31(5): Simplified Derivation of Relativistic Zeeman Splitting

Start with the relativistic classical hamiltonian:

$$H_1 = -\frac{e}{2m}\left(1-\frac{p_0^2}{m^2c^2}\right)^{-1/2}\underline{L_0}\cdot\underline{B} \quad -(1)$$

$$\sim -\frac{e}{2m}\left(1+\frac{1}{2}\frac{p_0^2}{m^2c^2}\right)\underline{L_0}\cdot\underline{B}.$$

Quantize by assuming that:

$$\hat{H}_1\phi = -\frac{e}{2m}\left(1+\frac{1}{2}\frac{p_0^2}{m^2c^2}\right)\underline{B}\cdot\underline{\hat{L}_0}\phi \quad -(2)$$

in which $\hat{L}_0$ is an operator and p_0^2 a function. If $\underline{B}$ is aligned in the Z axis:

$$\hat{H}_1\phi = -\frac{e}{2m}\left(1+\frac{1}{2}\frac{p_0^2}{m^2c^2}\right)B_Z\hat{L}_{0Z}\phi \quad -(3)$$

where

$$\hat{L}_{0Z}\phi = m_L\hbar\phi \quad -(4)$$

with

$$m_L = -L,\dots,L \quad -(5)$$

So the energy levels are:

$$H_1 = \langle\hat{H}_1\rangle = -\frac{e\hbar}{2m}\left(1+\frac{1}{2}\frac{p_0^2}{m^2c^2}\right)m_L \quad -(6)$$

Finally use:

2)

$$\frac{p_0^2}{2m} = \left\langle \frac{\hat{p}_0^2}{2m} \right\rangle \quad -(7)$$

So
$$H_1 = -\frac{e\hbar}{2m} m_L \left(1 + \frac{1}{mc^2} \left\langle \frac{\hat{p}_0^2}{2m} \right\rangle \right) \quad -(8)$$

$$= -\frac{e\hbar}{2m} m_L \left(1 - \frac{\hbar^2}{4m^2c^2} \int \psi^* \nabla^2 \psi \, d\tau \right)$$

In a rigorous development, ψ is the relativistic wave function of an atom or molecule.

In a rough first approximation, the non-relativistic wave functions of atomic H are used:

$$\left\langle \frac{\hat{p}_0^2}{2m} \right\rangle = \frac{m e^4}{32\pi^2 \epsilon_0^2 \hbar^2 n^2} \quad -(9)$$

So:
$$\boxed{H_1 = -\frac{e\hbar}{2m} m_L \left(1 + \left(\frac{e^4}{32\pi^2 \epsilon_0^2 \hbar^2 c^2} \right) \frac{1}{n^2} \right)} \quad -(10)$$

This result can be expressed as:

$$H_1 = -\frac{e\hbar}{2m} m_L \left(1 + \frac{1}{2} \left(\frac{\lambda_c}{a_0} \right) \frac{\alpha}{n^2} \right) \quad -(11)$$

where:

3) $$\lambda_c = \frac{\hbar}{mc} = 3.861591 \times 10^{-13}\, m \quad -(12)$$

is the Compton wavelength of the electron,

$$a_0 = \frac{4\pi\epsilon_0\hbar^2}{me^2} = 5.29177 \times 10^{-11}\, m \quad -(13)$$

is the Bohr radius, and

$$\alpha = \frac{e^2}{4\pi\hbar c\epsilon_0} = 0.007297351 \quad -(14)$$

is the fine structure constant.

So:

$$\boxed{H_1 = \langle H_1 \rangle = -\frac{e\hbar}{2m} m_L B_Z \left(1 + \frac{2.662567 \times 10^{-5}}{n^2} \right)} \quad -(15)$$

Except for a sign change, this is the result used in Note 331(3) to demonstrate relativistic Zeeman splitting when the Dirac approximation is no longer used.