}_-|k, j, m\rangle$ is equal to $\hbar^2[j(j+1) - m(m-1)]$ and thus goes to zero for $m = -j$. Since the norm of a vector goes to zero iff the vector is the null vector, we conclude that all vectors $\hat{J}_-|k, j, -j\rangle$ are null:

$$m = -j \quad \Rightarrow \quad \hat{J}_-|k, j, -j\rangle = 0$$

We can also establish the converse:

$$\hat{J}_-|k, l, m\rangle = 0 \quad \Rightarrow \quad m = -j$$

by letting $\hat{J}_+$ act on both sides of the equation above we get the relation

$$\begin{aligned} &\hbar^2\left[j(j+1) - m^2 + m\right]|k, j, m\rangle \\ &= \hbar^2 (j+m)(j-m+1)|k, j, m\rangle \quad = \quad 0 \end{aligned}$$

whose only solution is obtained for $m = -j$.

(2) Assuming that $m > -j$, the vector $\hat{J}_-|k, j, m\rangle$ is now a non-null vector since the square of its norm is different from zero. We will now establish that it is an eigenvector of both $\hat{J}^2$ and $\hat{J}_z$. We already know that $\hat{J}_-$ and $\hat{J}^2$ commute, that is:

$$\left[\hat{J}^2, \hat{J}_-\right]|k, j, m\rangle \;=\; 0$$

which we can write as follows

$$\begin{aligned}\hat{J}^2\hat{J}_-|k, j, m\rangle &= \hat{J}_-\hat{J}^2|k, j, m\rangle \\ &= j\,(j+1)\,\hbar^2\hat{J}_-|k, j, m\rangle\end{aligned}$$

This expression shows that $\hat{J}_-|k, j, m\rangle$ is an eigenvector of $\hat{J}^2$ with the eigenvalue $j\,(j+1)\,\hbar^2$.

Similarly we can write

$$\left[\hat{J}_z, \hat{J}_-\right]|k, j, m\rangle \quad = \quad -\hbar\hat{J}_-|k, j, m\rangle$$

that is:

$$\begin{aligned}
\hat{J}_z\hat{J}_-|k, j, m\rangle &= \hat{J}_-\hat{J}_z|k, j, m\rangle - \hbar\hat{J}_-|k, j, m\rangle \\
&= m\hbar\hat{J}_-|k, j, m\rangle - \hbar\hat{J}_-|k, j, m\rangle \\
&= (m - 1)\,\hbar\hat{J}_-|k, j, m\rangle
\end{aligned}$$

$\hat{J}_-|k, j, m\rangle$ is therefore an eigenvector of $\hat{J}_z$ with the eigenvalue $(m - 1)\hbar$.

γ. Lemma III (Properties of the vector $J_+|k, j, m\rangle$)

Let $|k, j, m\rangle$ be an eigenvector of $\hat{J}^2$ and $\hat{J}_z$ with the eigenvalues $j\,(j+1)\,\hbar^2$ and $m\hbar$.

1. If $m = j$, $\hat{J}_+|k, j, j\rangle = 0$.

2. If $m < j$, $\hat{J}_+|k, j, m\rangle$ is a non-null eigenvector of $\hat{J}^2$ and $\hat{J}_z$, with the eigenvalues $j\,(j+1)\,\hbar^2$ and $(m+1)\hbar$.

Proof: (1) The proof is based on similar argument as the proof of Lemma II. The square of the norm of $\hat{J}_+|k, j, m\rangle$ is zero if $m = j$, therefore:

$$m = j \quad \Rightarrow \quad \hat{J}_+|k, j, j\rangle = 0$$

The converse is proved similarly:

$$\hat{J}_+|k, j, m\rangle = 0 \quad \Leftrightarrow \quad j = m$$

(2) Assuming $m < j$, we get again in analogy with the Lemma II

$$\begin{aligned}\hat{J}^2 \hat{J}_+|k, j, m\rangle &= j\,(j+1)\,\hbar^2 \hat{J}_+|k, j, m\rangle \\ \hat{J}_z \hat{J}_+|k, j, m\rangle &= (m+1)\,\hbar \hat{J}_+|k, j, m\rangle\end{aligned}$$

b. DETERMINATION OF THE SPECTRUM OF J^2 AND J_z

Let $|k, j, m\rangle$ be a non-null eigenvector of $\hat{J}^2$ and $\hat{J}_z$ with the eigenvalues $j\,(j+1)\,\hbar^2$ and $m\hbar$. According to Lemma I: $-j \leq m \leq j$. That is, there exists a positive or zero integer p s.t.

$$-j \leq \quad m - p \quad < -j + 1$$

Consider now a series of vectors

$$|k, j, m\rangle, \hat{J}_{-}|k, j, m\rangle, \ldots, \left(\hat{J}_{-}\right)^{p} |k, j, m\rangle$$

According to Lemma II, each of the vectors $(\hat{J}_{-})^{n}|k, j, m\rangle$ of the series $(n = 0, 1, 2..., p)$ is a non-null eigenvector of $\hat{J}^2$ and $\hat{J}_z$ with the eigenvalues $j\,(j+1)\,\hbar^2$ and $(m-n)\hbar$.

Now let $\hat{J}_-$ act on $(\hat{J}_-)^p|k, j, m\rangle$ and assume that the eigenvalue $(m - p)\hbar$ of $\hat{J}_z$ associated with the vector $(\hat{J}_-)^p|k, j, m\rangle$ is greater than $-j\hbar$, i.e. $m - p > -j$.

By point (2) of Lemma II, $\hat{J}_-(\hat{J}_-)^p|k, j, m\rangle$ is then non-null and corresponds to the eigenvalues $j\,(j + 1)\,\hbar^2$ and $(m-p-1)\hbar$. However, this is in contradiction with Lemma I, since $m - p - 1 < -j$.

To remove the contradiction, we must therefore have $m-p = -j$ and $\hat{J}_-(\hat{J}_-)^p|k, j, m\rangle = 0$. This implies that there exists a positive integer p s.t.

$$\boxed{m - p = -j}$$

Completely analogous argument, based on Lemma III, shows that there exists a positive or zero integer q s.t.

$$\boxed{m + q = j}$$

since the vector series

$$|k, j, m\rangle, \hat{J}_+|k, j, m\rangle, ...\hat{J}_+^q|k, j, m\rangle$$

must be limited if there is to be no contradiction with Lemma I.

Combining $m - p = -j$ and $m + q = j$ leads to

$$\boxed{p + q = 2j}$$

which implies that j is equal to a positive or zero integer divided by 2, so

j **is necessarily either** *integer* **or** *half-integer***.**

Furthermore, if there exists a non-null eigenvector $|k, j, m\rangle$, all the vectors of the series

$$|k, j, m\rangle, \hat{J}_{-}|k, j, m\rangle, ...\hat{J}_{-}^{p}|k, j, m\rangle$$
$$|k, j, m\rangle, \hat{J}_{+}|k, j, m\rangle, ...\hat{J}_{+}^{q}|k, j, m\rangle$$

are also non-null eigenvectors of $\hat{J}^2$ with eigenvalue $j\,(j+1)\,\hbar^2$ as well as of $\hat{J}_z$ with the eigenvalues

$$j\hbar, (j-1)\,\hbar, (j-2)\,\hbar, ..., (-j+2)\,\hbar, (-j+1)\,\hbar, , -j\hbar$$

3. Standard $\{|k, j, m\rangle\}$ representations

a. THE BASIS STATES

Our goal is now to construct an orthonormal basis of the state space $\mathcal{E}$ composed of the eigenvectors common to $\hat{J}^2$ and $\hat{J}_z$.

Consider the subspace $\mathcal{E}(j,m)$ which is spanned by the eigenvectors of $\hat{J}^2$ and $\hat{J}_z$ corresponding to the eigenvalues $j\,(j+1)\,\hbar^2$ and $m\hbar$. Since these operators do not generally constitute a C.S.C.O., the dimension of this subspace $g(j,m)$ can be greater than 1. We choose an arbitrary orthonormal basis in $\mathcal{E}(j,m)$:

$$\{|k, j, m\rangle; k = 1, 2, ..., g(j,m)\}.$$

Note that

- If $m \neq j$, there exists a subspace $\mathcal{E}(j, m+1)$ spanned by the eigenvectors of $\hat{J}^2$ and $\hat{J}_z$ corresponding to the eigenvalues $j\,(j+1)\,\hbar^2$ and $(m+1)\hbar$.

- If $m \neq -j$, there exists a subspace $\mathcal{E}(j, m-1)$ spanned by the eigenvectors of $\hat{J}^2$ and $\hat{J}_z$ corresponding to the eigenvalues $j\,(j+1)\,\hbar^2$ and $(m-1)\hbar$.

In the cases where $m \neq \pm j$, we shall construct orthonormal bases in $\mathcal{E}(j, m+1)$ and $\mathcal{E}(j, m-1)$ from the basis chosen in $\mathcal{E}(j, m)$.

