## Lecture 6 Summary

## Phys 402

Having defined the total angular momentum of the Hydrogen atom $\vec{J}=\vec{L}+\vec{S}$ we now wish to find the possible values for the quantum number $j$ and write down expressions for eigenfunctions of $J^{2}$ and $J_{z}$. All of this was precipitated by the need to handle the spinorbit perturbing Hamiltonian, which is proportional to $\vec{S} \bullet \vec{L}=\frac{1}{2}\left(J^{2}-L^{2}-S^{2}\right)$.

If $\vec{J}=\vec{L}+\vec{S}$ and $J^{2}$ has eigenvalue $j(j+1) \hbar^{2}, L^{2}$ has eigenvalue $\ell(\ell+1) \hbar^{2}$, and $S^{2}$ has eigenvalue $s(s+1) \hbar^{2}$, then one might naively think that $j=\ell+s$. However this is not the whole story. Remember that both $\vec{L}$ and $\vec{S}$ have ladders of states associated with the $\ell$ and $s$ eigenvalues. Hence we need to find a way to combine different ladders of states.

If we apply $J_{z}$ to a souped-up Hydrogen atom product wave function which now includes spin, $\psi_{n \ell, m_{\ell}, s, m_{s}}(r, \theta, \phi) \propto R_{n \ell}(r) Y_{\ell}^{m_{\ell}}(\theta, \phi)\left|s m_{s}\right\rangle$, where the spinor is denoted with the ket $\left|s m_{s}\right\rangle(s=1 / 2$ for the electron), the result is:

$$
\begin{aligned}
J_{z} \psi_{n, \ell, m_{\ell}, s, m_{s}} & =m_{j} \hbar \psi_{n, \ell, m_{\ell}, s, m_{s}}, \text { and } \\
J_{z} \psi_{n, \ell, m_{\ell}, s, m_{s}} & =\left(L_{z}+S_{z}\right) \psi_{n, \ell, m_{\ell}, s, m_{s}}
\end{aligned}
$$

The $L_{z}$ operator sees only the spherical harmonic, while the $S_{z}$ operator sees only the spinor ket. The result is:

$$
\begin{aligned}
& J_{z} \psi_{n, \ell, m_{\ell}, s, m_{s}}=\left(m_{\ell} \hbar+m_{s} \hbar\right) \psi_{n, \ell, m_{\ell}, s, m_{s}}, \text { leading to the conclusion that } \\
& m_{j}=m_{\ell}+m_{s}
\end{aligned}
$$

However, if we operate with $J^{2}$ on this same Hydrogen atom wavefunction, the results are not so pretty. From the definition of $\vec{J}=\vec{L}+\vec{S}$, we know that $J^{2}=L^{2}+S^{2}+2 \vec{L} \bullet \vec{S}$ (note that $\vec{L}$ and $\vec{S}$ commute with each other), and the $\vec{L} \bullet \vec{S}$ operator can be expressed as:

$$
\begin{aligned}
2 \vec{L} \bullet \vec{S} & =2\left(L_{x} S_{x}+L_{y} S_{y}+L_{z} S_{z}\right) \\
& =2 L_{z} S_{z}+L_{+} S_{-}+L_{-} S_{+} .
\end{aligned}
$$

using our old friends the raising and lowering operators. $J^{2}$ can now be written as:

$$
J^{2}=L^{2}+S^{2}+2 L_{z} S_{z}+L_{+} S_{-}+L_{-} S_{+}
$$

Now consider applying this operator to a hydrogen atom product wavefunction of the form $\psi_{n, \ell, m_{\ell}, s, m_{s}}(r, \theta, \phi)=R_{n \ell}(r) Y_{\ell}^{m_{\ell}}(\theta, \phi)\left|\frac{1}{2} \frac{1}{2}\right\rangle$ for example (i.e. with a "spin up" electron):
$J^{2} \psi_{n, \ell, m_{\ell}, 1 / 2,1 / 2}=\left[\ell(\ell+1) \hbar^{2}+\frac{3}{4} \hbar^{2}+2 m_{\ell} \hbar \frac{\hbar}{2}\right] \psi_{n, \ell, m_{\ell}, 1 / 2,1 / 2}+\hbar \hbar \sqrt{\left(\ell-m_{\ell}\right)\left(\ell+m_{\ell}+1\right)} \psi_{n, \ell, m_{\ell}+1,1 / 2,-1 / 2}$
where we have used results from Eq. [4.121] and Eq. [4.136] on page 166 of Griffiths. Note that this is no longer an eigen-equation because the raising and lowering operators have changed the $m_{\ell}$ and $m_{s}$ values in the second term on the RHS. Apparently the
eigenfunctions of $J^{2}$ are linear combinations of Hydrogen atom product wavefunctions $\psi_{n, \ell, m_{\ell}, s, m_{s}}(r, \theta, \phi)$ with different values of $m_{\ell}$ and $m_{s}$. This is consistent with the statement we made in the last lecture that the $\vec{L} \bullet \vec{S}$ operator mixes together different unperturbed Hydrogen atom states.

