A spin ½ particle in a spherically symmetric potential

One of the most remarkable concepts that results from the Dirac theory of the hydrogen atom is that in addition to its orbital angular momentum the electron has an intrinsic angular momentum which we know as its *spin*. However unlike the orbital angular momentum which can have the values $\sqrt{\ell(\ell+1)}\hbar$ where ℓ is a positive integer, the spin angular momentum is always $\sqrt{\frac{1}{2}\left(\frac{1}{2}+1\right)}\hbar$ and while the orbital angular momentum can have projections on an external axis of $m_\ell\hbar$ where $-\ell \le m_\ell \le \ell$ the electron spin can only have two projections, $m_S\hbar$ with $m_S = \pm\frac{1}{2}$. The electron spin wave function with the $+\frac{\hbar}{2}$ projection is called α or the spin up state while the spin wavefunction with the $-\frac{\hbar}{2}$ projection is called β or the spin down state. Since spin is an angular momentum there is an operator $\hat{\vec{S}}$ associated with it which has the same commutation relations as the orbital angular momentum operator $\hat{\vec{L}}$, i.e., $\left[\hat{S}_\chi, \hat{S}_\sigma\right] = i\varepsilon_{\chi\sigma\gamma}\hat{S}_\gamma$. The spin wavefunctions are orthogonal $\langle\alpha|\beta\rangle = \langle\beta|\alpha\rangle = 0$ and normalized $\langle\alpha|\alpha\rangle = \langle\beta|\beta\rangle = 1$ and eigenfunctions of $\hat{S}^2$ & $\hat{S}_z$

$$\hat{S}^2\alpha = \frac{1}{2}\left(\frac{1}{2}+1\right)\hbar^2\alpha = \frac{3\hbar^2}{4}\alpha \;\;\&\;\; \hat{S}^2\beta = \frac{1}{2}\left(\frac{1}{2}+1\right)\hbar^2 = \frac{3\hbar^2}{4}\beta$$

and

$$\hat{S}_z\alpha = \frac{\hbar}{2}\alpha \;\;\&\;\; \hat{S}_z\beta = -\frac{\hbar}{2}\beta$$

The question at hand is how should the spin and orbital angular momentum be combined? Presumably the total angular momentum is the sum of the two and is given by

$\hat{\vec{J}} = \hat{\vec{L}} + \hat{\vec{S}}$ and since $\hat{\vec{L}}$ & $\hat{\vec{S}}$ commute we have $\left[\hat{J}_\alpha, \hat{J}_\beta\right] = i\hbar\varepsilon_{\alpha\beta\gamma}\hat{J}_\gamma$ and therefore $\left[\hat{\vec{J}}^2, \hat{J}_z\right] = 0$. Note also $\left[\hat{J}_z, \hat{\vec{L}}^2\right] = 0$ and $\left[\hat{J}_z, \hat{\vec{S}}^2\right] = 0$. Finally

$\left[\hat{\vec{J}}^2, \hat{\vec{L}}^2\right] = \left[(\hat{\vec{L}} + \hat{\vec{S}})^2, \hat{\vec{L}}^2\right] = \left[\hat{\vec{L}}^2 + \hat{\vec{S}}^2 + 2\hat{\vec{L}} \bullet \hat{\vec{S}}, \hat{\vec{L}}^2\right] = 0$ and similarly $\left[\hat{\vec{J}}^2, \hat{\vec{S}}^2\right] = 0$

From these commutation relations we deduce that if Φ is an eigenfunction of $\hat{\vec{J}}^2$ & $\hat{J}_z$ with eigenvalues $j(j+1)\hbar^2$ & $m_j\hbar$ and it is also an eignfunction of $\hat{\vec{L}}^2$ & $\hat{\vec{S}}^2$ with eigenvalues $\ell(\ell+1)\hbar^2$ & $\frac{1}{2}\left(\frac{1}{2}+1\right)\hbar^2$. In summary we have

$$\hat{\vec{J}}^2\Phi_{jm_j\ell 1/2} = j(j+1)\hbar^2\Phi_{jm_j\ell 1/2}$$
$$\hat{J}_z\Phi_{jm_j\ell 1/2} = m_j\hbar\Phi_{jm_j\ell 1/2}$$
$$\hat{\vec{L}}^2\Phi_{jm_j\ell 1/2} = \ell(\ell+1)\hbar^2\Phi_{jm_j\ell 1/2}$$
$$\hat{\vec{S}}^2\Phi_{jm_j\ell 1/2} = \frac{1}{2}(\frac{1}{2}+1)\hbar^2\Phi_{jm_j\ell 1/2}$$

Truly a remarkable amount of information!