We first show that if $k_1 \neq k_2$, the vectors $\hat{J}_+|k_1, j, m\rangle$ and $\hat{J}_+|k_2, j, m\rangle$ are orthogonal, and so are the vectors $\hat{J}_-|k_1, j, m\rangle$ and $\hat{J}_-|k_2, j, m\rangle$:

$$\begin{aligned}\langle k_2, j, m|\hat{J}_\mp \hat{J}_\pm|k_1, j, m\rangle &= \langle k_2, j, m|\left(\hat{J}^2 - \hat{J}_z^2 \mp \hbar \hat{J}_z\right)|k_1, j, m\rangle \\ &= \left[j\,(j+1) - m\,(m \pm 1)\right]\hbar^2 \langle k_2, j, m|k_1, j, m\rangle\end{aligned}$$

If $k_1 \neq k_2$, then $\langle k_2, j, m|k_1, j, m\rangle = 0$ and thus $\langle k_2, j, m|\hat{J}_\mp \hat{J}_\pm|k_1, j, m\rangle = 0$.

If $k_1 = k_2$, the square of the norm of $\hat{J}_\pm|k_1, j, m\rangle$ is equal to

$$\left[j\,(j+1) - m\,(m \pm 1)\right]\hbar^2$$

and thus we can define the set of $g(j, m)$ orthonormal vectors

$$|k, j, m+1\rangle = \frac{1}{\hbar\sqrt{j\,(j+1) - m\,(m+1)}}\hat{J}_+|k, j, m\rangle \tag{1.1}$$

which form a basis in $\mathcal{E}(j, m+1)$.

Similarly, we can show that the set of $g(j,m)$ orthonormal vectors

$$|k,j,m-1\rangle \quad = \quad \frac{1}{\hbar\sqrt{j\,(j+1)-m\,(m-1)}}\hat{J}_{-}|k,j,m\rangle \tag{1.2}$$

form an orthonormal basis in $\mathcal{E}(j,m-1)$.

We see in particular that the dimension of the subspaces $\mathcal{E}(j,m+1)$ and $\mathcal{E}(j,m-1)$ is the same as the dimension of $\mathcal{E}(j,m)$, and thus is independent on m:

$$g\,(j,m+1) = g\,(j,m-1) = g\,(j,m) = g(j)$$

We now proceed with our quest for finding the basis of $\mathcal{E}$ as follows:

- for each value of j, we choose one of the subspaces, for example the one with $m = j$: $\mathcal{E}(j, j)$;

- we choose an arbitrary orthonormal basis: $\{|k, j, j\rangle; k = 1, 2, ..., g(j)\}$;

- Using Eq. (1.2), we calculate by iteration the basis of each of the other $2j$ subspaces $\mathcal{E}(j, m)$.

$$
\begin{array}{lllll}
 & \multicolumn{4}{c}{\overbrace{\hspace{20em}}^{g(j)\ \text{different values of}\ k}} \\
 & k = 1, & 2, & \ldots, & g(j) \\ \cline{2-5}
\mathcal{E}(j, m = j) & |1, j, j\rangle & |2, j, j\rangle & \ldots & |g(j), j, j\rangle \\
\Downarrow \hat{J}_{-} & \Downarrow \hat{J}_{-} & \Downarrow \hat{J}_{-} & \ldots & \Downarrow \hat{J}_{-} \\
\mathcal{E}(j, m = j-1) & |1, j, j-1\rangle & |2, j, j-1\rangle & \ldots & |g(j), j, j-1\rangle \\
\Downarrow \hat{J}_{-} & \Downarrow \hat{J}_{-} & \Downarrow \hat{J}_{-} & \ldots & \Downarrow \hat{J}_{-} \\
\vdots & \vdots & \vdots & \vdots & \vdots \\
\mathcal{E}(j, m) & |1, j, m\rangle & |2, j, m\rangle & \ldots & |g(j), j, m\rangle \\
\Downarrow \hat{J}_{-} & \Downarrow \hat{J}_{-} & \Downarrow \hat{J}_{-} & \ldots & \Downarrow \hat{J}_{-} \\
\vdots & \vdots & \vdots & \vdots & \vdots \\
\mathcal{E}(j, m = -j) & |1, j, -j\rangle & |2, j, -j\rangle & \ldots & |g(j), j, -j\rangle \\ \cline{2-5}
 & \mathcal{E}(k = 1, j) & \mathcal{E}(k = 2, j) & & \mathcal{E}(k = g(j), j) \\
 & \multicolumn{4}{c}{\underbrace{\hspace{20em}}_{g(j)\ \text{spaces}\ \mathcal{E}(k, j)}}
\end{array}
$$

To carry out this construction for all values of j found in the problem under consideration (e.g. a particle in a central potential), we obtain

a *standard basis* of the space $\mathcal{E}$.

The orthonormalization and the completeness (also called closure) relation for such a basis are

$$\begin{aligned}\langle k, j, m | k', j', m' \rangle &= \delta_{kk'} \delta_{jj'} \delta_{mm'} \\ \sum_j \sum_{m=-j}^{j} \sum_{k=1}^{g(j)} |k, j, m\rangle \langle k, j, m| &= \hat{1}\end{aligned}$$

Comments:

- Note that the basis vectors of $\mathcal{E}(j, m-1)$ are proportional, with real and positive coefficient, to the vectors obtained by application of the lowering operator $\hat{J}_-$ onto the basis $\mathcal{E}(j, m)$.

- Equations (1.1) and (1.2) are compatible (Homework: apply $\hat{J}_+$ to both sides of Eq. (1.2) to find Eq. (1.1) with m replaced by $m-1$), so we can start from other values of m than $m = j$ to construct bases of $\mathcal{E}(j, m)$.

b. THE SPACES $\mathcal{E}(k, j)$

We will use the spaces $\mathcal{E}(k, j)$ rather than $\mathcal{E}(j, m)$ as those present some disadvantages:

- dimension $g(j)$ depends on the system and is not generally known;
- $\mathcal{E}(j, m)$ are not invariant under the action of $\hat{\vec{J}}$, giving nonzero matrix elements of $\mathcal{E}(j, m)$ and $\mathcal{E}(j, m \pm 1)$.

c. MATRICES REPRESENTING ANGULAR MOMENTUM OPERATORS

Using the subspaces $\mathcal{E}(k, j)$ considerably simplifies the search for the matrix representation in a standard basis of a component J_u of the angular momentum operator $\hat{\vec{J}}$ or an arbitrary function $F(\hat{\vec{J}})$ as the matrix elements between two vectors from different subspaces $\mathcal{E}(k, j)$ are zero. The angular momentum operators are then represented by a finite dimensional matrices inside of each of the subspaces $\mathcal{E}(k, j)$.

	$\mathcal{E}(k, j)$	$\mathcal{E}(k', j)$	$\mathcal{E}(k', j')$	$\dots$
$\mathcal{E}(k, j)$	matrix $(2j+1) \times (2j+1)$	0	0	0
$\mathcal{E}(k', j)$	0	matrix $(2j+1) \times (2j+1)$	0	0
$\mathcal{E}(k', j')$	0	0	matrix $(2j'+1) \times (2j'+1)$	0
$\vdots$	0	0	0	0

Moreover these finite-dimensional matrices are independent of k and of the physical system under study and depend only on j and on the operator to be represented. The definition of $|k, j, m\rangle$ implies

$$\boxed{\begin{array}{c} \hat{J}_z|k, j, m\rangle = m\hbar|k, j, m\rangle \\ \hat{J}_+|k, j, m\rangle = \hbar\sqrt{j(j+1) - m(m+1)}|k, j, m+1\rangle \\ \hat{J}_-|k, j, m\rangle = \hbar\sqrt{j(j+1) - m(m-1)}|k, j, m-1\rangle \end{array}}$$

that is

$$\begin{aligned} \langle k, j, m|\hat{J}_z|k', j', m'\rangle &= m\hbar\delta_{kk'}\delta_{jj'}\delta_{mm'} \\ \langle k, j, m|\hat{J}_\pm|k', j', m'\rangle &= \hbar\sqrt{j(j+1) - m(m\pm 1)}\delta_{kk'}\delta_{jj'}\delta_{m,m'\pm 1} \end{aligned} \quad (1.3)$$

Examples of the matrices $(J_u)^{(j)}$:

(i) $j = 0$

The subspace $\mathcal{E}(k, 0)$ is one-dimensional since the only positive value of m is zero; the corresponding basis vector is $\mathcal{B} = \{|j = 0, m = 0\rangle\}$. The matrix representation is then

$$(J_u)^{(0)} \quad = \quad 0$$

(ii) $j = 1/2$: $\mathcal{B} = \{|j = 1/2, m = 1/2\rangle, |j = 1/2, m = -1/2\rangle\}$

$$\left(\hat{J}_z\right)^{(1/2)} = \frac{\hbar}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} = \frac{\hbar}{2}\sigma_z$$

$$\left(\hat{J}_+\right)^{(1/2)} = \hbar\begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} \qquad \left(\hat{J}_-\right)^{(1/2)} = \hbar\begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}$$

$$\left(\hat{J}_x\right)^{(1/2)} = \frac{\hbar}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} = \frac{\hbar}{2}\sigma_x \qquad \left(\hat{J}_y\right)^{(1/2)} = \frac{\hbar}{2}\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} = \frac{\hbar}{2}\sigma_y$$

$$\left(\hat{J}^2\right)^{(1/2)} = \frac{3}{4}\hbar^2\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$

