Lecture 2

Electron Spin

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Electron Spin

As we noted last semester, the degeneracy of the energy eigenstates of the hydrogen atom and their splitting in the presence of an external magnetic field cannot be explained by only the spatial wave function of the electron. More information is needed to completely describe the state of the electron.

In addition, to a spatial part, the electron state has a part that transforms under rotations like a $j = 1/2$ state.

$$|\psi\rangle_{\text{space}} \otimes |\psi\rangle_{\text{spin}}$$

$|\psi\rangle_{\text{space}}$ is the spatial part that we are already familiar with. It is an element of an infinite dimensional vector space that when contracted with the spatial coordinates gives the wave function.

$$\psi(r, \theta, \phi) = \langle r, \theta, \phi | \psi \rangle_{\text{space}}$$

On the other hand, $|\psi\rangle_{\text{spin}}$ is something new. It is an element of a two dimensional vector space and is represented by a $1 \times 2$ complex matrix called a spinor.

$$\begin{pmatrix} a \\ b \end{pmatrix}_{\text{spin}}$$

where $|a|^2 + |b|^2 = 1$
Product Vector Space

The state of an electron is then an element of a product vector space (a space that is the product of two vector spaces.)

In this case, one part $|\psi\rangle_{\text{space}}$ is an element of an infinite dimensional vector space while $|\psi\rangle_{\text{spin}}$ is an element of a two dimensional vector space.

These two spaces are independent in the sense that any operator will operate on the elements of either one of the spaces or the other.

For example, the orbital angular momentum operator $\hat{\vec{L}}$ is the generator of rotations of the spatial part but does nothing (is the identity operator) when acting on the spin part.

$$\hat{\vec{L}} = \hat{\vec{L}}_{\text{space}} \otimes I_{\text{spin}}$$

Similarly, the operator $\hat{\vec{S}}$ is the generator of rotations of the spin part but does nothing (is the identity operator) when acting on the spatial part.

$$\hat{\vec{S}} = I_{\text{space}} \otimes \hat{\vec{S}}_{\text{spin}}$$
Spin Angular Momentum

The generator of rotations of an electron consists of two parts. One that rotates $|\psi\rangle_{\text{space}}$ and one that rotates $|\psi\rangle_{\text{spin}}$.

$$\hat{J} = \hat{L} + \hat{S}$$

Just as $\hat{L}$ is the orbital angular momentum operator and $\langle \psi | \hat{L}_i | \psi \rangle$ is the expectation value of measuring orbital angular $L_i$, $\hat{S}$ is the spin angular momentum operator and $\langle \psi | \hat{S}_i | \psi \rangle$ is the expectation value of measuring spin angular momentum $S_i$.

Spin is an intrinsic angular momentum carried by the electron (and all spin-1/2 objects). It has nothing to do with motion in space. Even if an electron is at rest it will have spin angular momentum.

If $[\hat{H}, \hat{L}] = [\hat{H}, \hat{S}] = 0$, then orbital and spin angular momentum are individually conserved. However, in general, the hydrogen atom is an example, $[\hat{H}, \hat{L}] \neq 0$ and $[\hat{H}, \hat{S}] \neq 0$ but $[\hat{H}, \hat{J}] = 0$. In that case the orbital and spin angular momenta are not individually conserved but rather $\hat{J}$ the total angular momentum is conserved.
Fundamental Spin 1/2 Particles

With the exception of the gauge particles:

\[ \text{photon, gluons, } W \text{ and } Z \]

and the still hypothetical Higgs particle, all of the fundamental particle have spin-1/2. These include the:

\[ \text{electron, muon, tau, neutrinos and quarks} \]

We will see later, that the existence of fundamental spin-1/2 particles is a basic consequence of relativistic quantum mechanics. One of the fundamental equations of relativistic quantum mechanics, the Dirac equation, is the equation of motion for spin-1/2 particles.

We’ll also find that the Dirac equation tells us that even for a free (non-interacting) electron, the orbital and spin angular momentum are not individually conserved but only the total angular momentum \( \vec{J} = \vec{L} + \vec{S} \).
Despite the fact the spatial part of a state is a superposition of only integral values of $j$, the $j = 1/2$ states have an important role to play in physics. They will be needed to describe the spin part of the electron wave function. We will describe that shortly, but first let’s see some general properties of $j = 1/2$ states.

