178(2): First Approximation to the Force Eigenvalues of the ESR and NMR Effects.

The relevant approximation to the fermion equation is:

$$\hat{H}_{rel}\,\phi = E_{rel}\,\phi \quad -(1)$$

in which:

$$\hat{H}_{rel} = mc^2 + V + \frac{\hat{p}^2}{2m} - \frac{e\hbar}{2m}\,\underline{\sigma}\cdot\underline{B}. \quad -(2)$$

Following Ryder, "Quantum Field Theory" (Cambridge Univ. Press, 1996) the non-relativistic limit is defined as:

$$(\hat{H}_{rel} - mc^2)\,\phi = (E_{rel} - mc^2)\,\phi \quad -(3)$$

i.e.

$$\hat{H}\,\phi = E\,\phi \quad -(4)$$

where

$$\hat{H} = \frac{\hat{p}^2}{2m} + V - \frac{e\hbar}{2m}\,\underline{\sigma}\cdot\underline{B}. \quad -(5)$$

If $\underline{B}$ is aligned in the Z direction then:

$$\underline{\sigma}\cdot\underline{B} = \begin{bmatrix} B_Z & 0 \\ 0 & -B_Z \end{bmatrix} \quad -(6)$$

So:

$$\hat{H}_+ = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V - \frac{e\hbar}{2m}B_Z, \quad -(7)$$

$$\hat{H}_- = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V + \frac{e\hbar}{2m}B_Z. \quad -(8)$$

2) In the first approximation, and for a weak magnetic field B_Z, the wavefunction ϕ can be taken to be those of the H atom, so there are two force equations:

$$\left(\hat{H}_+ - E\right)\frac{d\phi}{dx} = F_+ \phi \quad -(9)$$

and

$$\left(\hat{H}_- - E\right)\frac{d\phi}{dx} = F_- \phi \quad -(10)$$

so these equations can be evaluated by computer algebra to give F_+ and F_- for every orbital.