(iii) $j = 1$: $\mathscr{B} = \{|j = 1, m = 1\rangle, |j = 1, m = 0\rangle, |j = 1, m = -1\rangle\}$

$$\left(\hat{J}_z\right)^{(1)} = \hbar \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix} \qquad \left(\hat{J}^2\right)^{(1)} = 2\hbar^2 \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

$$\left(\hat{J}_+\right)^{(1)} = \hbar \begin{pmatrix} 0 & \sqrt{2} & 0 \\ 0 & 0 & \sqrt{2} \\ 0 & 0 & 0 \end{pmatrix} \qquad \left(\hat{J}_-\right)^{(1)} = \hbar \begin{pmatrix} 0 & 0 & 0 \\ \sqrt{2} & 0 & 0 \\ 0 & \sqrt{2} & 0 \end{pmatrix}$$

$$\left(\hat{J}_x\right)^{(1)} = \frac{\hbar}{\sqrt{2}} \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix} \qquad \left(\hat{J}_y\right)^{(1)} = \frac{\hbar}{\sqrt{2}} \begin{pmatrix} 0 & -i & 0 \\ i & 0 & -i \\ 0 & i & 0 \end{pmatrix}$$

(iv) j *arbitrary*

The matrix $(J_z)^{(j)}$ is diagonal and its elements are the $(2j + 1)$ values of $m\hbar$. The only nonzero elements of $(J_x)^{(j)}$ and $(J_y)^{(j)}$ are obtained using Eq. (1.3). $(J_x)^{(j)}$ is symmetric and real and $(J_y)^{(j)}$ is antisymmetric and purely imaginary:

$$\langle k, j, m|\hat{J}_x|k', j', m'\rangle = \frac{\hbar}{2}\delta_{kk'}\delta_{jj'}$$
$$\times\left[\hbar\sqrt{j(j+1) - m(m+1)}\delta_{m,m'+1} + \sqrt{j(j+1) - m(m-1)}\delta_{m,m'-1}\right]$$
$$\langle k, j, m|\hat{J}_y|k', j', m'\rangle = \frac{\hbar}{2i}\delta_{kk'}\delta_{jj'}$$
$$\times\left[\hbar\sqrt{j(j+1) - m(m+1)}\delta_{m,m'+1} - \sqrt{j(j+1) - m(m-1)}\delta_{m,m'-1}\right]$$

$(\hat{J}^2)^{(j)}$ is proportional to a unit matrix:

$$\langle k, j, m|\hat{J}^2|k', j', m'\rangle = j(j+1)\hbar^2\delta_{kk'}\delta_{jj'}\delta_{mm'}$$

An orthonormal basis $\{|k, j, m\rangle\}$ of the state space, composed of eigenvectors common to $\hat{J}^2$ and $\hat{J}_z$:

$$\hat{J}^2|k, j, m\rangle = j(j+1)\hbar^2|k, j, m\rangle$$
$$\hat{J}_z|k, j, m\rangle = m\hbar|k, j, m\rangle$$

is called a “standard basis” if the action of the operators $\hat{J}_+$ and $\hat{J}_-$ on the basis vectors is given by:

$$\hat{J}_+|k, j, m\rangle = \hbar\sqrt{j(j+1) - m(m+1)}|k, j, m+1\rangle$$
$$\hat{J}_-|k, j, m\rangle = \hbar\sqrt{j(j+1) - m(m-1)}|k, j, m-1\rangle$$

D. APPLICATION TO ORBITAL ANGULAR MOMENTUM

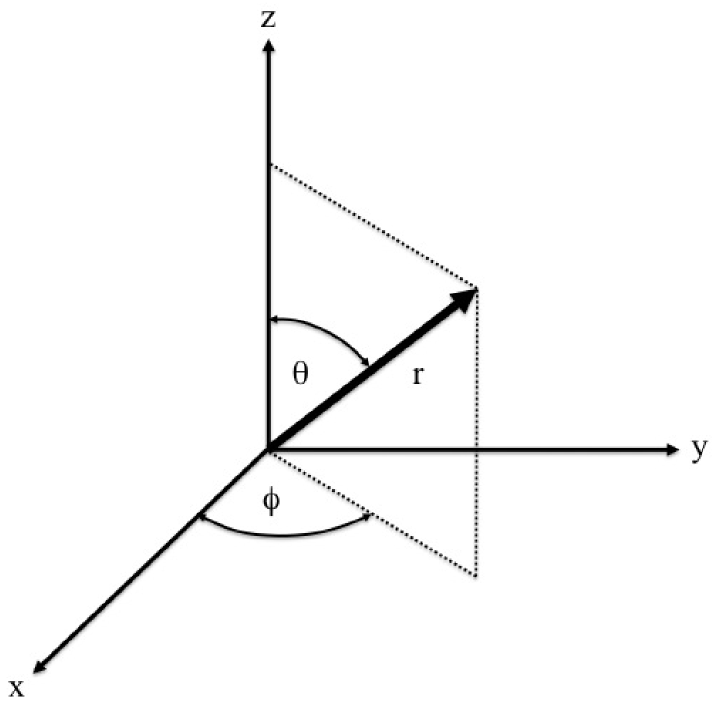
1. Eigenvalues and eigenfunctions of $\hat{L}^2$ and $\hat{L}_z$

a. EIGENVALUE EQUATION IN THE $\{|\vec{r}\rangle\}$ REPRESENTATION

In the coordinate representation, the components of the orbital angular momentum $\hat{\vec{L}} = \hat{\vec{R}} \times \hat{\vec{P}}$, where $\hat{\vec{R}} = \vec{r}$ are the position operators and $\hat{\vec{P}} = -i\hbar\vec{\nabla}$ are the momentum operators, are given as

$$\begin{aligned} \hat{L}_x &= \frac{\hbar}{i}\left(y\frac{\partial}{\partial z} - z\frac{\partial}{\partial y}\right) \\ \hat{L}_y &= \frac{\hbar}{i}\left(z\frac{\partial}{\partial x} - x\frac{\partial}{\partial z}\right) \\ \hat{L}_z &= \frac{\hbar}{i}\left(x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x}\right) \end{aligned}$$

It is convenient to work in spherical (polar) coordinates as the various angular momentum operators act only on the angular variables θ and ϕ:



$$\begin{cases} x = r\sin\theta\cos\phi \\ y = r\sin\theta\sin\phi \\ z = r\cos\theta \end{cases}$$

with:

$$\begin{cases} r \geq 0 \\ 0 \leq \theta \leq \pi \\ 0 \leq \phi \leq 2\pi \end{cases}$$

The volume element $d^3\vec{r} = dxdydz$ is given in the spherical coordinates as:

$$\mathrm{d}^3\vec{r} \quad = \quad r^2 \sin\theta \,\mathrm{d}r\,\mathrm{d}\theta\,\mathrm{d}\phi = r^2\,\mathrm{d}r\,\mathrm{d}\Omega$$

where

$$\mathrm{d}\Omega \quad = \quad \sin\theta\,\mathrm{d}\theta\,\mathrm{d}\phi$$

In the spherical coordinate representation, the relevant operators are (homework: check that the last three operators follow from the first three):

$$
\begin{aligned}
\hat{L}_x &= i\hbar\left(\sin\phi\frac{\partial}{\partial\theta} + \frac{\cos\phi}{\tan\theta}\frac{\partial}{\partial\phi}\right)\\
\hat{L}_y &= i\hbar\left(-\cos\phi\frac{\partial}{\partial\theta} + \frac{\sin\phi}{\tan\theta}\frac{\partial}{\partial\phi}\right)\\
\hat{L}_z &= \frac{\hbar}{i}\frac{\partial}{\partial\phi}\\
\hat{L}^2 &= -\hbar^2\left(\frac{\partial^2}{\partial\theta^2} + \frac{1}{\tan\theta}\frac{\partial}{\partial\theta} + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2}\right)\\
\hat{L}_+ &= \hbar e^{i\phi}\left(\frac{\partial}{\partial\theta} + i\cot\theta\frac{\partial}{\partial\phi}\right)\\
\hat{L}_- &= \hbar e^{-i\phi}\left(-\frac{\partial}{\partial\theta} + i\cot\theta\frac{\partial}{\partial\phi}\right)
\end{aligned}
$$

In the coordinate representation, the eigenfunctions of $\hat{L}^2$ and $\hat{L}_z$ associated with the eigenvalues $l\,(l+1)\,\hbar^2$ and $m\hbar$ are the solutions of the partial differential equations:

$$
\begin{aligned}
-\left\{\frac{\partial^2}{\partial\theta^2}+\frac{1}{\tan\theta}\frac{\partial}{\partial\theta}+\frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2}\right\}\psi(r,\theta,\phi) &= l(l+1)\psi(r,\theta,\phi)\\
-i\frac{\partial}{\partial\phi}\psi(r,\theta,\phi) &= m\psi(r,\theta,\phi)
\end{aligned}
$$

From the general theory of angular momentum we know that l is either integer or half-integer and m take the values $l, l-1, ..., -l+1, -l$.

