249 (B4): Spin Orbit Coupling with the Zeeman Effect

Consider the classical kinetic energy of an electron:

$$H = \frac{1}{2m} p^2 . \quad -(1)$$

In the minimal prescription, consider the interaction of this electron with the vector potential in the minimal prescription:

$$H = \frac{1}{2m} (\underline{p} - e\underline{A}) \cdot (\underline{p} - e\underline{A}) \quad -(2)$$

$$= \frac{p^2}{2m} - \frac{e}{2m}(\underline{p} \cdot \underline{A} + \underline{A} \cdot \underline{p}) + \frac{e^2}{2m} A^2$$

For a uniform magnetic field:

$$\underline{A} = \frac{1}{2} \underline{B} \times \underline{r} . \quad -(3)$$

Consider the Hamiltonian:

$$H_1 = -\frac{e}{4m} \left(\underline{p} \cdot (\underline{B} \times \underline{r}) + (\underline{B} \times \underline{r}) \cdot \underline{p} \right) \quad -(4)$$

By vector algebra:

$$\underline{p} \times (\underline{B} \times \underline{r}) = \underline{B} \cdot (\underline{r} \times \underline{p}) = \underline{B} \cdot \underline{L} \quad -(5)$$

where the orbital angular momentum is:

$$\underline{L} = \underline{r} \times \underline{p} \quad -(6)$$

So

$$\boxed{H_1 = -\frac{e}{2m} \underline{L} \cdot \underline{B}} \quad -(7)$$

2) Here $e/(2m)$ is the gyromagnetic ratio and the magnetic dipole moment is:

$$\underline{m} = \frac{e}{2m}\underline{L} \quad -(8)$$

So

$$\boxed{H_1 = -\underline{m}\cdot\underline{B}} \quad -(9)$$

The classical hamiltonian responsible for eq. (9) is:

$$H_1 = -\frac{e}{2m}\left(\underline{p}\cdot\underline{A} + \underline{A}\cdot\underline{p}\right). \quad -(10)$$

Now consider eq. (10) in the SU(2) basis:

$$H_1 = -\frac{e}{2m}\left(\underline{\sigma}\cdot\underline{p}\,\underline{\sigma}\cdot\underline{A} + \underline{\sigma}\cdot\underline{A}\,\underline{\sigma}\cdot\underline{p}\right). \quad -(11)$$

Using Pauli algebra:

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

$$\underline{\sigma}\cdot\underline{A}\,\underline{\sigma}\cdot\underline{p} = \underline{A}\cdot\underline{p} + i\,\underline{\sigma}\cdot\underline{A}\times\underline{p} \quad -(13)$$

So the same result (9) is obtained.

However, as in note 249(3) eqs. (6) and (7):

$$\underline{\sigma}\cdot\underline{p} = \frac{1}{r^2}\underline{\sigma}\cdot\underline{r}\left(\underline{r}\cdot\underline{p} + i\,\underline{\sigma}\cdot\underline{L}\right) \quad -(14)$$

$$\underline{\sigma}\cdot\underline{A} = \frac{1}{r^2}\underline{\sigma}\cdot\underline{r}\left(\underline{r}\cdot\underline{A} + i\,\underline{\sigma}\cdot\underline{r}\times\underline{A}\right). \quad -(15)$$

Using

$$\frac{1}{r^2}\underline{\sigma}\cdot\underline{r}\,\underline{\sigma}\cdot\underline{r} = 1 \quad -(16)$$

3) it follows that:

$$\underline{\sigma}\cdot\underline{p}\,\underline{\sigma}\cdot\underline{A} = \frac{1}{r^2}\Big(\underline{r}\cdot\underline{p}\,\underline{r}\cdot\underline{A} + i\underline{\sigma}\cdot\underline{L}\,\underline{r}\cdot\underline{A} + i\underline{r}\cdot\underline{p}\,\underline{\sigma}\cdot\underline{r}\times\underline{A} - \underline{\sigma}\cdot\underline{L}\,\underline{\sigma}\cdot\underline{r}\times\underline{A}\Big) \quad -(17)$$

From comparison of the real and imaginary parts of eqs. (12) and (17):

$$-\underline{p}\cdot\underline{A} = \frac{1}{r^2}\Big(\underline{r}\cdot\underline{p}\,\underline{r}\cdot\underline{A} - \underline{\sigma}\cdot\underline{L}\,\underline{\sigma}\cdot\underline{r}\times\underline{A}\Big) \quad -(18)$$

$$\underline{\sigma}\cdot\underline{p}\times\underline{A} = \underline{\sigma}\cdot\underline{L}\,\underline{r}\cdot\underline{A} + \underline{r}\cdot\underline{p}\,\underline{\sigma}\cdot\underline{r}\times\underline{A} \quad -(19)$$

In eq. (18) and (19) it follows that:

$$\underset{\sim}{r}\cdot\underline{A} = \frac{1}{2}\,\underset{\sim}{r}\cdot\underline{B}\times\underline{r} = \frac{1}{2}\,\underline{B}\cdot\underline{r}\times\underline{r} = \underline{0} \quad -(20)$$

