253(8): Relativistic Corrections in the Operator Representation

Start with the relativistically corrected operator rep.:

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

where:

$$v^2 = \frac{1}{m^2}\,\underline{\sigma}\cdot(\underline{p}-e\underline{A})\,\underline{\sigma}\cdot(\underline{p}-e\underline{A}) \quad -(2)$$

Consider the term:

$$H_1\phi = -\frac{1}{8m^3c^2}\left(\underline{\sigma}\cdot(\underline{p}-e\underline{A})\underline{\sigma}\cdot(\underline{p}-e\underline{A})\underline{\sigma}\cdot(\underline{p}-e\underline{A})\underline{\sigma}\cdot(\underline{p}-e\underline{A})\right)\phi \quad -(3)$$

The operator representation is defined by

$$\underline{p} \rightarrow -i\hbar\underline{\nabla} \quad -(4)$$

From previous notes:

$$\frac{1}{2m}\left(\underline{\sigma}\cdot(-i\hbar\underline{\nabla}-e\underline{A})\underline{\sigma}\cdot(-i\hbar\underline{\nabla}-e\underline{A})\right)\phi$$

$$= -\frac{e\hbar}{2m}\underline{\sigma}\cdot\underline{B}\phi + \ldots \quad -(5)$$

So:

$$H_1\phi = -\frac{1}{m^2c^2}\left(\left(\underline{\sigma}\cdot(-i\hbar\underline{\nabla}-e\underline{A})\underline{\sigma}\cdot(-i\hbar\underline{\nabla}-e\underline{A})\right)\left(-\frac{e\hbar}{2m}\underline{\sigma}\cdot\underline{B}\phi\right)\right.$$

$$\left. + \ldots\right) \quad -(6)$$

2)

$$= \frac{e\hbar}{8m^3c^2}\left(-\hbar^2\nabla^2 + ie\hbar\left(\underline{\nabla}\cdot\underline{A} + \underline{A}\cdot\underline{\nabla}\right) + e^2A^2\right)\left(\underline{\sigma}\cdot\left(\underline{B}\psi\right)\right) \quad -(7)$$

Therefore:

$$\text{Real } H_1\psi = -\frac{e\hbar^3}{8m^3c^2}\underline{\nabla}\cdot\underline{\nabla}\left(\underline{\sigma}\cdot\underline{B}\psi\right) \quad -(8)$$

$$+ \frac{e^3\hbar A^2}{8m^3c^2}\underline{\sigma}\cdot\underline{B}\psi$$

For a uniform magnetic field:

$$\underline{A} = \frac{1}{2}\underline{B}\times\underline{r} \quad -(9)$$

so

$$A^2 = \frac{1}{4}\underline{B}\times\underline{r}\cdot\underline{B}\times\underline{r} \quad -(10)$$

$$= \frac{1}{4}\left(B^2 r^2 - \left(\underline{B}\cdot\underline{r}\right)\left(\underline{B}\cdot\underline{r}\right)\right)$$

For a Z axis magnetic field:

$$\underline{\sigma}\cdot\underline{B}\psi = \sigma_Z B_Z\psi \quad -(11)$$

$$A^2 = \frac{1}{4}B_Z^2\left(r^2 - Z^2\right) \quad -(12)$$

$$= \frac{1}{4}B_Z^2 r^2\left(1-\cos^2\theta\right)$$

in spherical polar coordinates.

3) So:

$$\text{Real } H_1 \phi = H_{11}\phi + H_{12}\phi \quad -(13)$$

where

$$H_{11}\phi = -\frac{e\hbar^3}{8m^3c^2}\nabla^2(\sigma_Z B_Z \phi)$$

$$= -\frac{e\hbar^3 \sigma_Z B_Z}{8m^3c^2}\nabla^2\phi \quad -(14)$$

and

$$H_{12}\phi = \frac{e^3\hbar \,\sigma_Z B_Z^3}{32m^3c^2} r^2(1-\cos^2\theta)\phi \quad -(15)$$

where

$$\sigma_Z = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} \quad -(16)$$

Resonance occurs between states of $\sigma_Z$.

The energy expectation values are:

$$E_{11} = -\frac{e\hbar^3 \sigma_Z B_Z}{8m^3c^2}\int \phi^* \nabla^2 \phi \, d\tau \quad -(17)$$

$$E_{12} = \frac{e^3\hbar \,\sigma_Z B_Z^3}{32m^3c^2}\int \phi^* r^2(1-\cos^2\theta)\phi \, d\tau \quad -(18)$$

These are relativistic corrections to the ESR energy:

4)

$$E_0 = -\frac{e\hbar}{2m} \sigma_Z B_Z \quad -(19)$$

The resonance frequencies are:

$$\omega_0 = \frac{eB_Z}{m} \quad -(20)$$

$$\omega_{11} = \frac{e\hbar^2 B_Z}{4m^3c^2} \int \psi^* \nabla^2 \psi \, d\tau \quad -(21)$$

and

$$\omega_{12} = \frac{e^3 B_Z^3}{16m^3c^2} \int \psi^* r^2 (1-\cos^2\theta) \psi \, d\tau \quad -(22)$$

The relativistic resonance frequencies depend on the orbital in which the electron is situated. Eqs. (21) and (22) can be worked out for the hydrogenic wave functions.

<u>Units Check</u>

The units of $eB_Z/m$ are $s^{-1}$, so:

$$\omega_{11} = \frac{J^2 s^2 s^{-1} m^{-2}}{kgm^2 m^2 s^{-2}} = \frac{J^2 s^{-1}}{kgm^2 m^4 s^{-4}} = s^{-1}$$

$$\omega_{12} = \frac{s^{-3} m^2}{m^2 s^{-2}} = s^{-1}$$