Note that there is no r dependence in the differential equations above, so we can consider r as a parameter, and take into account only the θ- and ϕ-dependence of ψ:

$$\psi_{l,m}(r,\theta,\phi) = f(r)Y_l^m(\theta,\phi)$$

$f(r)$ is square-integrable function of the radial coordinate r and it appears as an integration constant in the differential equations above. By $Y_l^m(\theta,\phi)$ we denote a common eigenfunction of $\hat{L}^2$ and $\hat{L}_z$ with the eigenvalues $l(l+1)\hbar^2$ and $m\hbar$:

$$\begin{aligned} \hat{L}^2 Y_l^m(\theta,\phi) &= l(l+1)\hbar^2 Y_l^m(\theta,\phi) \\ \hat{L}_z Y_l^m(\theta,\phi) &= m\hbar Y_l^m(\theta,\phi) \end{aligned}$$

To normalize $\psi_{l,m}(r,\theta,\phi)$, we normalize $Y_l^m(\theta,\phi)$ and $f(r)$ separately:

$$\begin{aligned}
\int_0^{2\pi} \mathrm{d}\phi \int_0^{\pi} \sin\theta \left|Y_l^m(\theta,\phi)\right|^2 \mathrm{d}\theta &= 1 \\
\int_0^{\infty} r^2 \left|f(r)\right|^2 \mathrm{d}r &= 1
\end{aligned}$$

b. VALUES OF l and m

α. l and m must be integral

Using that $\hat{L}_z = \frac{\hbar}{i}\frac{\partial}{\partial\phi}$ we can write the eigenvalue equation for $\hat{L}_z$

$$\frac{\hbar}{i}\frac{\partial}{\partial\phi}Y_l^m(\theta,\phi) \quad = \quad m\hbar Y_l^m(\theta,\phi)$$

which shows that $Y_l^m(\theta,\phi)$ factorizes as

$$Y_l^m(\theta,\phi) \quad = \quad F_l^m(\theta)e^{im\phi}$$

Since the function $Y_l^m(\theta, \phi)$ must be continuous, the following condition must hold for $\phi = 0$ and $\phi = 2\pi$:

$$Y_l^m(\theta, \phi = 0) = Y_l^m(\theta, \phi = 2\pi)$$

which implies that

$$e^{2im\pi} = 1$$

This shows that

in the case of an orbital angular momentum, m must be an integer, and consequently also l must be an integer.

β. All integral values (positive or zero) of l can be found

Choose an integral value of $l \geq 0$. We know that, based on the general theory, $Y_l^l(\theta, \phi)$ must satisfy

$$\hat{L}_+ Y_l^l(\theta, \phi) = 0$$

By applying the relations we have derived earlier

$$\begin{aligned} Y_l^m(\theta, \phi) &= F_l^m(\theta) e^{im\phi} \\ \hat{L}_+ &= \hbar e^{i\phi} \left(\frac{\partial}{\partial \theta} + i \cot\theta \frac{\partial}{\partial \phi} \right) \end{aligned}$$

we obtain for $m = l$ the differential equation

$$\left\{ \frac{\mathrm{d}}{\mathrm{d}\theta} - l \cot\theta \right\} F_l^l(\theta) = 0$$

The equation

$$\left\{\frac{\mathrm{d}}{\mathrm{d}\theta} - l\cot\theta\right\} F_l^l(\theta) \quad = \quad 0$$

can be integrated using

$$\cot\theta\mathrm{d}\theta \quad = \quad \frac{\mathrm{d}(\sin\theta)}{\sin\theta}$$

to yield the solution

$$F_l^l(\theta) \quad = \quad c_l\,(\sin\theta)^l$$

where c_l is the normalization constant.

Consequently for each positive or zero value of l, there exists a unique (up to a constant) function

$$Y_l^l(\theta, \phi) \quad = \quad c_l \, (\sin\theta)^l \, e^{il\phi}$$

Through repeated application of $\hat{L}_-$ we construct

$$Y_l^{l-1}(\theta, \phi), ..., Y_l^m(\theta, \phi), ..., Y_l^{-l}(\theta, \phi)$$

To the eigenvalues $l\,(l+1)\,\hbar^2$ and $m\hbar$, there corresponds one and only one eigenfunction $Y_l^m\,(\theta, \phi)$. These functions are called *spherical harmonics*.

Explicitely:

$$
\begin{aligned}
Y_l^m(\theta,\phi) &= \sqrt{\frac{(l+m)!}{(2l)!(l-m)!}}\left(\frac{\hat{L}_-}{\hbar}\right)^{l-m} Y_l^l(\theta,\phi) \\
&= \frac{(-1)^l}{2^l l!}\sqrt{\frac{(2l+1)(l+m)!}{4\pi(l-m)!}} e^{im\phi}(sin\theta)^{-m}\frac{d^{l-m}}{d(cos\theta)^{l-m}}(sin\theta)^{2l}
\end{aligned}
$$

Examples:

$$
\begin{aligned}
Y_0^0(\theta,\phi) &= \frac{1}{\sqrt{4\pi}} \\
Y_1^{\pm1}(\theta,\phi) &= \mp\sqrt{\frac{3}{8\pi}}\ sin\theta\ e^{\pm i\phi} \\
Y_1^0(\theta,\phi) &= \sqrt{\frac{3}{4\pi}}\ cos\theta \\
Y_2^{\pm2}(\theta,\phi) &= \sqrt{\frac{15}{32\pi}}\ sin^2\theta\ e^{\pm 2i\phi} \\
Y_2^{\pm1}(\theta,\phi) &= \mp\sqrt{\frac{15}{8\pi}}\ sin\theta\ cos\theta\ e^{\pm i\phi} \\
Y_2^0(\theta,\phi) &= \sqrt{\frac{5}{16\pi}}(3cos^2\theta - 1)
\end{aligned}
$$

c. FUNDAMENTAL PROPERTIES OF THE SPHERICAL HARMONICS

α. Recurrence relations

$$\hat{L}_{\pm} Y_l^m(\theta,\phi) = \hbar \sqrt{l(l+1) - m(m\pm 1)}\, Y_l^{m\pm 1}(\theta,\phi)$$

$$\begin{aligned}
e^{i\phi}\left(\frac{\partial}{\partial\theta} - m\cot\theta\frac{\partial}{\partial\phi}\right) Y_l^m(\theta,\phi) &= \sqrt{l(l+1) - m(m+1)}\, Y_l^{m+1}(\theta,\phi) \\
e^{-i\phi}\left(-\frac{\partial}{\partial\theta} - m\cot\theta\frac{\partial}{\partial\phi}\right) Y_l^m(\theta,\phi) &= \sqrt{l(l+1) - m(m-1)}\, Y_l^{m-1}(\theta,\phi)
\end{aligned}$$

β. Orthonormalization and completeness (closure) relations

$$\int_0^{2\pi} \mathrm{d}\phi \int_0^{\pi} \sin\theta \mathrm{d}\theta \, Y_{l'}^{m'*}(\theta,\phi) Y_l^m(\theta,\phi) \quad = \quad \delta_{l'l}\delta_{m'm}$$

Any function $f(\theta,\phi)$ can be expanded in terms of spherical harmonics

$$f(\theta,\phi) \quad = \quad \sum_{l=0}^{\infty} \sum_{m=-l}^{+l} c_{l,m} Y_l^m(\theta,\phi)$$

with

$$c_{l,m} \quad = \quad \int_0^{2\pi} \mathrm{d}\phi \int_0^{\pi} \sin\theta \mathrm{d}\theta \, Y_l^{m*}(\theta,\phi) f(\theta,\phi)$$

Thus the spherical harmonics form a basis of the space $\mathcal{E}_\Omega$ of functions of θ and ϕ.

Completeness:

$$\sum_{l=0}^{\infty} \sum_{m=-l}^{l} Y_l^m(\theta, \phi)\, Y_l^{m*}(\theta', \phi') = \delta\left(\cos\theta - \cos\theta'\right) \delta\left(\phi - \phi'\right)$$
$$= \frac{1}{\sin\theta} \delta\left(\theta - \theta'\right) \delta\left(\phi - \phi'\right)$$

where $\delta(\theta - \theta')$ and $\delta(\phi - \phi')$ are the delta-functions.