So

$$\boxed{\underline{p}\cdot\underline{A} = -\frac{1}{r^2}\,\underline{\sigma}\cdot\underline{L}\,\underline{\sigma}\cdot\underline{r}\times\underline{A}} \quad -(21)$$

$$\boxed{\underline{\sigma}\cdot\underline{p}\times\underline{A} = \underline{r}\cdot\underline{p}\,\underline{\sigma}\cdot\underline{r}\times\underline{A}} \quad -(22)$$

Therefore the Hamiltonian (10) is:

$$H_1 = -\frac{e}{m}\,\underline{p}\cdot\underline{A} \quad -(23)$$

$$= \frac{e}{mr^2}\,\underline{\sigma}\cdot\underline{L}\,\underline{\sigma}\cdot\underline{r}\times\underline{A}$$

$$= -\frac{e}{2m}\,\underline{L}\cdot\underline{B}$$

$$= -\underline{m}_D\cdot\underline{B}$$

Finally use eqs. (3) and (23) to find:

$$H_1 = \frac{e}{2mr^2}\,\underline{\sigma}\cdot\underline{L}\;\underline{\sigma}\cdot\underline{r}\times(\underline{B}\times\underline{r}) \quad -(24)$$

$$= \frac{e}{2mr^2}\,\underline{\sigma}\cdot\underline{L}\;\underline{\sigma}\cdot\left(r^2\underline{B} - \underset{\sim}{r}(\underline{B}\cdot\underline{r})\right)$$

$$= \frac{e}{2m}\left(\underline{\sigma}\cdot\underline{L}\;\underline{\sigma}\cdot\underline{B} - \frac{\underset{\sim}{r}}{r^2}\,\underline{B}\cdot\underline{r}\right)$$

$$= -\underline{m}_D\cdot\underline{B}$$

It can be seen that the hamiltonian responsible for the Zeeman effect has been developed into a hamiltonian that gives electron spin resonance. The usual hamiltonian for electron spin resonance is:

$$H_2 = -\frac{e\hbar}{2m}\,\underline{\sigma}\cdot\underline{B} \quad -(25)$$

ESR from eq. (25) occurs at

$$\omega_2 = \frac{eB}{m} \quad -(26)$$

ESR from eq. (24) occurs at:

$$\omega_1 = \frac{e\,\sigma \cdot \underline{L}\,B}{\cancel{2}\hbar m} = \frac{2 m_D B}{\cancel{2}\hbar} \quad - (27)$$

Therefore the new ESOR phenomenon is defined by the resonance frequency:

$$\boxed{\omega_1 = \frac{2 m_D B}{\cancel{2}\hbar}} \quad - (28)$$

where m_D is the magnetic dipole moment:

$$m_D = \frac{eL}{2m} \quad - (29)$$

This is a purely classical calculation, so electron ~~spin~~ resonance occurs for any orbital angular momentum. This is named electron orbital resonance, (EOR). If the angular momentum is that of an atom or molecule its observable magnitude is

$$L_Z = m_L \hbar \quad - (30)$$

where

$$m_L = -L, \ldots, L \quad - (31)$$

and

$$L = 0, \ldots, n-1 \quad - (32)$$

where n is the principal quantum number.

If the relevant hamiltonian:

6)

$$H_2 = \frac{e}{2\cancel{4}m} \underline{\sigma} \cdot \underline{L} \; \underline{\sigma} \cdot \underline{B} \quad - (33)$$

is regarded as a spin - orbit hamiltonian then the spin operator is:

$$\underline{\hat{S}} = \frac{1}{2} \hbar \underline{\hat{\sigma}} \quad - (34)$$

So

$$\hat{H}_2 \psi = \frac{e}{\cancel{2}m\hbar} \underline{\sigma} \cdot \underline{B} \; \underline{\hat{S}} \cdot \underline{\hat{L}} \psi \quad - (35)$$

$$= \frac{eB\hbar}{\cancel{2}m} \left(\hat{J}^2 - \hat{L}^2 - \hat{S}^2 \right) \psi$$

So electron orbital resonance occurs at:

$$\boxed{\omega_1 = \frac{e}{\cancel{2}m} \left(J(J+1) - L(L+1) - S(S+1) \right) B} \quad - (36)$$

The Complete Hamiltonian

This is:

$$H = - \frac{e}{2m} \underline{L} \cdot \underline{B} - \frac{e\hbar}{2m} \underline{\sigma} \cdot \underline{B}$$

$$= \frac{e}{2m} \left(\underline{\sigma} \cdot \underline{L} \; \underline{\sigma} \cdot \underline{B} - \frac{\underline{r}}{r^2} \underline{B} \cdot \underline{r} \right) - \frac{e\hbar}{2m} \underline{\sigma} \cdot \underline{B} \quad - (37)$$

and gives rise to many new effects