An interesting feature is that the two-component $j = 1/2$ states $|1/2, m\rangle$ change sign under rotation by 360 degrees. In order to get the same phase back again, we must rotate by 720 degrees!

Note that in terms of observation this doesn’t matter since all that we can observe is the norm squared of the state, $\langle jm|jm\rangle$, which doesn’t change sign.

Let’s see why a two-component state must change sign under a 360 degree rotation.
Rotation of $j = 1/2$ State by 180°

For $j = 1/2$, in the $|jm\rangle$ basis the representations of the generators of rotations are:

\[
J_x = \frac{\hbar}{2} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \quad J_y = \frac{\hbar}{2} \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \quad J_z = \frac{\hbar}{2} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}
\]

Under rotation by $\phi$ about the $z$-axis the state $\begin{pmatrix} a \\ b \end{pmatrix}$ transforms as:

\[
\begin{pmatrix} a \\ b \end{pmatrix} \rightarrow \begin{pmatrix} e^{-i\phi/2} & 0 \\ 0 & e^{i\phi/2} \end{pmatrix} \begin{pmatrix} a \\ b \end{pmatrix}
\]

If $\phi = 2\pi$:
\[
\begin{pmatrix} a \\ b \end{pmatrix} \rightarrow -\begin{pmatrix} a \\ b \end{pmatrix} \propto \begin{pmatrix} a \\ b \end{pmatrix} \quad \text{same state, different phase}
\]

If $\phi = \pi$:
\[
\begin{pmatrix} a \\ b \end{pmatrix} \rightarrow i \begin{pmatrix} -a \\ b \end{pmatrix} \propto \begin{pmatrix} -a \\ b \end{pmatrix} \quad \text{different state}
\]

Let’s see if there is a contradiction if a two-component system transforms like:

\[
\begin{pmatrix} a \\ b \end{pmatrix} \rightarrow \begin{pmatrix} e^{-i\phi} & 0 \\ 0 & e^{i\phi} \end{pmatrix} \begin{pmatrix} a \\ b \end{pmatrix}
\]
Rotation of $\hat{J}_x$ Eigenstate

In the $|jm\rangle$ basis, the eigenstates of $\hat{J}_x$ with eigenvalues $+\hbar/2$ and $-\hbar/2$ are:

$|+\rangle_x = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \end{pmatrix}$  

$|−\rangle_x = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -1 \end{pmatrix}$

If \( \begin{pmatrix} a \\ b \end{pmatrix} \rightarrow \begin{pmatrix} e^{-i\phi} & 0 \\ 0 & e^{i\phi} \end{pmatrix} \begin{pmatrix} a \\ b \end{pmatrix} \) under a rotation by $\pi$:

$|+\rangle_x \rightarrow -|+\rangle_x$

which is still an eigenstate of $\hat{J}_x$ with eigenvalue $+\hbar/2$.

But, under a $180^\circ$ rotation about $z$, the eigenvalue of $\hat{J}_x$ must change sign.

$\langle \psi | \hat{J}_x | \psi \rangle \rightarrow -\langle \psi | \hat{J}_x | \psi \rangle$

$\Rightarrow \quad |\uparrow\rangle_x \rightarrow c |\downarrow\rangle_x$

Therefore, $j$ must be $1/2$. \( \begin{pmatrix} 1 \\ 1 \end{pmatrix} \rightarrow -i \begin{pmatrix} 1 \\ -1 \end{pmatrix} \)
In summary, under a $180^\circ$ rotation, we must get a different state. In the case of a two-component system, this requires that the relative sign of the components changes under the rotation. This in turn requires that the rotation matrix be

$$
\begin{pmatrix}
e^{-i\pi/2} & 0 \\
0 & e^{i\pi/2}
\end{pmatrix}
= -i
\begin{pmatrix}
1 & 0 \\
0 & -1
\end{pmatrix}
$$

while under a $360^\circ$ rotation

$$
\begin{pmatrix}
e^{-i\pi} & 0 \\
0 & e^{i\pi}
\end{pmatrix}
= -
\begin{pmatrix}
1 & 0 \\
0 & 1
\end{pmatrix}
$$