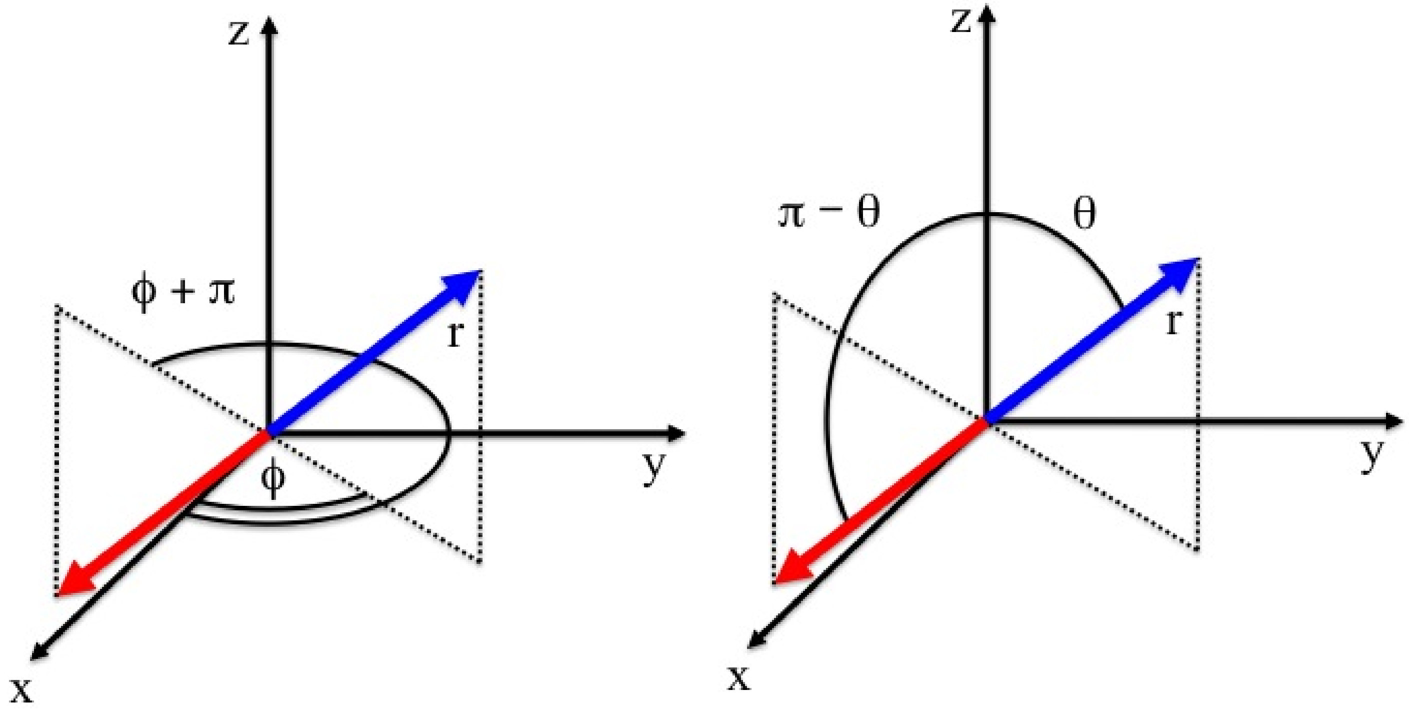
γ. Complex conjugation and parity

Complex conjugation:

$$\left[Y_l^m(\theta,\phi)\right]^* \quad = \quad (-1)^m Y_l^{-m}(\theta,\phi)$$

We are now interested in parity of the spherical harmonics, i.e. their behaviour upon the reflection through the coordinate origin $\vec{r} \rightarrow -\vec{r}$ which in spherical coordinates is given as

$$\begin{aligned} r &\Rightarrow r \\ \theta &\Rightarrow \pi - \theta \\ \phi &\Rightarrow \pi + \phi \end{aligned}$$


z
ϕ + π
r
ϕ
y
x
z
π − θ
θ
r
y
x

It can be shown (Cohen-Tannoudji, Complement A_{VI}) that

$$Y_l^m(\pi - \theta, \pi + \phi) \quad = \quad (-1)^l Y_l^m(\theta, \phi)$$

This means that the spherical harmonics are functions of a definite parity which is independent of m:

they are even if l is even and odd if l is odd.

d. STANDARD BASES OF THE WAVEFUNCTION SPACE OF A SPINLESS PARTICLE

The operators $\hat{L}^2$ and $\hat{L}_z$ do not constitute C.S.C.O. in the wavefunction space of a spinless particle.

Let $\mathcal{E}(l, m = l)$ be a subspace spanned by eigenfunctions of $\hat{L}^2$ and $\hat{L}_z$ with eigenvalues $l\,(l+1)\,\hbar^2$ and $m\hbar$. Choose an arbitrary basis in each $\mathcal{E}(l, m = l)$: $\mathcal{B} = \{\psi_{k,l,l}(\vec{r})\}$, and construct $\psi_{k,l,m}(\vec{r})$ by repeated application of the lowering operator $\hat{L}_-$. The eigenvalue equations become

$$\begin{aligned}\hat{L}^2\psi_{k,l,m}(\vec{r}) &= l(l+1)\hbar^2\psi_{k,l,m}(\vec{r})\\ \hat{L}_z\psi_{k,l,m}(\vec{r}) &= m\hbar\psi_{k,l,m}(\vec{r})\end{aligned}$$

and

$$\hat{L}_{\pm}\psi_{k,l,m}(\vec{r}) \;=\; \hbar\sqrt{l(l+1)-m(m\pm 1)}\,\psi_{k,l,m\pm 1}(\vec{r})$$

The eigenfunctions of $\hat{L}^2$ and $\hat{L}_z$ with eigenvalues $l\,(l+1)\,\hbar^2$ and $m\hbar$ have the same angular dependence, i.e. that of $Y_l^m(\theta,\phi)$ (only radial dependence differs). We can write

$$\psi_{k,l,m}(\vec{r}) \;=\; R_{k,l,m}(r)Y_l^m(\theta,\phi)$$

If $\psi_{k,l,m}(\vec{r})$ constitute a standard basis, the radial wavefunctions $R_{k,l,m}(\vec{r})$are independent of m:

$$
\begin{aligned}
\hat{L}_{\pm}\psi_{k,l,m}(\vec{r}) &= R_{k,l,m}(r)\hat{L}_{\pm}Y_l^m(\theta,\phi) \\
&= \hbar\sqrt{l(l+1)-m(m\pm1)}R_{k,l,m}(r)Y_l^{m\pm1}(\theta,\phi)
\end{aligned}
$$

comparison with

$$
\hat{L}_{\pm}\psi_{k,l,m}(\vec{r}) = \hbar\sqrt{l(l+1)-m(m\pm1)}\psi_{k,l,m\pm1}(\vec{r})
$$

show that

$$
R_{k,l,m\pm1}(r) = R_{k,l,m}(r)
$$

and are thus independent of m.

The functions $\psi_{k,l,m}(\vec{r})$ of a standard basis of the wavefunction space of a spinless particle are therefore

$$\psi_{k,l,m}(\vec{r}) \quad = \quad R_{k,l}(r) Y_l^m(\theta, \phi)$$

and satisfy the orthonormality condition

$$\begin{aligned}
\int \mathrm{d}^3\vec{r}\psi^*_{k,l,m}(\vec{r})\,\psi_{k',l',m'}(\vec{r}) \quad &= \quad \int_0^\infty r^2 \mathrm{d}r\, R^*_{k,l}(r) R_{k',l'}(r) \\
&\times \quad \int_0^{2\pi} \mathrm{d}\phi \int_0^\pi \sin\theta \mathrm{d}\theta\, Y_l^{m*}(\theta,\phi) Y_{l'}^{m'}(\theta,\phi) \\
&= \quad \delta_{kk'}\delta_{ll'}\delta_{mm'}
\end{aligned}$$

Since the spherical harmonics are orthonormal, we obtain

$$\int_0^\infty r^2 \mathrm{d}r\, R^*_{k,l}(r) R_{k',l'}(r) \quad = \quad \delta_{kk'}$$

2. Physical considerations

a. STUDY OF A $|k,l,m\rangle$ STATE

Consider a spinless particle in an eigenstate $|k,l,m\rangle$ of $\hat{L}^2$ and $\hat{L}_z$. Suppose we wish to measure the component of the angular momentum along the x axis or y axis, i.e. $\hat{L}_x$ or $\hat{L}_y$. Since these operators do not commute with $\hat{L}_z$, we can not predict the result of the measurement with certainty.

What are the mean values and root-mean square deviations of such measurements?

$$\begin{aligned}
\hat{L}_x &= \frac{1}{2}\left(\hat{L}_+ + \hat{L}_-\right) \\
\hat{L}_y &= \frac{1}{2i}\left(\hat{L}_+ - \hat{L}_-\right)
\end{aligned}$$

Since $\hat{L}_x|k,l,m\rangle$ and $\hat{L}_y|k,l,m\rangle$ will be superpositions of $|k,l,m\pm 1\rangle$, that means that

$$\langle k,l,m|\hat{L}_x|k,l,m\rangle = \langle k,l,m|\hat{L}_y|k,l,m\rangle \quad = \quad 0$$

Furthermore, using $\hat{L}_+\hat{L}_- + \hat{L}_-\hat{L}_+ = 2\left(\hat{L}^2 - \hat{L}_z^2\right)$:

$$\begin{aligned}
\langle k,l,m|\hat{L}_x^2|k,l,m\rangle &= \frac{1}{4}\langle k,l,m|\left(\hat{L}_+^2 + \hat{L}_-^2 + \hat{L}_+\hat{L}_- + \hat{L}_-\hat{L}_+\right)|k,l,m\rangle \\
&= \frac{1}{4}\langle k,l,m|2\left(\hat{L}^2 - \hat{L}_z^2\right)|k,l,m\rangle \\
&= \frac{\hbar^2}{2}[l(l+1) - m^2] \\
\langle k,l,m|\hat{L}_y^2|k,l,m\rangle &= -\frac{1}{4}\langle k,l,m|\left(\hat{L}_+^2 + \hat{L}_-^2 - \hat{L}_+\hat{L}_- - \hat{L}_-\hat{L}_+\right)|k,l,m\rangle \\
&= \frac{\hbar^2}{2}[l(l+1) - m^2]
\end{aligned}$$

