One Electron Spin Operators

An individual electron has two degenerate spin states, α & β and both are eigenfunctions of $\hat{s}^2$ with eigenvalue $\frac{1}{2}\left(\frac{1}{2}+1\right)\hbar^2=\frac{3}{4}\hbar^2$. They are also eigenfunctions of $\hat{s}_z$ with eigenvalues $\pm\frac{\hbar}{2}$ respectively. In what follows we will use atomic units and will measure the spin angular momentum in units of $\hbar$, so the eigenvalue equations become

$$\hat{s}^2\alpha=\frac{3}{4}\alpha \;\;\&\;\; \hat{s}^2\beta=\frac{3}{4}\beta$$

and

$$\hat{s}_z\alpha=\frac{1}{2}\alpha \;\;\&\;\; \hat{s}_z\beta=-\frac{1}{2}\beta$$

The spin eigenfunctions $\alpha \,\&\, \beta$ are orthonormal

$$\int\alpha^*(\xi)\alpha(\xi)\,d\xi=\langle\alpha|\alpha\rangle=1$$

$$\int\beta^*(\xi)\beta(\xi)\,d\xi=\langle\beta|\beta\rangle=1$$

$$\int\alpha^*(\xi)\beta(\xi)\,d\xi=\langle\alpha|\beta\rangle=0$$

We will also make use of the raising and lowering operators defined by

$$\hat{s}_\pm=\hat{s}_x\pm i\hat{s}_y$$

and the commutation relations

$$\left[\hat{s}_x,\hat{s}_y\right]=i\hat{s}_z \;\;\&\;\; \left[\hat{s}_y,\hat{s}_z\right]=i\hat{s}_x \;\;\&\;\; \left[\hat{s}_z,\hat{s}_x\right]=i\hat{s}_y$$

Note that $\hat{s}_+\hat{s}_-=(\hat{s}_x+i\hat{s}_y)(\hat{s}_x-i\hat{s}_y)=\hat{s}_x^2+\hat{s}_y^2-i\hat{s}_x\hat{s}_y+i\hat{s}_y\hat{s}_x=\hat{s}_x^2+\hat{s}_y^2-i\left[\hat{s}_x,\hat{s}_y\right]$

So $\hat{s}_+\hat{s}_-=\hat{s}_x^2+\hat{s}_y^2+\hat{s}_z$

and $\hat{s}^2=\hat{s}_x^2+\hat{s}_y^2+\hat{s}_z^2=\hat{s}_+\hat{s}_--\hat{s}_z+\hat{s}_z^2=\hat{s}_-\hat{s}_++\hat{s}_z+\hat{s}_z^2$

a relationship we will use frequently in what follows.

Using the commutators given above we can show that

$\left[\hat{s}_z,\hat{s}_+\right]=\hat{s}_+$ & $\left[\hat{s}_z,\hat{s}_-\right]=-\hat{s}_-$

from which we see

$$\hat{s}_+\beta=\left[\hat{s}_z,\hat{s}_+\right]\beta=\hat{s}_z\hat{s}_+\beta-\hat{s}_+\hat{s}_z\beta=\hat{s}_z\hat{s}_+\beta+\frac{1}{2}\hat{s}_+\beta$$

and $\hat{s}_z\hat{s}_+\beta=\frac{1}{2}\hat{s}_+\beta$ so $\hat{s}_+\beta$ is an eigenfunction of $\hat{s}_z$ with an eigenvalue $+\frac{1}{2}$ and $\therefore$ $\hat{s}_+\beta=\alpha$

in a similar way one may show that

$$\hat{s}_+\alpha=0 \text{ \& } \hat{s}_+\beta=\alpha$$

$$\hat{s}_-\alpha=\beta \text{ \& } \hat{s}_-\beta=0$$

$\hat{s}_+$ is a raising operator because it raises the $m_s=-\frac{1}{2}$ function β to the $m_s=+\frac{1}{2}$ function α. Likewise $\hat{s}_-$ is a lowering operator because it lowers the $m_s=+\frac{1}{2}$ function α to the $m_s=-\frac{1}{2}$ function β.