Lecture 22

Eigenfunctions of L^2 and L_z

The eigenfunctions f_ℓ^m of L^2 and L_z are determined from

$$L^2 f_\ell^m = \hbar^2 \ell(\ell+1) f_\ell^m$$

$$L_z f_\ell^m = \hbar m f_\ell^m ,$$

where $\hbar^2 \ell(\ell+1)$ and $m\hbar$ are the corresponding eigenvalues that we found using algebraic method during the last lecture.

First, we need to write these operators in spherical coordinates to establish what equations we are dealing with here.

We start with the definition for the angular momentum:

$$\mathbf{L} = -i\hbar\, \mathbf{r} \times \nabla$$

Using the expressions for **r** and ∇ in spherical coordinates:

$$\mathbf{r} = r\hat{r}$$

$$\nabla = \hat{r}\frac{\partial}{\partial r} + \hat{\theta}\frac{1}{r}\frac{\partial}{\partial \theta} + \hat{\phi}\frac{1}{r\sin\theta}\frac{\partial}{\partial \phi}$$

we can show (see pages 167-169 of the textbook) that

$$L_z = -i\hbar\frac{\partial}{\partial \phi}$$

$$L^2 = -\hbar^2\left[\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right) + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2}\right].$$

Therefore,

$$L^2 f_\ell^m = -\hbar^2\left[\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right)+\frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2}\right]f_\ell^m = \hbar^2\ell(\ell+1)f_\ell^m$$

But, this is exactly the angular equation for $Y_\ell^m(\theta,\phi)$ that we got when we have done the separation of variables:

Angular equation:

$$\frac{1}{Y}\left\{\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial Y}{\partial\theta}\right)+\frac{1}{\sin^2\theta}\frac{\partial^2 Y}{\partial\phi^2}\right\} = -\ell(\ell+1)$$

You can now see the reason for calling the separation constant $\ell(\ell+1)$!

The second equation is

$$L_z f_\ell^m = -i\hbar\frac{\partial}{\partial\phi}f_\ell^m = m\hbar f_\ell^m.$$

This is equivalent to the equation for Φ that we got when we separated variables θ and ϕ :

$$\boxed{\frac{1}{\Phi}\frac{d^2\Phi}{d\phi^2} = -m^2}$$

Again, this is why we called the separation constant m^2.

Therefore, we already solved this system of equations and know the answer; the **eigenfunctions that we are looking for are spherical harmonics** $Y_\ell^m(\theta,\phi)$.

In fact, when we separated the variables, we constructed the eigenfunctions of H, L^2, and L_z:

$$H\psi = E\psi,\quad L^2\psi = \hbar^2\ell(\ell+1),\quad L_z\psi = \hbar m\psi.$$

Spin

We note now that our algebraic solution allows both integer and half-integer values of ℓ and m, but separation of variable gave only integer values of ℓ and m. What about the half-integer solutions?

To understand the significance of half-integer solutions, we return back in time to 1922, when O. Stern and W. Gerlach conducted experiment to measure the magnetic dipole moments of atoms. The results of these experiments could not be explained by classical mechanics. First, let's discuss why would atom poses a **magnetic moment**.

Even in Bohr's model of the hydrogen atom, an electron, which is a charged particle, occupies a circular orbit, rotating with orbital angular momentum **L**. A moving charge is equivalent to electric current, so an electron moving in a closed orbit forms a current loop and this, therefore, creates a magnetic dipole. The corresponding magnetic dipole moment is given by:

$$\vec{\mu} = -\frac{e}{2m}\vec{L}.$$

If the atom with a magnetic moment $\vec{\mu}$ is placed in a magnetic field **B**, it will experience a net force **F**,