Thus in the state $|k, l, m\rangle$

$$\left\langle \hat{L}_x \right\rangle = \left\langle \hat{L}_y \right\rangle \quad = \quad 0$$

and

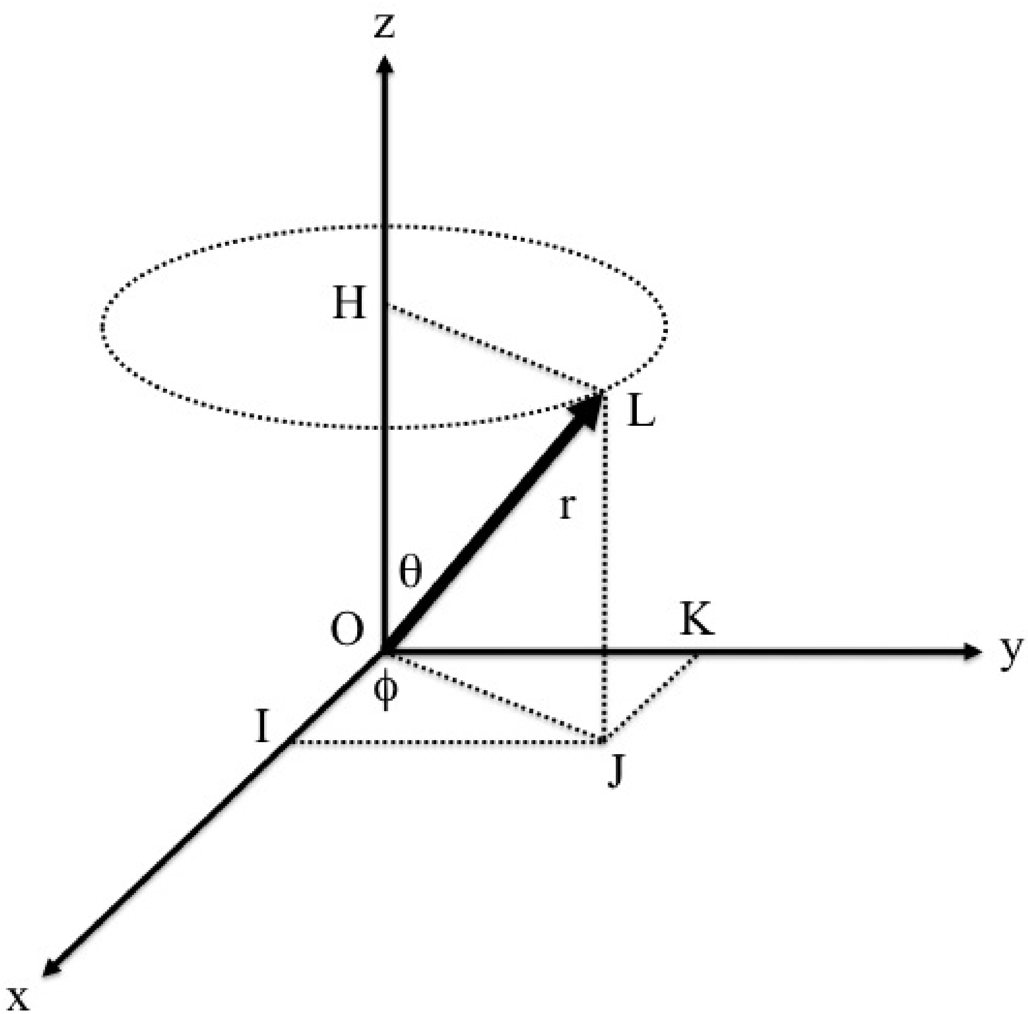
$$\Delta L_x = \Delta L_y \quad = \quad \hbar \sqrt{\frac{1}{2}\left[l(l+1) - m^2\right]}$$

where $\Delta \hat{O}$ is defined as $\Delta \hat{O} = \sqrt{\left\langle \hat{O}^2 \right\rangle - \left\langle \hat{O} \right\rangle^2}$.

Interpretation:

Consider a classical angular momentum of the modulus $\hbar\sqrt{l(l+1)}$ whose projection onto the z axis is $m\hbar$:

$$\begin{aligned} \left|\vec{OL}\right| &= \hbar\sqrt{l(l+1)} \\ \overline{OH} &= m\hbar \end{aligned}$$


z
H
L
r
θ
O
K
y
ϕ
I
J
x

$$
\begin{aligned}
\left|\vec{OL}\right| &= \hbar\sqrt{l(l+1)} \\
\overline{OH} &= m\hbar
\end{aligned}
$$

Since the triangle OLJ has a right angle at J, and $OH = JL$, we get

$$
OJ = \sqrt{OL^2 - OH^2} \;=\; \hbar\sqrt{l(l+1) - m^2}
$$

Consequently, the components of this classical angular momentum would be

$$
\begin{aligned}
\overline{OI} &= \hbar\sqrt{l(l+1) - m^2}\cos\phi \\
\overline{OK} &= \hbar\sqrt{l(l+1) - m^2}\sin\phi \\
\overline{OH} &= \hbar\sqrt{l(l+1)}\cos\theta = m\hbar
\end{aligned}
$$

Let us assume that $|OL|$ and θ are known and that ϕ is a random variable which takes with equal probability values from the interval $[0, 2\pi]$. We then average over ϕ:

$$\begin{aligned}\left\langle\overline{OI}\right\rangle &\propto \int_0^{2\pi} \cos\phi \, \mathrm{d}\phi = 0 \\ \left\langle\overline{OK}\right\rangle &\propto \int_0^{2\pi} \sin\phi \, \mathrm{d}\phi = 0\end{aligned}$$

which corresponds to our quantum results for the state $|k, l, m\rangle$:

$$\left\langle\hat{L}_x\right\rangle = \left\langle\hat{L}_y\right\rangle = 0$$

In addition, the root-mean-square deviations

$$\left\langle \overline{OI}^2 \right\rangle \;=\; \frac{1}{2\pi}\hbar^2 \left[l(l+1) - m^2 \right] \int_0^{2\pi} \cos^2\phi \, \mathrm{d}\phi = \frac{\hbar^2}{2} \left[l(l+1) - m^2 \right]$$

and similarly

$$\left\langle \overline{OK}^2 \right\rangle \;=\; \frac{\hbar^2}{2} \left[l(l+1) - m^2 \right]$$

are in agreement with our quantum results.

However, we must be careful interpreting quantum mechanical results using classical analogy. Recall that the individual measurements of $\hat{L}_x$ and $\hat{L}_y$ on a particle in the state $|k, l, m\rangle$ can not yield any arbitrary value between $\pm\hbar\sqrt{l(l+1) - m^2}$, like classical picture suggests. The only possible results are the eigenvalues of $\hat{L}_x$ and $\hat{L}_y$ (which are the same as those of $\hat{L}_z$).

b. CALCULATION OF THE PHYSICAL PREDICTIONS CONCERNING MEASUREMENTS OF $\hat{L}^2$ AND $\hat{L}_z$

Consider a particle in a state

$$\langle \vec{r} | \psi \rangle = \psi\left(\vec{r}\right) \quad = \quad \psi(r, \theta, \phi)$$

Measurement of $\hat{L}^2$ can yield only the results

$$0, 2\hbar^2, 6\hbar^2, ..., l(l+1)\hbar^2$$

How can we calculate probabilities of these different results from $\psi(r, \theta, \phi)$?

α. *General formulas*

Let $\mathcal{P}_{\hat{L}^2,\hat{L}_z}(l,m)$ be the probability of finding in a simultaneous measurement of $\hat{L}^2$ and $\hat{L}_z$ the results $l(l+1)\hbar^2$ and $m\hbar$.
Expanding the wavefunction $\psi(\vec{r})$ in a standard basis

$$\{\psi_{k,l,m}(\vec{r}) \;=\; R_{k,l}(r)Y_l^m(\theta,\phi)\}$$

we can write $\psi(\vec{r})$ as

$$\psi(\vec{r}) \;=\; \sum_k \sum_l \sum_m c_{k,l,m}R_{k,l}(r)Y_l^m(\theta,\phi)$$

where the coefficients $c_{k,l,m}$ can be calculated using the formula

$$\begin{aligned} c_{k,l,m} &= \int \mathrm{d}^3\vec{r}\,\psi^*_{k,l,m}(\vec{r})\,\psi(\vec{r}) \\ &= \int_0^\infty r^2\,\mathrm{d}r\,R^*_{k,l}(r)\int_0^{2\pi}\mathrm{d}\phi\int_0^\pi \sin\theta\,\mathrm{d}\theta\,Y_l^{m*}(\theta,\phi)\,\psi(r,\theta,\phi) \end{aligned}$$

The probability is then given as

$$\mathcal{P}_{\hat{L}^2,\hat{L}_z}(l,m) \;=\; \sum_k \left|c_{k,l,m}\right|^2$$

If we measure only $\hat{L}^2$, the probability of finding the result $l(l+1)\hbar^2$ is

$$\mathcal{P}_{\hat{L}^2}(l) \;=\; \sum_{m=-l}^{+l} \mathcal{P}_{\hat{L}^2,\hat{L}_z}(l,m) = \sum_k \sum_{m=-l}^{+l} \left|c_{k,l,m}\right|^2$$

Similarly, if we measure only $\hat{L}_z$, the probability of finding the value $m\hbar$ is

$$\mathcal{P}_{\hat{L}_z}(m) \;=\; \sum_{l\geq|m|} \mathcal{P}_{\hat{L}^2,\hat{L}_z}(l,m) = \sum_k \sum_{l\geq|m|} \left|c_{k,l,m}\right|^2$$