Under a $180^\circ$ rotation about $z$:

$$
|+\rangle_x \rightarrow -i |−\rangle_x \quad |−\rangle_x \rightarrow -i |+\rangle_x
$$

while under $360^\circ$ rotation about $z$:

$$
|+\rangle_x \rightarrow -|+\rangle_x \quad |−\rangle_x \rightarrow -|−\rangle_x
$$

For $j = 1$ also, the eigenstate of $\hat{J}_x$ with eigenvalue $+\hbar$ must transform into a different state, i.e., the eigenstate with eigenvalue $-\hbar$ under rotation by $180^\circ$ about $z$. So, why can we have an integral $j$ for a three-component system?
\( j = 1 \) States

In the case of a \( j = 1 \) three-component system, we have under a 180° rotation about \( z \):

\[
\begin{pmatrix} a \\ b \\ c \end{pmatrix} \rightarrow \begin{pmatrix} e^{-i\pi} & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & e^{i\pi} \end{pmatrix} \begin{pmatrix} a \\ b \\ c \end{pmatrix} = \begin{pmatrix} -a \\ b \\ -c \end{pmatrix}
\]

and we get a different state (with a change in the relative sign of the middle component with respect to the other two) even though \( j \) is an integer.

Here we have:

\[
|+\rangle_x = \frac{1}{2} \begin{pmatrix} 1 \\ \sqrt{2} \\ 1 \end{pmatrix} \quad |0\rangle_x = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 0 \\ 1 \end{pmatrix} \quad |\rangle_x = \frac{1}{2} \begin{pmatrix} 1 \\ -\sqrt{2} \\ 1 \end{pmatrix}
\]

Under a 180° rotation about \( z \):

\[
|+\rangle_x \rightarrow -|\rangle_x \quad |0\rangle_x \rightarrow -|0\rangle_x \quad |\rangle_x \rightarrow -|+\rangle_x
\]

while under a 360° rotation about \( z \):

\[
|+\rangle_x \rightarrow |+\rangle_x \quad |0\rangle_x \rightarrow |0\rangle_x \quad |\rangle_x \rightarrow |\rangle_x
\]
Pauli Spin Matrices

In the case of $j = 1/2$, it is useful to remove the factor of $\hbar/2$ from the generator matrices. This gives the Pauli spin matrices.

$$
\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \quad \sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \quad \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}
$$

These matrices obey several important identities.

1) $[J_i, J_j] = i\hbar \epsilon_{ijk} J_k \Rightarrow [\sigma_i, \sigma_j] = 2i\epsilon_{ijk} \sigma_k$

2) $\sigma_i \sigma_j = -\sigma_j \sigma_i$ for $i \neq j$

3) $(\hat{n} \cdot \vec{\sigma})^2 = I$

4) $\sigma_i \sigma_j = \delta_{ij} I + i \epsilon_{ijk} \sigma_k$

5) $\{\sigma_i, \sigma_j\} = 2\delta_{ij} I$

6) $\left( \vec{A} \cdot \vec{\sigma} \right) \left( \vec{B} \cdot \vec{\sigma} \right) = \left( \vec{A} \cdot \vec{B} \right) I + i \left( \vec{A} \times \vec{B} \right) \cdot \vec{\sigma}$
The three Pauli matrices with the identity matrix form a complete set

\[ \sigma_0 = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \quad \sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \quad \sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \quad \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \]

Any $2 \times 2$ complex matrix can be written as a linear superposition of these matrices

\[ M = \sum_{\alpha=0}^{3} c_{\alpha} \sigma_{\alpha} \]

where since \( \text{Tr}(\sigma_i \sigma_j) = 2 \delta_{ij} I \)

\[ c_{\beta} = \frac{\text{Tr}(M \sigma_{\beta})}{2} \]
Finite Rotation Matrices for $j = 1/2$

Since the basis states $|jm\rangle$ are eigenstates of $\hat{J}_z$, it is straightforward to find the matrix representation of finite rotations about the $z$ axis.

$$\hat{U}[R(\phi\hat{k})] = e^{-i\phi\hat{J}_z/\hbar} = \begin{pmatrix} e^{-i\phi/2} & 0 \\ 0 & e^{i\phi/2} \end{pmatrix}$$

