174(3): Relevant Operator Properties

The basic operator in relativistic quantum mechanics is

$$\hat{\kappa} = \underline{\hat{\sigma}} \cdot \underline{\hat{L}} + \hbar \quad -(1)$$

which written in full is:

$$\hat{\kappa} = \begin{bmatrix} \underline{\hat{\sigma}} \cdot \underline{\hat{L}} + \hbar & 0 \\ 0 & -\underline{\hat{\sigma}} \cdot \underline{\hat{L}} - \hbar \end{bmatrix} \quad -(2)$$

so

$$\hat{\kappa}\phi = -\kappa\hbar\phi \quad -(3)$$

$$\kappa = \pm\left(j + \frac{1}{2}\right). \quad -(4)$$

Thus:

$$\begin{aligned}\hat{\kappa}^2 &= \left(\underline{\hat{\sigma}} \cdot \underline{\hat{L}} + \hbar\right)^2 \\ &= \underline{\hat{\sigma}} \cdot \underline{\hat{L}}\, \underline{\hat{\sigma}} \cdot \underline{\hat{L}} + 2\hbar\, \underline{\hat{\sigma}} \cdot \underline{\hat{L}} + \hbar^2\end{aligned} \quad -(5)$$

We have:

$$\underline{\hat{\sigma}} \cdot \underline{\hat{L}}\, \underline{\hat{\sigma}} \cdot \underline{\hat{L}} = \hat{L}^2 + i\underline{\hat{\sigma}} \cdot \underline{\hat{L}} \times \underline{\hat{L}} \quad -(6)$$

The basic commutator relations are:

$$[\hat{L}_X, \hat{L}_Y] = i\hbar \hat{L}_Z \quad -(7)$$

et cyclicum,

i.e.

$$\underline{\hat{L}} \times \underline{\hat{L}} = i\hbar \underline{\hat{L}}. \quad -(8)$$

So:

$$\boxed{\underline{\hat{\sigma}} \cdot \underline{\hat{L}}\, \underline{\hat{\sigma}} \cdot \underline{\hat{L}} = \hat{L}^2 - \hbar\, \underline{\hat{\sigma}} \cdot \underline{\hat{L}}} \quad -(9)$$

From eq. (9) in eq. (5):

2)

$$\hat{K}^2 = \hat{L}^2 + \hbar \underline{\hat{\sigma}} \cdot \underline{\hat{L}} + \hbar^2 \quad -(10)$$

As in previous notes:

$$\underline{\sigma} \cdot \underline{\hat{L}} \, \phi^R = \hbar \left(j - \frac{1}{2} \right) \phi^R \quad -(11)$$

$$\underline{\sigma} \cdot \underline{\hat{L}} \, \phi^L = -\hbar \left(j + \frac{3}{2} \right) \phi^L \quad -(12)$$

The total angular momentum operator is:

$$\underline{\hat{J}} = \underline{\hat{L}} + \frac{\hbar}{2} \underline{\hat{\sigma}} \quad -(13)$$

$$= \underline{\hat{L}} + \underline{\hat{S}} \quad -(14)$$

where the intrinsic spin angular momentum operator is:

$$\underline{\hat{S}} = \frac{1}{2} \hbar \underline{\hat{\sigma}} \quad -(15)$$

So:

$$\hat{J}^2 = \hat{L}^2 + \hbar \underline{\hat{\sigma}} \cdot \underline{\hat{L}} + \frac{\hbar^2}{4} \underline{\hat{\sigma}} \cdot \underline{\hat{\sigma}}$$

$$= \hat{L}^2 + \hbar \underline{\hat{\sigma}} \cdot \underline{\hat{L}} + \frac{3}{4} \hbar^2 \quad -(16)$$

$$= \hat{L}^2 + \hbar \underline{\hat{\sigma}} \cdot \underline{\hat{L}} + \underline{\hat{S}} \cdot \underline{\hat{S}}$$

$$= \hat{L}^2 + 2 \underline{\hat{S}} \cdot \underline{\hat{L}} + \underline{\hat{S}} \cdot \underline{\hat{S}}$$

in which we have used:

$$\underline{\hat{\sigma}} \cdot \underline{\hat{\sigma}} = 3. \quad -(17)$$

We have:

$$\hat{J}^2 \phi = \hbar^2 j (j+1) \phi \quad -(18)$$

$\therefore$

3)