Since $\hat{L}^2$ and $\hat{L}_z$ act only on θ and ϕ, r can be treated as a parameter

$$\psi(r,\theta,\phi) = \sum_l \sum_m a_{l,m}(r) Y_l^m(\theta,\phi)$$

where $a_{l,m}(r)$ depends on r only

$$a_{l,m}(r) = \int_0^{2\pi} \mathrm{d}\phi \int_0^{\infty} \sin\theta \, \mathrm{d}\theta \, Y_l^{m*}(\theta,\phi)\psi(r,\theta,\phi)$$

$$a_{l,m} = \sum_k c_{k,l,m} R_{k,l}(r)$$

Comparing with the expression for $c_{k,l,m}$

$$c_{k,l,m} = \int_0^{\infty} r^2 \mathrm{d}r \, R_{k,l}^*(r) a_{l,m}(r)$$

and using the orthogonality condition $\int_0^\infty r^2 \mathrm{d}r\, R^*_{k,l}(r) R_{k',l'}(r) = \delta_{kk'}$ we also obtain

$$\int_0^\infty r^2 \mathrm{d}r \left|a_{l,m}(r)\right|^2 = \sum_k \left|c_{k,l,m}\right|^2$$

and then the desired probabilities

$$\begin{aligned}
\mathcal{P}_{\hat{L}^2,\hat{L}_z}(l,m) &= \int_0^\infty r^2 \mathrm{d}r \left|a_{l,m}(r)\right|^2 \\
\mathcal{P}_{\hat{L}^2}(l) &= \sum_{m=-l}^{+l} \int_0^\infty r^2 \mathrm{d}r \left|a_{l,m}(r)\right|^2 \\
\mathcal{P}_{\hat{L}_z}(m) &= \sum_{l \geq |m|} \int_0^\infty r^2 \mathrm{d}r \left|a_{l,m}(r)\right|^2
\end{aligned}$$

Consequently, to obtain the physical predictions concerning measurements of $\hat{L}^2$ and $\hat{L}_z$, we may consider the wavefunction as depending only on θ and ϕ. We can then expand it in terms of spherical harmonics

$$\psi(r,\theta,\phi) = \sum_l \sum_m a_{l,m}(r) Y_l^m(\theta,\phi) \tag{1.4}$$

and apply the formulas for $\mathcal{P}_{\hat{L}^2,\hat{L}_z}(l,m)$, $\mathcal{P}_{\hat{L}^2}(l)$, $\mathcal{P}_{\hat{L}_z}(m)$.

Similarly, since $\hat{L}_z$ acts only on ϕ, it is ϕ dependence of the wavefunction which is important for $\mathcal{P}_{\hat{L}_z}(m)$:

$$Y_l^m(\theta,\phi) \quad = \quad Z_l^m(\theta)\frac{e^{im\phi}}{\sqrt{2\pi}}$$

where each of the functions on r.h.s. is normalized:

$$\int_0^{2\pi} \mathrm{d}\phi \frac{e^{-im\phi}}{\sqrt{2\pi}}\frac{e^{im'\phi}}{\sqrt{2\pi}} \quad = \quad \delta_{mm'}$$

Substituting this to orthonormalization formula for the spherical harmonics, we get

$$\int_0^{\pi} \sin\theta \, \mathrm{d}\theta \, Z_l^{m*}(\theta) Z_{l'}^{m}(\theta) = \delta_{ll'} \tag{1.5}$$

If we consider the expansion of $\psi(r, \theta, \phi)$ into the Fourier series

$$\psi(r, \theta, \phi) = \sum_m b_m(r, \theta) \frac{e^{im\phi}}{\sqrt{2\pi}}$$

where

$$b_m(r, \theta) = \frac{1}{\sqrt{2\pi}} \int_0^{2\pi} \mathrm{d}\phi \, e^{-im\phi} \psi(r, \theta, \phi)$$

and compare the last two formulas with Eq.(1.4), we obtain

$$b_m(r,\theta) \quad = \quad \sum_l a_{l,m}(r) Z_l^m(\theta)$$

with

$$a_{l,m}(r) \quad = \quad \int_0^\pi \sin\theta \, \mathrm{d}\theta \, Z_l^{m*}(\theta) b_m(r,\theta)$$

and then, taking into account the normalization (1.5), we arrive at

$$\int_0^\pi \sin\theta \, \mathrm{d}\theta \, |b_m(r,\theta)|^2 \quad = \quad \sum_l \left| a_{l,m}(r) \right|^2$$

Substituting this into the formula for $\mathcal{P}_{\hat{L}_z}(m)$ gives

$$\mathcal{P}_{\hat{L}_z}(m) \quad = \quad \int_0^\infty r^2 \mathrm{d}r \int_0^\pi \sin\theta \, \mathrm{d}\theta \, |b_m(r,\theta)|^2$$

β. Special cases and examples

(i) Suppose $\psi(r,\theta,\phi) = f(r)g(\theta,\phi)$. We can always assume that $f(r)$ and $g(\theta,\phi)$ can be normalized separately

$$\begin{aligned}\int_0^\infty r^2 \mathrm{d}r\, |f(r)|^2 &= 1 \\ \int_0^{2\pi} \mathrm{d}\phi \int_0^\pi \sin\theta\, \mathrm{d}\theta\, |g(\theta,\phi)|^2 &= 1\end{aligned}$$

We can expand

$$g(\theta,\phi) = \sum_l \sum_m d_{l,m} Y_l^m(\theta,\phi)$$

with

$$d_{l,m} = \int_0^{2\pi} \mathrm{d}\phi \int_0^\pi \sin\theta\, \mathrm{d}\theta\, Y_l^{m*}(\theta,\phi) g(\theta,\phi)$$

In this case therefore, the coefficients $a_{l,m}(r)$ are proportional to $f(r)$:

$$a_{l,m}(r) \;=\; d_{l,m} f(r)$$

and then

$$\mathcal{P}_{\hat{L}^2,\hat{L}_z}(l,m) \;=\; \left|d_{l,m}\right|^2$$

is independent on the radial part $f(r)$ of the wavefunction.

(ii) Consider $\psi(r,\theta,\phi) = f(r)h(\theta)k(\phi)$ where each factor normalizes separately

$$\int_0^\infty r^2 \mathrm{d}r\,|f(r)|^2 = \int_0^\pi \sin\theta\,\mathrm{d}\theta\,|h(\theta)|^2 = \int_0^{2\pi} \mathrm{d}\phi\,|k(\phi)|^2 \quad = \quad 1$$

If we are interested in $\hat{L}_z$ only

$$k(\phi) \quad = \quad \sum_m e_m \frac{e^{im\phi}}{\sqrt{2\pi}}$$

where

$$e_m \quad = \quad \frac{1}{\sqrt{2\pi}} \int_0^{2\pi} \mathrm{d}\phi\, e^{-im\phi} k(\phi)$$

and then

$$b_m(r,\theta) \quad = \quad e_m f(r) h(\theta)$$

The desired probability is given as

$$\mathcal{P}_{\hat{L}_z}(m) \;=\; \int_0^\infty r^2 \mathrm{d}r \int_0^\pi \sin\theta \, \mathrm{d}\theta \, |b_m(r,\theta)|^2 = |e_m|^2$$

where we have used the fact that $f(r)$ and $h(\theta)$ are normalized functions.

Simple examples:

1) Let us assume $\psi(\vec{r})$ is independent of θ and ϕ, i.e.

$$\begin{cases} h(\theta) = \dfrac{1}{\sqrt{2}} \\ k(\phi) = \dfrac{1}{\sqrt{2\pi}} \end{cases}$$

then

$$g(\theta, \phi) \quad = \quad \frac{1}{\sqrt{4\pi}} = Y_0^0(\theta, \phi)$$

and thus the measurement of $\hat{L}^2$ and $\hat{L}_z$ must yield zero.

2) Consider

$$\begin{cases} h(\theta) = \sqrt{\frac{3}{2}}\cos\theta \\ k(\phi) = \frac{1}{\sqrt{2\pi}} \end{cases}$$

then

$$g(\theta,\phi) \quad = \quad \sqrt{\frac{3}{4\pi}} = Y_1^0(\theta,\phi)$$

and thus the measurement of $\hat{L}^2$ yields $2\hbar^2$ and of $\hat{L}_z$ gives zero.

Consider the case when

$$\begin{cases} h(\theta) = \frac{1}{\sqrt{2}} \\ k(\phi) = \frac{e^{i\phi}}{\sqrt{2\pi}} \end{cases}$$

then $g(\theta, \phi)$ is no longer a single spherical harmonics and

$$\mathcal{P}_{\hat{L}_z}(m = 1) \quad = \quad 1$$

for $m = 1$, and it equals to zero for all other values of m.

For $\hat{L}^2$, we must expand the function

$$g(\theta, \phi) \quad = \quad \frac{1}{\sqrt{4\pi}} e^{i\phi}$$

and all the spherical harmonics $Y_l^m(\theta, \phi)$ with odd l and $m = 1$ will be needed, so we are no longer sure of the result of the measurement of $\hat{L}^2$.

