248(8): Derivation of Spin Orbit Coupling and the Thomas Factor.

These results emerge from the $\hat{H}_{22}$ hamiltonian. For a real valued vector potential:

$$\hat{H}_{22}\,\phi = \frac{e}{4m^2c^2}\left(\underline{\sigma}\cdot(\underline{p}-e\underline{A})\,\phi\,\underline{\sigma}\cdot(\underline{p}-e\underline{A})\right)\phi \quad -(1)$$

In the textbook derivation of spin-orbit coupling several assumptions are made as follows:

1) the vector potential $\underline{A}$ is assumed to be zero, so only electric field effects are considered.

2) It is assumed that the first $\underline{p}$ is an operator:

$$\underline{p} = -i\hbar\,\underline{\nabla} \quad -(2)$$

but that the second $\underline{p}$ is a function.

Then eq. (1) reduces to:

$$\hat{H}_{22}\,\phi = -\frac{ie\hbar}{4m^2c^2}\left(\underline{\sigma}\cdot\underline{\nabla}\,\phi\,\underline{\sigma}\cdot\underline{p}\right)\phi \quad -(3)$$

The $\underline{\nabla}$ operator acts on $\phi\,\underline{\sigma}\cdot\underline{p}\,\phi$, so by the Leibnitz theorem:

$$\underline{\nabla}\left(\phi\,\underline{\sigma}\cdot\underline{p}\,\phi\right) = \underline{\nabla}\left(\underline{\sigma}\cdot\underline{p}\right)\phi\,\phi + \underline{\sigma}\cdot\underline{p}\;\underline{\nabla}\left(\phi\,\phi\right) \quad -(4)$$

If $\underline{p}$ has no gradient then:

$$\underline{\nabla}\left(\underline{\sigma}\cdot\underline{p}\right) = \underline{0} \quad -(5)$$

2) However if $\underline{p}$ has a non-zero gradient there are other effects present. If eq. (5) is true then:

$$\hat{H}_{22}\phi = -\frac{ie\hbar}{4m^2c^2}\left(\underline{\sigma}\cdot\underline{\nabla}(\phi\,\phi)\,\underline{\sigma}\cdot\underline{p}\right) \quad -(6)$$

The Leibnitz theorem asserts that:

$$\underline{\nabla}(\phi\,\phi) = (\underline{\nabla}\phi)\phi + \phi(\underline{\nabla}\phi) \quad -(7)$$

If the wavefunction has no gradient then

$$\underline{\nabla}\phi = 0. \quad -(8)$$

w.r.t. the assumption (8):

$$\hat{H}_{22}\phi = -\frac{ie\hbar}{4m^2c^2}\left(\underline{\sigma}\cdot\underline{\nabla}\phi\,\underline{\sigma}\cdot\underline{p}\right)\phi \quad -(9)$$

The standard physics asserts that:

$$\underline{E} = -\underline{\nabla}\phi \quad -(10)$$

So

$$\hat{H}_{22} = -\frac{ie\hbar}{4m^2c^2}\left(\underline{\sigma}\cdot\underline{E}\,\underline{\sigma}\cdot\underline{p}\right). \quad -(11)$$

Now use the Pauli algebra:

$$\underline{\sigma}\cdot\underline{E}\,\underline{\sigma}\cdot\underline{p} = \underline{E}\cdot\underline{p} + i\,\underline{\sigma}\cdot\underline{E}\times\underline{p} \quad -(12)$$

The real part of $\hat{H}_{22}$ from eqs. (11) and (12) is:

3)

$$\hat{H}_{22} = \frac{e\hbar}{4m^2c^2} \left(\underline{\sigma} \cdot \underline{E} \times \underline{p} \right) \quad -(13)$$

in which $\underline{p}$ is regarded as a function, and not as an operator. If this second $\underline{p}$ is regarded as an operator then new effects appear. In the derivation of the Zeeman effect, ESR, NMR and g factor of the electron, both $\underline{p}$'s are regarded as operators, but in the derivation of the spin orbit coupling, only the first $\underline{p}$ is regarded as an operator.

Finally the Coulomb potential of electrostatics is chosen for ϕ:

$$\phi = -\frac{e}{4\pi r \epsilon_0} \quad -(14)$$

and the standard physics formula used for $\underline{E}$:

$$\underline{E} = -\underline{\nabla}\phi = -\frac{e}{4\pi\epsilon_0}\frac{\underline{r}}{r^3} \quad -(15)$$

so

$$\hat{H}_{22} = \frac{-e\hbar}{8\pi c^2 \epsilon_0 m^2 r^3} \underline{\sigma} \cdot \underline{r} \times \underline{p} \quad -(16)$$

The orbital angular momentum is:

$$\underline{L} = \underline{r} \times \underline{p} \quad -(17)$$

So:

$$\hat{H}_{22} = -\frac{e\hbar}{8\pi c^2 \epsilon_0 m^2 r^3}\,\underline{\sigma}\cdot\underline{L} \quad -(18)$$

In atomic and molecular spectra both $\underline{\sigma}$ and $\underline{L}$ are regarded as operators acting on ψ, with:

$$\hat{\underline{S}} = \hbar\,\hat{\underline{\sigma}} \quad -(19)$$

so

$$\hat{H}_{22}\psi = -\frac{e}{8\pi c^2 \epsilon_0 m^2 r^3}\,\hat{\underline{S}}\cdot\hat{\underline{L}}\,\psi \quad -(20)$$

$$:= -\zeta\left(\hat{\underline{S}}\cdot\hat{\underline{L}}\right)\psi$$

The Thomas factor is contained in eq. (1) as part of the denominator.

There are many developments possible of this theory in ECE physics, introducing the spin connection. In atomic and molecular spectra the classical operators $\hat{\underline{S}}\cdot\hat{\underline{L}}$ are developed with the Cartan ~~theory~~. The mysterious thing is why the theory works with only one $\hat{p}$ ~~are~~ as an operator.