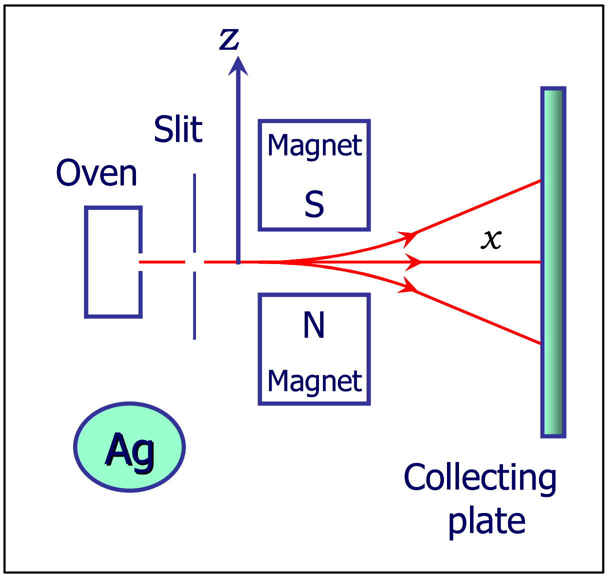
$$F_x = \vec{\mu}\cdot\frac{\partial \vec{B}}{\partial x} \qquad F_y = \vec{\mu}\cdot\frac{\partial \vec{B}}{\partial y} \qquad F_z = \vec{\mu}\cdot\frac{\partial \vec{B}}{\partial z}.$$

Stern suggested to measure the magnetic moments of atoms by deflecting atomic beam by inhomogeneous magnetic field. In the experimental setup, the only force on the atoms is in z direction and

$$F_z = \mu_z \frac{\partial B_z}{\partial z}.$$

The direction of magnetic moment in the beam is random, so every value of μ_z in the range $-\mu \le \mu_z \le \mu$ is expected. As a result, the deposit on the collecting plate is expected to be spread continuously over a symmetrical region about the point of no displacement.

The Stern-Gerlach experiment



Expected: uniform distribution deflections as the direction of the atomic magnetic moment is at random and every value of μ_z the can occur in z direction.

Found: two distinct traces
(beam was split to two components)
So multiplicity $\alpha=2l+1=2$ $l=1/2$?
Ag, Au, Cu, Na, K, Cs, H

<u>Electronic configurations of atoms in Stern-Gerlach experiments:</u>

H $1s$
Na $\{1s^2 2s^2 2p^6\} 3s^1$
K $\{1s^2 2s^2 2p^6 3s^2 3p^6\} 4s^1$
Cu $\{1s^2 2s^2 2p^6 3s^2 3p^6 3d^{10}\} 4s^1$
Ag $\{1s^2 2s^2 2p^6 3s^2 3p^6 3d^{10} 4s^2 4p^6 4d^{10}\} 5s^1$
Cs $\{[Ag] 5s^2 5p^6\} 6s^1$
Au $\{[Cs] 5d^{10} 4f^{14}] 6s^1$

$\ell = 0$ ← orbital angular momentum

$\boxed{\text{spin (intrinsic angular momentum)} = 1/2}$

s means $\ell=0$ | d means $\ell=2$
p means $\ell-1$ | f means $\ell=3$

Conclusion: elementary particles carry intrinsic angular momentum **S** in addition to **L**. Spin of elementary particles has nothing to do with rotation, does not depend on coordinates θ and ϕ , and is purely a quantum mechanical phenomena.

Fundamental commutation relations:

$$\boxed{\begin{aligned}[S_x, S_y] &= i\hbar S_z\\ [S_y, S_z] &= i\hbar S_x\\ [S_z, S_x] &= i\hbar S_y\end{aligned}}$$

Therefore, all our results from algebraic derivations apply, and we can write:

$$S^2 |s\, m\rangle = \hbar^2 s(s+1) |s\, m\rangle$$

$$S_z |s\, m\rangle = \hbar m |s\, m\rangle. \qquad m \equiv m_s$$

$|s\, m\rangle$ are the eigenfunctions.

Both integer and half-integer values of s and m are possible.
All elementary particles have specific value of s, it is always the same for the same type of particle. For example, photons have spin 1 and electrons have spin $1/2$.

Also,

$$S_\pm |s\, m\rangle = \hbar \sqrt{s(s+1) - m(m \pm 1)}\; |s\, (m \pm 1)\rangle$$

where

$$S_\pm = S_x \pm i S_y.$$

Spin $1/2$

$s=\frac{1}{2}$, therefore $m=\pm\frac{1}{2}$ and there are two eigenstates $|s\,m\rangle=|\frac{1}{2}\,\frac{1}{2}\rangle$, $|s\,m\rangle=|\frac{1}{2}\,(-\frac{1}{2})\rangle$.

We will call them spin up $\uparrow$ $|\frac{1}{2}\,\underbrace{\tfrac{1}{2}}_{m=\frac{1}{2}}\rangle$ and spin down $\downarrow$ $|\frac{1}{2}\,\underbrace{-\tfrac{1}{2}}_{m=-\frac{1}{2}}\rangle$.