Let's consider the explicit form of $\Phi_{jm_j\ell 1/2}$. Since it's an eigenfunction of $\hat{\vec{L}}^2$ & $\hat{\vec{S}}^2$ it must be expandable in the direct product space spanned by $\alpha Y_\ell^m(\theta,\phi)$ & $\beta Y_\ell^{m'}(\theta,\phi)$ and have the form

$$\Phi_{jm_j\ell 1/2} = C_\alpha \alpha Y_\ell^m(\theta,\phi) + C_\beta \beta Y_\ell^{m'}(\theta,\phi)$$

The coefficients C_α & C_β are determined by requiring that $\Phi_{jm_j\ell 1/2}$ be an eigenfunction of $\hat{\vec{J}}^2$ & $\hat{J}_z$. This is a bit tedious so we defer it to the appendix. The result is

$$\Phi_{jm_j\ell 1/2} = \frac{1}{\sqrt{2\ell+1}}\left(\pm\sqrt{\ell \pm m_j + 1/2}\ \alpha Y_\ell^{m_j-1/2}(\theta,\phi) + \sqrt{\ell \mp m_j + 1/2}\ \beta Y_\ell^{m_j+1/2}(\theta,\phi)\right)$$

where $j = \ell \pm 1/2$.

Let's write out a few of these angular functions explicitly using the Dirac Bra Ket notation.

For $\ell = 0$, j can only be $1/2$ (it must be positive) so the function is

$$\left| j = 1/2, m_j, \ell = 0 \right\rangle = \left(\sqrt{m_j + 1/2}\ \alpha Y_0^{m_j - 1/2} + \sqrt{-m_j + 1/2}\ \beta Y_0^{m_j + 1/2} \right)$$

and the two possible values of $m_j = \pm 1/2$ result in

$\left| j = 1/2, m_j = +1/2, \ell = 0 \right\rangle = \alpha Y_0^0$ and $\left| j = 1/2, m_j = -1/2, \ell = 0 \right\rangle = \beta Y_0^0$

from which we see that since $\ell = 0$ the total angular momentum is simply that due to the electron spin.

For $\ell = 1$ we can have $j = 1/2 \,\&\, 3/2$ so

$$\left| j = 1/2, m_j, \ell = 1 \right\rangle = \frac{1}{\sqrt{3}} \left(-\sqrt{-m_j + 3/2}\ \alpha Y_1^{m_j - 1/2} + \sqrt{m_j + 3/2}\ \beta Y_1^{m_j + 1/2} \right)$$

and since $m_j = \pm 1/2$ we have

$$\left| j = 1/2, 1/2, \ell = 1 \right\rangle = \frac{1}{\sqrt{3}} \left(-\ \alpha Y_1^0 + \frac{2}{\sqrt{2}}\ \beta Y_1^1 \right)$$

and

$$\left| j = 1/2, -1/2, \ell = 1 \right\rangle = \frac{1}{\sqrt{3}} \left(-\frac{2}{\sqrt{2}}\ \alpha Y_1^{-1} + \beta Y_1^0 \right)$$

The $j = 3/2$ functions are

$$\left| j = 3/2, m_j, \ell = 1 \right\rangle = \frac{1}{\sqrt{3}} \left(+\sqrt{m_j + 3/2}\ \alpha Y_1^{m_j - 1/2} + \sqrt{-m_j + 3/2}\ \beta Y_1^{m_j + 1/2} \right)$$

and since $m_j = \pm 1/2 \,\&\, \pm 3/2$ we have the four functions

$$\left| j = 3/2, -3/2, \ell = 1 \right\rangle = \beta Y_1^{-1}$$

$$\left| j = 3/2, -1/2, \ell = 1 \right\rangle = \frac{1}{\sqrt{3}} \left(\ \alpha Y_1^{-1} + \sqrt{2}\ \beta Y_1^0 \right)$$

$$\left| j = 3/2, 1/2, \ell = 1 \right\rangle = \frac{1}{\sqrt{3}} \left(+\sqrt{2}\ \alpha Y_1^0 +\ \beta Y_1^1 \right)$$

$$\left| j = 3/2, 3/2, \ell = 1 \right\rangle = \alpha Y_1^1$$