Spin Operators in Many Electron Systems

In an *N* electron system the spin angular momentum operators are formed by summing the operators for the individual spins as follows:

$$\hat{S}_{\mu} = \sum_{j=1}^N \hat{s}_{\mu}(j)$$

where $\mu = x, y, z$

and $\hat{s}_{\mu}(j)$ is the μ^{th} component of the spin operator for the j^{th} electron. Because the spin operators for different electrons commute the commutation relations for the many-electron operators are then

$$\left[\hat{S}_{\mu},\hat{S}_{\nu}\right] = i\varepsilon_{\mu\nu\gamma}\hat{S}_{\gamma}$$

The operator representing the square of the total spin angular momentum is

$$\hat{S}^2 = \hat{S}_x^2 + \hat{S}_y^2 + \hat{S}_z^2$$

Which may be written as

$$\hat{S}^2 = \hat{S}_{\pm}\hat{S}_{\mp} \mp \hat{S}_z + \hat{S}_z^2$$

Where the many electron raising and lowering operators are

$$\hat{S}_{\pm} = \sum_{j=1}^{N} \hat{s}_{\pm}(j)$$

Exercise Prove that $\hat{S}^2 = \hat{S}_{\pm}\hat{S}_{\mp} \mp \hat{S}_z + \hat{S}_z^2$

Note that \hat{S}^2 commutes with the spin free Hamiltonian

$$\hat{H} = \sum_{i=1}^{N} \hat{f}(i) + \sum_{i < j}^{N} g(i, j)$$

 $\begin{bmatrix} \hat{S}^2, \hat{H} \end{bmatrix} = 0$ and each of its components $\begin{bmatrix} \hat{S}^2, \hat{S}_{\mu} \end{bmatrix} = 0$ but because the individual components do not commute we may choose the eigenfunctions of \hat{H} to be

eigenfunctions of \hat{S}^2 and one of its components (most often chosen to be the z component) so the many electron eigenfunction $\psi(1,2,3,\cdots N)$ of satisfies the equations

$$\hat{S}^2 \psi = S(S+1)\psi \& \hat{S}_z \psi = M\psi$$

where $-S \le M \le S$ in multiples of 1.