↑ I will omit ( ).

Taking these eigenstates to be basis vectors, we can express any spin state of a particle with spin $1/2$ as:

$$\chi=\begin{pmatrix}a\\b\end{pmatrix}=a\chi_+ + b\chi_-$$

represents spin up ↑

$$\chi_+=\begin{pmatrix}1\\0\end{pmatrix}$$

represents spin down ↓

$$\chi_-=\begin{pmatrix}0\\1\end{pmatrix}$$

All our spin operators are 2x2 matrixes for spin $1/2$, which we can find out from how they act on our basis set states χ_+ and χ_-.

Example: find matrix representation of S^2.

Solution:

$$S^2\chi_+ = s(s+1)\hbar^2\chi_+ = \frac{3}{4}\hbar^2\chi_+$$

$$S^2\chi_- = s(s+1)\hbar\,\chi_- = \frac{3}{4}\hbar^2\chi_-$$

We write matrix S^2 as $S^2=\begin{pmatrix}c&d\\e&f\end{pmatrix}$ with 4 unknowns $c, d, e,$ and f.

$$S^2\chi_+ = \frac{3}{4}\hbar^2\chi_+$$

$$\begin{pmatrix}c&d\\e&f\end{pmatrix}\begin{pmatrix}1\\0\end{pmatrix}=\frac{3}{4}\hbar^2\begin{pmatrix}1\\0\end{pmatrix} \Rightarrow \begin{pmatrix}c\\e\end{pmatrix}=\begin{pmatrix}3/4\,\hbar^2\\0\end{pmatrix}$$

$$e = 0$$
$$c = \frac{3}{4}\hbar^2.$$

Now, we take the second equation for χ_-.

$$S^2 \chi_- = \frac{3}{4}\hbar^2 \chi_-$$
$$\downarrow \quad \downarrow \qquad\qquad \downarrow$$
$$\begin{pmatrix} c & d \\ e & f \end{pmatrix}\begin{pmatrix} 0 \\ 1 \end{pmatrix} = \frac{3}{4}\hbar^2 \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

$$\begin{pmatrix} d \\ f \end{pmatrix} = \begin{pmatrix} 0 \\ 3/4\,\hbar^2 \end{pmatrix} \Rightarrow \quad d = 0, \quad c = \frac{3}{4}\hbar^2.$$

Putting it all together, we get our matrix S^2:

$$\left.\begin{aligned} c &= \frac{3}{4}\hbar^2 \\ d &= 0 \\ e &= 0 \\ f &= \frac{3}{4}\hbar^2 \end{aligned}\right\} \quad S^2 = \begin{pmatrix} c & d \\ e & f \end{pmatrix} = \begin{pmatrix} 3/4\,\hbar^2 & 0 \\ 0 & \frac{3}{4}\hbar^2 \end{pmatrix}$$

$$\boxed{S^2 = \frac{3}{4}\hbar^2 \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}}$$

Class exercise 8

Find matrix representations for S_z, S_x, and S_y for spin $1/2$.

Hint: to find S_z use $S_z |s\,m\rangle = m\hbar |s\,m\rangle$, i.e.

$$\boxed{S_z \chi_+ = \frac{\hbar}{2}\chi_-, \quad S_z \chi_- = -\frac{\hbar}{2}\chi_-.}$$

To find S_x and S_y, first use

$$\boxed{S_\pm |s\,m\rangle = \hbar\sqrt{s(s+1)-m(m\pm 1)}\,|s\,(m\pm 1)\rangle}$$

to find S_+ and S_-. Next, use definitions $S_\pm = S_x \pm i S_y$ and to find S_x and S_y.

Solution

① S_z

$$S_z \chi_+ = \frac{\hbar}{2}\chi_+ \qquad\qquad S_z \chi_- = -\frac{\hbar}{2}\chi_-$$

$$\begin{pmatrix} c & d \\ e & f \end{pmatrix}\begin{pmatrix} 1 \\ 0 \end{pmatrix} = \frac{\hbar}{2}\begin{pmatrix} 1 \\ 0 \end{pmatrix} \qquad\qquad \begin{pmatrix} c & d \\ e & f \end{pmatrix}\begin{pmatrix} 0 \\ 1 \end{pmatrix} = -\frac{\hbar}{2}\begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