What about for a finite rotation about $x$, $y$ or an arbitrary direction $\hat{n}$?

$$\hat{U}[R(\theta\hat{n})] = e^{-i\theta\hat{n}\cdot\vec{J}/\hbar} = e^{-i\theta\hat{n}\cdot\vec{\sigma}/2}$$

$$= \sum_{n=0}^{\infty} \frac{(-i\theta\hat{n}\cdot\vec{\sigma}/2)^n}{n!} = \sum_{n=0}^{\infty} \left( \frac{-i\theta}{2} \right)^n \frac{1}{n!} (\hat{n} \cdot \vec{\sigma})^n$$

$$(\hat{n} \cdot \vec{\sigma})^{2n} = I \quad (\hat{n} \cdot \vec{\sigma})^{2n+1} = \hat{n} \cdot \vec{\sigma}$$

$$\Rightarrow \quad \hat{U}[R(\theta\hat{n})] = \sum_{n=0}^{\infty} \left[ \frac{(i\theta/2)^{2n}}{(2n)!} I - \frac{(i\theta/2)^{2n+1}}{(2n+1)!} (\hat{n} \cdot \vec{\sigma}) \right]$$

$$= \cos(\theta/2)I - i (\hat{n} \cdot \vec{\sigma}) \sin(\theta/2)$$
General Rotation of a Two-Component Spinor

Let’s rotate the state $|+\rangle_z$ into the state $|+\rangle_{\hat{n}}$

where $\hat{n} = (\sin \theta \cos \phi, \sin \theta \sin \phi, \cos \theta)$

To do this we rotate by the angle $\theta$ about the axis in the direction $\hat{\theta}$ which is the unit vector perpendicular to $\hat{k}$ and $\hat{n}$.

$$\hat{\theta} = \frac{\hat{k} \times \hat{n}}{|\hat{k} \times \hat{n}|} = \left( \frac{1}{\sin \theta} \right) (-\sin \theta \sin \phi, \sin \theta \cos \phi, 0)$$

$$= (-\sin \phi, \cos \phi, 0)$$

The rotation matrix is then

$$e^{-i\theta \vec{\sigma} \cdot \hat{\theta}/2} = \cos(\theta/2)I - i(\vec{\sigma} \cdot \hat{\theta}) \sin(\theta/2)$$

$$= \begin{pmatrix} \cos(\theta/2) & -(\cos \phi + i \sin \phi) \sin(\theta/2) \\ (\cos \phi - i \sin \phi) \sin(\theta/2) & \cos(\theta/2) \end{pmatrix}$$

$$= \begin{pmatrix} \cos(\theta/2) & -\sin(\theta/2)e^{i\phi} \\ \sin(\theta/2)e^{-i\phi} & \cos(\theta/2) \end{pmatrix}$$
Eigenstate of $\vec{J} \cdot \hat{n}$

Let’s put this in a more symmetric form by rotating by $-\phi$ about $z$ first

$$\begin{pmatrix}
\cos(\theta/2) & -\sin(\theta/2)e^{i\phi} \\
\sin(\theta/2)e^{-i\phi} & \cos(\theta/2)
\end{pmatrix}
\begin{pmatrix}
e^{i\phi/2} & 0 \\
0 & e^{-i\phi/2}
\end{pmatrix}
\begin{pmatrix}
\cos(\theta/2)e^{i\phi/2} & -\sin(\theta/2)e^{i\phi/2} \\
\sin(\theta/2)e^{-i\phi/2} & \cos(\theta/2)e^{-i\phi/2}
\end{pmatrix}
$$

If we now rotate the state $|+\rangle_z = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$ we get:

$$|+\rangle_{\hat{n}} = \begin{pmatrix}
\cos(\theta/2)e^{i\phi/2} & -\sin(\theta/2)e^{i\phi/2} \\
\sin(\theta/2)e^{-i\phi/2} & \cos(\theta/2)e^{-i\phi/2}
\end{pmatrix}
\begin{pmatrix} 1 \\ 0 \end{pmatrix}
$$