The eigenfunctions of $J^{2}$ can be expressed as linear combinations of states with different values of $m_{\ell}$ and $m_{s}$ using the world-famous Clebsch-Gordan coefficients $\left(C_{m_{\ell}}^{\ell} s_{m_{s}}{ }^{j} m_{j}\right)$ as:

$$
\left|j m_{j}\right\rangle=\sum_{\substack{m_{\ell} \text { and } \\ m_{\ell}+m_{s}=m_{j}}} C_{m_{l} \text { such that }}^{\ell} \stackrel{s}{m_{s}}{\underset{m}{j}}_{m_{j}}^{j}\left|\ell m_{\ell}\right\rangle\left|s m_{s}\right\rangle
$$

where the ket $\left|\ell m_{\ell}\right\rangle$ represents the spherical harmonics $Y_{\ell}^{m_{\ell}}$. The C-G coefficient values are given in Table 4.8 on page 179 of Griffiths. Remember that all of the coefficients should appear under a square root, with the minus sign (if any) out front. Also note that we have dropped the radial part of the wavefunction ( $R_{n \ell}$ ) because it plays no role in combining angular momenta. Don't forget to put it back later.

Where do these CG coefficients come from? Consider starting with a product wavefunction at the top of the $m_{j}$ ladder (it is a product of the wavefunctions with maximum values of $m_{\ell}$ and $m_{s}$ ). Now apply the $\hat{J}_{-}=\hat{L}_{-}+S_{-}$lowering operator, and construct orthonormal states on lower rungs of the ladder. The coefficients on the terms of those wavefunctions are the C-G coefficients.

We did a specific example of a hydrogen atom with $\ell=1$ and spin $s=1 / 2$. In this case the angular momentum vector and spin vector can either be "parallel" or "anti-parallel." Consider the two cases:

1) "Parallel" $\vec{L}$ and $\vec{S}$ : The maximum value of $m_{\ell}$ is +1 , while the value of $m_{s}$ is $+1 / 2$ for the "parallel" case. This means that $m_{j}=m_{\ell}+m_{s}=3 / 2$. This is the state at the top of the ladder. There must also be states with $m_{j}=+1 / 2,-1 / 2,-3 / 2$. This is a set of 4 states on the ladder of $j=3 / 2$. Thus the eigenvalues of $J^{2}$ for this ladder must be $\frac{3}{2}\left(\frac{3}{2}+1\right) \hbar^{2}=\frac{15}{4} \hbar^{2}$. Note that $\langle\vec{L} \bullet \vec{S}\rangle>0$ in this case, giving a positive spin-orbit Hamiltonian perturbation.
2) "Anti-Parallel" $\vec{L}$ and $\vec{S}$ : The maximum value of $m_{\ell}$ is +1 , while the value of $m_{s}$ is $-1 / 2$ for the "anti-parallel" case. This means that $m_{j}=m_{\ell}+m_{s}=1 / 2$. This is the state at the top of the ladder. There must also be a state with $m_{j}=-1 / 2$. This is a set of 2 states on the ladder of $j=1 / 2$. Thus the eigenvalues of $J^{2}$ for this ladder must be $\frac{1}{2}\left(\frac{1}{2}+1\right) \hbar^{2}=\frac{3}{4} \hbar^{2}$. Note that $\langle\vec{L} \bullet \vec{S}\rangle<0$ in this case, giving a negative spin-orbit Hamiltonian perturbation.

There are a total of 6 states possible by simply combining the orbital angular momentum with $\ell=1$ and spin angular momentum with $s=1 / 2!$ Just imagine what happens when you combine 3 or more angular momentum vectors!

Now for an example of how to construct states that are simultaneous eigenfunctions of $L^{2}, S^{2}, J^{2}$ and $J_{z}$. Take the case again of hydrogen with $\ell=1$ and spin $s=1 / 2$. How do we find the state with $j=3 / 2$ and $m_{j}=-1 / 2$ in terms of the $Y_{\ell}^{m_{\ell}}$ and spinors? Look at the $1 \times \frac{1}{2}$ CG Table on page 188 . We are led to this table because we are combining an angular momentum vector with $\ell=1$ and spin vector with $s=1 / 2$. Now look under the column labeled " $3 / 2$ ". It says:

$$
\begin{aligned}
& \left|\frac{3}{2}-\frac{1}{2}\right\rangle=\sum_{m_{\ell}+m_{s}=-1 / 2} C_{m_{\ell}}^{1} \begin{array}{ccc}
1 / 2 & m_{s} & 3 / 2 \\
-1 / 2
\end{array}\left|1 m_{\ell}\right\rangle\left|\frac{1}{2} m_{s}\right\rangle \\
& \left|\frac{3}{2}-\frac{1}{2}\right\rangle=\sqrt{\frac{2}{3}}|10\rangle\left|\frac{1}{2}-\frac{1}{2}\right\rangle+\sqrt{\frac{1}{3}}|1-1\rangle\left|\frac{1}{2} \frac{1}{2}\right\rangle
\end{aligned}
$$

This can be written in a more familiar way in terms of spherical harmonics and spinors as:

$$
\left\langle\vec{r} \left\lvert\, \frac{3}{2}-\frac{1}{2}\right.\right\rangle=\sqrt{\frac{2}{3}} Y_{1}^{0}(\theta, \phi) \chi_{-}+\sqrt{\frac{1}{3}} Y_{1}^{-1}(\theta, \phi) \chi_{+}
$$

where the spinors are being written as $\chi_{ \pm}=\left|\frac{1}{2} \pm \frac{1}{2}\right|$.
One can move back and forth between the coupled and un-coupled representations using the Clebsch-Gordan table on page 179. Here is the schematic layout for the CG table for combining two spins (called $\left.\vec{S}_{1}, \vec{S}_{2}\right)$ to form a total spin $\vec{S}=\vec{S}_{1}+\vec{S}_{2}\left(S^{2}\right.$ has eigenvalue $\left.s(s+1) \hbar^{2}\right)$ :

General Schematic of the C-G Table