Addendum: Angular momentum and rotations

(Cohen-Tannoudji et al.: QM I, Complement B_{VI})

Consider a quantum mechanical system in a state $|\psi\rangle \in \mathcal{E}$. We perform a rotation $\mathcal{R}$ on this system whose state now changes to $|\psi'\rangle \neq |\psi\rangle$.:

$$|\psi'\rangle = \hat{R}|\psi\rangle$$

We need to distinguish between the geometric rotation $\mathcal{R}$ and its effect $\hat{R}$ in the Hilbert space:

$$\mathcal{R} \rightarrow \hat{R}$$

Consider a wavefunction $\psi(\vec{r}) = \langle\vec{r}|\psi\rangle$ and let us perform a rotation $\mathcal{R}$ on this system:

$$\vec{r}' = \mathcal{R}\vec{r}$$

After the rotation, we can assume that the value of the initial wavefunction at the point $\vec{r}$ will be found after rotation, to be the value of the final wave function $\psi'(\vec{r}')$ at the point $\vec{r}'$

$$\psi'(\vec{r}') = \psi(\vec{r})$$

that is

$$\psi'(\vec{r}') = \psi(\mathcal{R}^{-1}\vec{r}')$$

as this must hold for any point in space which we can rewrite it as

$$\psi'(\vec{r}) = \psi(\mathcal{R}^{-1}\vec{r})$$

We can define the rotation operator

$$|\psi'\rangle = \hat{R}|\psi\rangle$$

which in the coordinate representation becomes

$$\langle\vec{r}|\hat{R}|\psi\rangle = \langle\mathcal{R}^{-1}\vec{r}|\psi\rangle$$

where $|\mathcal{R}^{-1}\vec{r}\rangle$ is the basis ket of this representation determined by the components of the vector $\mathcal{R}^{-1}\vec{r}$.

The rotation operator is linear and unitary and they form a group
(for proofs see Cohen-Tannoudji et al. QM I, B_{VI}).

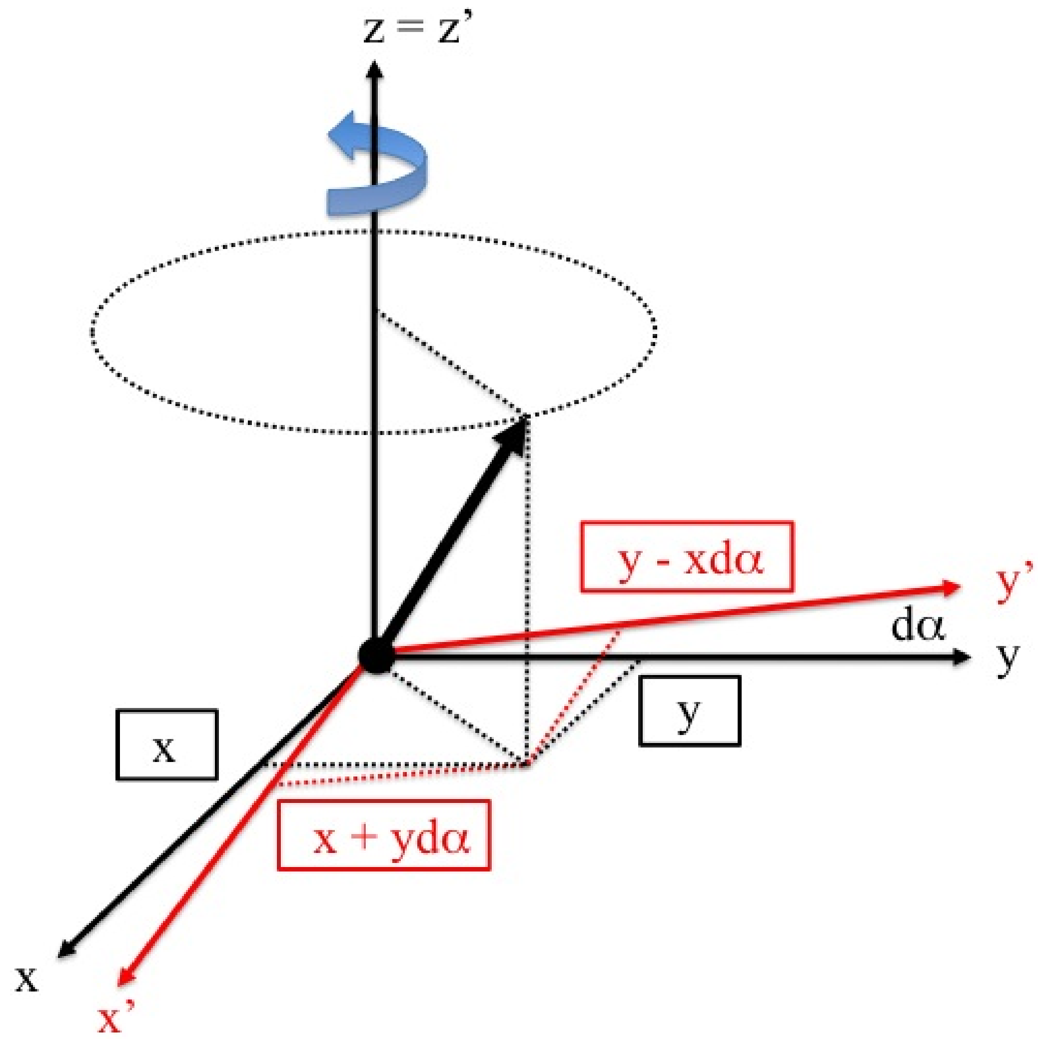
Expressions for rotation operators in terms of angular momentum operators

An infinitesimal rotation $\mathcal{R}_{\vec{e}_z}(\mathrm{d}\alpha)$ around the z axis, defined by the unit vector $\vec{e}_z$, transforms the wavefunction $\psi(\vec{r})$ as follows:

$$\psi'(\vec{r}) = \psi[\mathcal{R}_{\vec{e}_z}^{-1}(\mathrm{d}\alpha)\vec{r}]$$

Since the components of $\vec{r} = (x, y, z)$, we can calculate

$$\begin{aligned} \mathcal{R}_{\vec{e}_z}^{-1}(\mathrm{d}\alpha)\vec{r} &= \mathcal{R}_{-\vec{e}_z}(\mathrm{d}\alpha)\vec{r} = (\vec{r} - \mathrm{d}\alpha\vec{e}_z \times \vec{r}) \\ &= (x + y\,\mathrm{d}\alpha, y - x\,\mathrm{d}\alpha, z) \end{aligned}$$


z = z'
y - xdα
y'
dα
y
y
x
x + ydα
x
x'

The wavefunction $\psi'(x,y,z)$ can now be written as

$$\psi'(x,y,z) = \psi(x + y\,\mathrm{d}\alpha, y - x\,\mathrm{d}\alpha, z)$$

which yields to first order in $\mathrm{d}\alpha$

$$\begin{aligned}
\psi'(x,y,z) &= \psi(x,y,z) + \mathrm{d}\alpha\left[y\frac{\partial\psi}{\partial x} - x\frac{\partial\psi}{\partial y}\right] \\
&= \psi(x,y,z) - \mathrm{d}\alpha\left[x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x}\right]\psi(x,y,z)
\end{aligned}$$

We recognize that the last term in the bracket is proportional to the operator $\hat{L}_z$ in the coordinate representation, so

$$\psi'(\vec{r}) = \langle\vec{r}|\psi'\rangle = \langle\vec{r}|\left(1 - \frac{i}{\hbar}\mathrm{d}\alpha\hat{L}_z\right)|\psi\rangle$$

and the rotation operator is then:

$$\hat{R}_{\vec{e}_z}(\mathrm{d}\alpha) = 1 - \frac{i}{\hbar}\mathrm{d}\alpha\hat{L}_z$$

We can generalize this result to an infinitesimal rotation around an arbitrary axis, defined by a unit vector $\vec{u}$:

$$\hat{R}_{\vec{u}}(\mathrm{d}\alpha) = 1 - \frac{i}{\hbar}\mathrm{d}\alpha\vec{u}.\hat{\vec{L}}$$

Finite rotations

Consider a rotation $\mathcal{R}_{\vec{e}_z}(\alpha)$ by an arbitrary angle α around the z axis. It has to satisfy that

$$\hat{R}_{\vec{e}_z}(\alpha + \mathrm{d}\alpha) = \hat{R}_{\vec{e}_z}(\alpha)\hat{R}_{\vec{e}_z}(\mathrm{d}\alpha) = \hat{R}_{\vec{e}_z}(\alpha)\left(1 - \frac{i}{\hbar}\mathrm{d}\alpha\hat{L}_z\right)$$

We can rewrite the last expression as

$$\hat{R}_{\vec{e}_z}(\alpha + \mathrm{d}\alpha) - \hat{R}_{\vec{e}_z}(\alpha) = -\frac{i}{\hbar}\mathrm{d}\alpha\hat{R}_{\vec{e}_z}(\alpha)\hat{L}_z$$

$$\hat{R}_{\vec{e}_z}(\alpha + \mathrm{d}\alpha) - \hat{R}_{\vec{e}_z}(\alpha) = -\frac{i}{\hbar}\mathrm{d}\alpha \hat{R}_{\vec{e}_z}(\alpha)\hat{L}_z$$

Since $\hat{R}_{\vec{e}_z}(\alpha)$ and $\hat{L}_z$ commute, The solution of this equation is formally

$$\hat{R}_{\vec{e}_z}(\alpha) = e^{-\frac{i}{\hbar}\alpha \hat{L}_z}$$

which generalizes for an arbitrary rotation as

$$\hat{R}_{\vec{u}}(\alpha) = e^{-\frac{i}{\hbar}\alpha \vec{u}.\hat{\vec{L}}}$$