Let’s check that this is an eigenstate of $\vec{J} \cdot \hat{n}$ with eigenvalue $+\hbar/2$. 
Eigenstate of $\vec{J} \cdot \hat{n}$

$$\vec{J} \cdot \hat{n} = \frac{\hbar}{2} \begin{pmatrix} n_z & n_x - in_y \\ n_x + in_y & -n_z \end{pmatrix}$$

$$= \frac{\hbar}{2} \begin{pmatrix} \cos \theta & \sin \theta e^{-i\phi} \\ \sin \theta e^{i\phi} & -\cos \theta \end{pmatrix}$$

For the state: $$\begin{pmatrix} \cos(\theta/2)e^{i\phi/2} \\ \sin(\theta/2)e^{-i\phi/2} \end{pmatrix}$$

$$\langle \vec{J} \cdot \hat{n} \rangle =$$

$$\frac{\hbar}{2} \left( \cos \frac{\theta}{2} e^{-i\phi/2}, \sin \frac{\theta}{2} e^{i\phi/2} \right) \begin{pmatrix} \cos \theta & \sin \theta e^{-i\phi} \\ \sin \theta e^{i\phi} & -\cos \theta \end{pmatrix} \begin{pmatrix} \cos \frac{\theta}{2} e^{i\phi/2} \\ \sin \frac{\theta}{2} e^{-i\phi/2} \end{pmatrix} =$$

$$\frac{\hbar}{2} \left[ \cos \frac{\theta}{2} \left( \cos \theta \cos \frac{\theta}{2} + \sin \theta \sin \frac{\theta}{2} \right) + \sin \frac{\theta}{2} \left( \sin \theta \cos \frac{\theta}{2} - \cos \theta \sin \frac{\theta}{2} \right) \right]$$

$$= \frac{\hbar}{2} \left[ \cos \theta \left( \cos^2 \frac{\theta}{2} - \sin^2 \frac{\theta}{2} \right) + 2 \sin \theta \cos \frac{\theta}{2} \sin \frac{\theta}{2} \right]$$

$$= \frac{\hbar}{2} \left( \cos^2 \theta + \sin^2 \theta \right) = 1$$
A Check on Consistency

Under a $-\pi/2$ rotation about the $x$-axis, the expectation valuer of $\hat{S}_y$ for the rotated system should equal the expectation value of $\hat{S}_z$ for the non-rotated system.

$$\langle \psi' | \hat{S}_y | \psi' \rangle = \langle \psi | \hat{S}_z | \psi \rangle$$

Let’s check it.

$$\langle \psi | \hat{S}_z | \psi \rangle = \langle \psi | e^{-i\pi \sigma_x/4} e^{i\pi \sigma_x/4} \hat{S}_z e^{-i\pi \sigma_x/4} e^{i\pi \sigma_x/4} | \psi \rangle$$

$$= \langle \psi' | e^{i\pi \sigma_x/4} \hat{S}_z e^{-i\pi \sigma_x/4} | \psi' \rangle$$

Now, does

$$e^{i\pi \sigma_x/4} \hat{S}_z e^{-i\pi \sigma_x/4} = \hat{S}_y$$
Generalization of the Anticommutation Relations

\[
\sigma_i \sigma_j = -\sigma_j \sigma_i \quad \text{for} \quad i \neq j
\]

\[
\Rightarrow \quad \sigma_i \sigma_j^n = (-1)^n \sigma_j^n \sigma_i = (-\sigma_j)^n \sigma_i
\]

Then for any analytic function of \( \sigma_j \), i.e. and function that can be expanded as a power series, we have

\[
\sigma_i f(\sigma_j) = f(-\sigma_j) \sigma_i
\]

Using this result we have

\[
e^{i\pi \sigma_x / 4} \hat{S}_z e^{-i\pi \sigma_x / 4} = \frac{\hbar}{2} e^{i\pi \sigma_x / 4} \sigma_z e^{-i\pi \sigma_x / 4}
\]

\[
= \frac{\hbar}{2} e^{i\pi \sigma_x / 4} e^{i\pi \sigma_x / 4} \sigma_z = \frac{\hbar}{2} e^{i\pi \sigma_x / 2} \sigma_z
\]

\[
= \frac{\hbar}{2} (\cos \frac{\pi}{2} + i\sigma_x \sin \frac{\pi}{2}) \sigma_z = \frac{\hbar}{2} i\sigma_x \sigma_z = \frac{\hbar}{2} \sigma_y = \hat{S}_y
\]

It checks.