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 $\vec{S} \cdot \vec{L} = \frac{1}{2} (J^2 - L^2 - S^2)$.

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 ℓ 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, $\psi_{n,\ell,m_\ell,s,m_s}(r,\theta,\phi) \propto R_{n\ell}(r)Y_\ell^{m_\ell}(\theta,\phi) |s m_s\rangle$, where the spinor is denoted with the ket $|s m_s\rangle$ (s = 1/2 for the electron), the result is:

$$J_{z}\psi_{n,\ell,m_{\ell},s,m_{s}} = m_{j}\hbar\psi_{n,\ell,m_{\ell},s,m_{s}}, \text{ and}$$
$$J_{z}\psi_{n,\ell,m_{\ell},s,m_{s}} = (L_{z} + S_{z})\psi_{n,\ell,m_{\ell},s,m_{s}}$$

The L_z operator sees only the spherical harmonic, while the S_z operator sees only the spinor ket. The result is:

 $J_z \psi_{n,\ell,m_\ell,s,m_s} = (m_\ell \hbar + m_s \hbar) \psi_{n,\ell,m_\ell,s,m_s}, \text{ leading to the conclusion that}$ $m_j = m_\ell + m_s$

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 $J^2 = L^2 + S^2 + 2\vec{L} \cdot \vec{S}$ (note that \vec{L} and \vec{S} commute with each other), and the $\vec{L} \cdot \vec{S}$ operator can be expressed as:

$$2\vec{L} \bullet \vec{S} = 2(L_x S_x + L_y S_y + L_z S_z)$$
$$= 2L_z S_z + L_+ S_- + L_- S_+.$$

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

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

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):

$$J^{2}\psi_{n,\ell,m_{\ell},1/2,1/2} = \left[\ell(\ell+1)\hbar^{2} + \frac{3}{4}\hbar^{2} + 2m_{\ell}\hbar\frac{\hbar}{2}\right]\psi_{n,\ell,m_{\ell},1/2,1/2} + \hbar\hbar\sqrt{(\ell-m_{\ell})(\ell+m_{\ell}+1)}\psi_{n,\ell,m_{\ell}+1,1/2,-1/2}$$

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_{ℓ} 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_ℓ and m_s . This is consistent with the statement we made in the last lecture that the $\vec{L} \cdot \vec{S}$ 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_{ℓ} and m_s using the world-famous Clebsch-Gordan coefficients $(C_{m_{\ell}}^{\ell s j} m_{s}^{j} m_{s})$ as:

$$|j \ m_j\rangle = \sum_{\substack{m_\ell \text{ and } m_s \text{ such that} \\ m_\ell + m_s = m_j}} C_{m_l}^{\ell} \sum_{\substack{m_s \ m_s \\ m_l}}^{j} |\ell \ m_\ell\rangle |s \ m_s\rangle$$

where the ket $|\ell m_{\ell}\rangle$ 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_ℓ and m_s). Now apply the $\hat{f}_- = \hat{L}_- + S_-$ 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_{ℓ} 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 $\frac{3}{2}(\frac{3}{2}+1)\hbar^2 = \frac{15}{4}\hbar^2$. Note that $\langle \vec{L} \cdot \vec{S} \rangle > 0$ in this case, giving a positive spin-orbit Hamiltonian perturbation.

2) "Anti-Parallel" \vec{L} and \vec{S} : The maximum value of m_{ℓ} 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 $\frac{1}{2}(\frac{1}{2}+1)\hbar^2 = \frac{3}{4}\hbar^2$. Note that $\langle \vec{L} \cdot \vec{S} \rangle < 0$ 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 <u>example</u> 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 " $\frac{3/2}{-1/2}$ ". It says:

$$\left| \frac{3}{2} - \frac{1}{2} \right\rangle = \sum_{m_{\ell} + m_s = -1/2} C_{m_{\ell} - m_s - 1/2}^{1 - 1/2} \left| 1 m_{\ell} \right\rangle \left| \frac{1}{2} m_s \right\rangle$$
$$\left| \frac{3}{2} - \frac{1}{2} \right\rangle = \sqrt{\frac{2}{3}} \left| 1 0 \right\rangle \left| \frac{1}{2} - \frac{1}{2} \right\rangle + \sqrt{\frac{1}{3}} \left| 1 - 1 \right\rangle \left| \frac{1}{2} - \frac{1}{2} \right\rangle$$

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

$$\left\langle \vec{r} \left| \frac{3}{2} - \frac{1}{2} \right\rangle = \sqrt{\frac{2}{3}} Y_1^0(\theta, \phi) \chi_- + \sqrt{\frac{1}{3}} Y_1^{-1}(\theta, \phi) \chi_+$$

where the spinors are being written as $\chi_{\pm} = |\frac{1}{2} \pm \frac{1}{2}$.

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 \vec{S}_1 , \vec{S}_2) to form a total spin $\vec{S} = \vec{S}_1 + \vec{S}_2$ (S^2 has eigenvalue $s(s+1)\hbar^2$):

General Schematic of the C-G Table

$$\vec{S} = \vec{S}_1 + \vec{S}_2$$

$$S_1 \times S_2$$

$$S_1 \times S_2$$

$$M_s$$

$$Coupled Representation
$$M_s$$

$$CG\#$$$$

Un-Coupled Representation