$$\hat{L}^2 \phi^R = \hbar^2 l_- (l_- + 1) \phi^R \quad -(19)$$

$$\hat{L}^2 \phi^L = \hbar^2 l_+ (l_+ + 1) \phi^L \quad -(20)$$

where

$$l_\pm = j \pm \frac{1}{2}. \quad -(21)$$

Now consider:

$$\underline{\hat{\sigma}} \cdot \underline{\hat{p}} = \underline{\hat{\sigma}} \cdot \frac{\underline{r}}{r} \left(\frac{\underline{r}}{r} \cdot \underline{\hat{p}} + i \frac{\underline{\hat{\sigma}} \cdot \underline{\hat{L}}}{r} \right) \quad -(22)$$

then:

$$\underline{\hat{\sigma}} \cdot \underline{\hat{p}} \; \underline{\hat{\sigma}} \cdot \underline{\hat{p}} = \frac{\underline{r}}{r} \cdot \underline{\hat{p}} \frac{\underline{r}}{r} \cdot \underline{\hat{p}} - \frac{\underline{\hat{\sigma}} \cdot \underline{\hat{L}} \; \underline{\hat{\sigma}} \cdot \underline{\hat{L}}}{r^2} + i \frac{\underline{r}}{r} \cdot \underline{\hat{p}} \frac{\underline{\hat{\sigma}} \cdot \underline{\hat{L}}}{r} + i \frac{\underline{\hat{\sigma}} \cdot \underline{\hat{L}}}{r} \frac{\underline{r}}{r} \cdot \underline{\hat{p}} \quad -(23)$$

Therefore the real part of this equation is:

$$\text{Real } \underline{\hat{\sigma}} \cdot \underline{\hat{p}} \; \underline{\hat{\sigma}} \cdot \underline{\hat{p}} = \frac{\underline{r}}{r} \cdot \underline{\hat{p}} \frac{\underline{r}}{r} \cdot \underline{\hat{p}} - \frac{\underline{\hat{\sigma}} \cdot \underline{\hat{L}} \; \underline{\hat{\sigma}} \cdot \underline{\hat{L}}}{r^2} \quad -(24)$$

where we have used:

$$\underline{\hat{\sigma}} \cdot \frac{\underline{r}}{r} \; \underline{\hat{\sigma}} \cdot \frac{\underline{r}}{r} = 1. \quad -(25)$$

Now use:

$$\frac{\underline{r}}{r} \cdot \underline{\hat{p}} \frac{\underline{r}}{r} \cdot \underline{\hat{p}} = -\hbar^2 \frac{\partial^2}{\partial r^2} \quad -(26)$$

and eq. (9) to find:

$$\underline{\hat{\sigma}} \cdot \underline{\hat{p}} \; \underline{\hat{\sigma}} \cdot \underline{\hat{p}} = -\hbar^2 \frac{\partial^2}{\partial r^2} - \frac{\hat{L}^2}{r^2} + \frac{\hbar}{r^2} \underline{\hat{\sigma}} \cdot \underline{\hat{L}} \quad -(27)$$

+) However we know that:

$$\hat{\underline{\sigma}}\cdot\hat{\underline{p}}\;\hat{\underline{\sigma}}\cdot\hat{\underline{p}} = \hat{p}^2 = -\hbar^2\hat{\nabla}^2 \quad -(28)$$

so:

$$\boxed{\hat{\nabla}^2 = \frac{\partial^2}{\partial r^2} + \frac{\hat{L}^2}{\hbar^2 r^2} - \frac{1}{\hbar r^2}\hat{\underline{\sigma}}\cdot\hat{\underline{L}}} \quad -(29)$$

To make clear that these are all operator equations, the symbol $\wedge$ has been placed above all operators.

The fine structure of hydrogen can be understood in all detail using just angular momentum operators (P. W. Atkins, "Molecular Quantum Mechanics", OUP, 1983, 2nd edition). Using:

$$\hat{J}^2 = \hat{L}^2 + \hat{S}^2 + 2\hat{\underline{L}}\cdot\hat{\underline{S}} \quad -(30)$$

the energy levels of spin orbit coupling are given by:

$$\hat{\underline{L}}\cdot\hat{\underline{S}}\,\psi = \frac{1}{2}\left(j^2 - l^2 - s^2\right)\psi \quad -(31)$$

and

$$E_{so} = \frac{1}{2}\hbar^2\Big(j(j+1) - l(l+1) - s(s+1)\Big)\langle\psi^*|\xi(r)|\psi\rangle \quad -(32)$$

The entire H spectrum is given by eq. (32).

In the next note it will be explained how these operators are relevant to the fermion equation and its approximation.