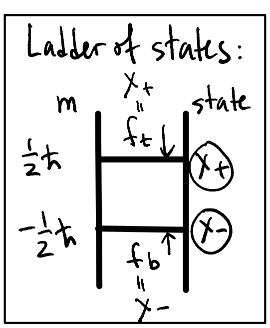
$$\begin{pmatrix} c \\ e \end{pmatrix} = \begin{pmatrix} \hbar/2 \\ 0 \end{pmatrix} \qquad\qquad \begin{pmatrix} d \\ f \end{pmatrix} = \begin{pmatrix} 0 \\ -\hbar/2 \end{pmatrix}$$

$$c = \hbar/2 \qquad\qquad d = 0$$
$$e = 0 \qquad\qquad f = -\hbar/2$$

$$\boxed{S_z = \begin{pmatrix} \hbar/2 & 0 \\ 0 & -\hbar/2 \end{pmatrix} = \frac{\hbar}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}}$$

② $S_\pm$

$$S_\pm |s\,m\rangle = \hbar\sqrt{s(s+1)-m(m\pm 1)}\,|s\,(m\pm 1)\rangle \quad (1)$$



$$\left.\begin{aligned} S_+ \chi_+ &= 0 \\ S_- \chi_- &= 0 \end{aligned}\right\}$$

Note that these also come from definitions of $S_\pm$ operators, since $\chi_+ = f_t$ "top rung of ladder"
$\chi_- = f_b$ "bottom rung of ladder"

Plugging s, m into formula (1) will give zero too, of course.

$$S_\pm |s\, m\rangle = \hbar \sqrt{s(s+1) - m(m\pm 1)}\, |s\,(m\pm 1)\rangle$$

$$S_+ \chi_- = \hbar \sqrt{\tfrac{1}{2}\cdot\tfrac{3}{2} - \left(-\tfrac{1}{2}\right)\left(-\tfrac{1}{2}+1\right)}\ \chi_+ = \hbar \chi_+$$

$$\begin{bmatrix} s = 1/2 \\ m = -1/2 \end{bmatrix}$$

$$S_- \chi_+ = \hbar \sqrt{\tfrac{3}{4} - \tfrac{1}{2}\left(\tfrac{1}{2} - 1\right)}\ \chi_- = \hbar \chi_-$$

Summary:

$$S_+ \chi_+ = 0 \qquad\qquad S_- \chi_- = 0$$

$$S_+ \chi_- = \hbar \chi_+ \qquad\qquad S_- \chi_+ = \hbar \chi_-$$

$$\begin{pmatrix} c & d \\ e & f \end{pmatrix}\begin{pmatrix} 1 \\ 0 \end{pmatrix} = 0 \Rightarrow \begin{matrix} c = 0 \\ e = 0 \end{matrix} \qquad\qquad \begin{pmatrix} c & d \\ e & f \end{pmatrix}\begin{pmatrix} 0 \\ 1 \end{pmatrix} = 0 \Rightarrow \begin{matrix} d = 0 \\ f = 0 \end{matrix}$$

$$\begin{pmatrix} c & d \\ e & f \end{pmatrix}\begin{pmatrix} 0 \\ 1 \end{pmatrix} = \hbar \begin{pmatrix} 1 \\ 0 \end{pmatrix} \qquad\qquad \begin{pmatrix} c & d \\ e & f \end{pmatrix}\begin{pmatrix} 1 \\ 0 \end{pmatrix} = \hbar \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

$$\begin{pmatrix} d \\ f \end{pmatrix} = \begin{pmatrix} \hbar \\ 0 \end{pmatrix} \Rightarrow \begin{matrix} d = \hbar \\ f = 0 \end{matrix} \qquad\qquad \begin{pmatrix} c \\ e \end{pmatrix} = \begin{pmatrix} 0 \\ \hbar \end{pmatrix} \Rightarrow \begin{matrix} c = 0 \\ e = \hbar \end{matrix}$$

$$\boxed{S_+ = \hbar \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}} \qquad\qquad \boxed{S_- = \hbar \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}}$$

$$\left.\begin{matrix} S_+ = S_x + i S_y \\ S_- = S_x - i S_y \end{matrix}\right\} \qquad \begin{matrix} S_x = \frac{1}{2}(S_+ + S_-) \\ S_y = \frac{1}{2i}(S_+ - S_-) \end{matrix}$$

$$\boxed{S_x = \frac{\hbar}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}} \qquad \boxed{S_y = \frac{\hbar}{2i}\begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} = \frac{\hbar}{2}\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}}$$