249(3): New First Order ESR and NMR Effects

Consider the fermion equation in the usual approximation:

$$E = mc^2 + e\phi + \frac{1}{2m}(\underline{p} - e\underline{A})\left(1 + \frac{e\phi}{2mc^2}\right)(\underline{p} - e\underline{A}) \quad -(1)$$

which quantizes to $\hat{H}\psi = E\psi \quad -(2)$

Now consider the Hamiltonian:

$$\hat{H}_1 = \frac{1}{2m}\underline{\sigma}\cdot(-i\hbar\underline{\nabla} - e\underline{A})\,\underline{\sigma}\cdot(\underline{p} - e\underline{A}) \quad -(3)$$

in which the first p is considered to be the operator $-i\hbar\underline{\nabla}$ and the second $\underline{p}$ the function. Thus:

$$\hat{H}_1 = -\frac{i\hbar}{2m}\underline{\sigma}\cdot\underline{\nabla}\,\underline{\sigma}\cdot\underline{p} - \frac{e}{2m}\underline{\sigma}\cdot\underline{A}\,\underline{\sigma}\cdot\underline{p} + \frac{ie\hbar}{2m}\underline{\sigma}\cdot\underline{\nabla}\,\underline{\sigma}\cdot\underline{A} + \frac{e^2}{2m}\underline{\sigma}\cdot\underline{A}\,\underline{\sigma}\cdot\underline{A} \quad -(4)$$

Now consider the first order Hamiltonian:

$$\boxed{\hat{H}_{12} = -\frac{e}{2m}\underline{\sigma}\cdot\underline{A}\,\underline{\sigma}\cdot\underline{p}} \quad -(5)$$

and use the Pauli algebra:

$$\underline{\sigma}\cdot\underline{p} = \frac{1}{r^2}\underline{\sigma}\cdot\underline{r}\,(\underline{r}\cdot\underline{p} + i\underline{\sigma}\cdot\underline{L}) \quad -(6)$$

$$\sigma\cdot\underline{A} = \frac{1}{r^2}\underline{\sigma}\cdot\underline{r}\,(\underline{r}\cdot\underline{A} + i\underline{\sigma}\cdot\underline{r}\times\underline{A}) \quad -(7)$$

2) using: $\frac{1}{r^2}\,\underline{\sigma}\cdot\underline{r}\;\underline{\sigma}\cdot\underline{r} = 1$ — (8)

it follows ~~that~~:

$$\underline{\sigma}\cdot\underline{p}\;\underline{\sigma}\cdot\underline{A} = \left[\left(\underline{r}\cdot\underline{p} + i\underline{\sigma}\cdot\underline{L}\right)\left(\underline{r}\cdot\underline{A} + i\underline{\sigma}\cdot(\underline{r}\times\underline{A})\right)\right]/r^2$$

$$= \frac{1}{r^2}\Big(\underline{r}\cdot\underline{p}\,\underline{r}\cdot\underline{A} + i\underline{\sigma}\cdot\underline{L}\,\underline{r}\cdot\underline{A} + i\underline{r}\cdot\underline{p}\;\underline{\sigma}\cdot\underline{r}\times\underline{A} - \underline{\sigma}\cdot\underline{L}\;\underline{\sigma}\cdot(\underline{r}\times\underline{A})\Big) \quad -(9)$$

So
$$\boxed{\hat{H}_{12} = \frac{e}{2mr^2}\,\underline{\sigma}\cdot\underline{L}\;\underline{\sigma}\cdot(\underline{r}\times\underline{A}) + \cdots} \quad -(10)$$

This gives an entirely new type of ESR, NMR and MRI.

In standard physics:

$$\underline{B} = \underline{\nabla}\times\underline{A}\,, \quad \underline{A} = \frac{1}{2}\underline{B}\times\underline{r} \quad -(11)$$

so:
$$\hat{H}_{12} = \frac{e}{4mr^2}\,\underline{\sigma}\cdot\underline{L}\;\underline{\sigma}\cdot\left(\underline{r}\times(\underline{B}\times\underline{r})\right) + \cdots \quad -(12)$$

where
$$\underline{r}\times(\underline{B}\times\underline{r}) = r^2\underline{B} - \underline{r}\,(\underline{B}\cdot\underline{r}) \quad -(13)$$

Therefore we arrive at a result of great utility:

3)
$$\boxed{\hat{H}_{12} = \frac{e}{4m} \underline{\sigma} \cdot \underline{L}\, \underline{\sigma} \cdot \underline{B} + \cdots} \quad -(14)$$

On average:

$$\boxed{\hat{H}_{12} = \frac{e}{4m} \underline{\sigma} \cdot \underline{L}\, \underline{\sigma} \cdot \underline{B} + \cdots} \quad -(15)$$

This is a new type of Zeeman effect, ESR, NMR and MRI and a new type of spin orbit coupling considered into one hamiltonian. Writing it out in full:

$$\hat{H}_{12} \phi = \frac{e}{4m} \underline{\sigma} \cdot \underline{B}\, \underline{\sigma} \cdot \underline{L}\, \phi \quad -(16)$$

In quantum mechanics:

$$\hat{\underline{S}} = \frac{1}{2} \hbar \hat{\underline{\sigma}} \quad -(17)$$

but the $\hat{H}_{12}$ hamiltonian is a classical function multiplied by the wave function ϕ.

When acting on a wave function:

$$\hat{H}_{12} \phi = \frac{e}{4m} \underline{\sigma} \cdot \underline{B} \left(\hat{\underline{\sigma}} \cdot \hat{\underline{L}}\, \phi \right) \quad -(18)$$

t)

$$= \frac{e}{4m} \underline{\sigma} \cdot \underline{B} \cdot \frac{1}{2} \left(J^2 - L^2 - S^2 \right) \phi$$

so the final result is:

$$\hat{H}_{12} \phi = \frac{e}{8m} \underline{\sigma} \cdot \underline{B} \left(J^2 - L^2 - S^2 \right) \phi \quad -(19)$$

The interaction energy is:

$$\boxed{E = \frac{e}{8m} \left(J^2 - L^2 - S^2 \right) \underline{\sigma} \cdot \underline{B}} \quad -(20)$$

where J, L and S are quantum numbers in atoms or molecules. The ESR resonance frequency is:

$$\omega = \frac{e}{4\hbar m} \left(J^2 - L^2 - S^2 \right) B \quad -(21)$$

giving a completely new type of ESR.

There will also be a completely new type of NMR