RelCorrection

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Relativistic Correction

$$T = E_{TOT} - mc^2 = \sqrt{m^2c^4 + p^2c^2} - mc^2 =$$

$$= mc^2\sqrt{1 + \frac{p^2}{m^2c^2}} - mc^2 = //$$

$$\sqrt{1+x} \approx 1 + \frac{1}{2}x - \frac{1}{8}x^2$$

$$T = mc^2\left(1 + \frac{1}{2}\frac{p^2}{m^2c^2} - \frac{1}{8}\frac{p^4}{m^4c^4}\right) - mc^2 =$$

$$= \frac{p^2}{2m} - \frac{1}{8}\frac{p^4}{m^3c^2} \sim \frac{p^2}{c^2} \sim \frac{v^2}{c^2}$$

Relativistic Correction

$$\Rightarrow H_0 = \frac{p^2}{2m} - \frac{Ze^2}{r}$$

$$H = \underbrace{\frac{p^2}{2m}}_{T_0} + H_{Rel} - \frac{Ze^2}{r}$$

$$H_{Rel} = -\frac{1}{8}\frac{p^4}{m^3c^2} = -\frac{1}{2m}\frac{p^4}{4m^2c^2} = -\frac{1}{2mc^2}T_0^2$$

$$\boxed{H_{Rel} = -\frac{1}{2mc^2}T_0^2}$$

In Natural Units

$$\hat{H}_{Rel} = -\frac{1}{2m}\hat{T}_0^2 \equiv \hat{H}_{Kin}$$

1st order Correction

$$\Delta_{Kin} = \langle \phi^{nl}_{jm} | \hat{H}_{Kin} | \phi^{nl}_{jm} \rangle =$$

$$= -\frac{1}{2m}\langle \phi^{nl}_{jm} | H_0 - V |^2 \phi^{nl}_{jm} \rangle = -\frac{1}{2}\langle \phi | H_0^2 - H_0V - VH_0 + V^2 | \phi \rangle$$

1) $\boxed{\langle \phi^{nl}_{jm} | H_0^2 | \phi^{nl}_{jm} \rangle = E_n^{0\,2}}$

2) $\langle \phi | H_0 V | \phi \rangle = \langle \phi | H_0 | \phi \rangle \langle \phi | V | \phi \rangle$

$$= E_n^0 \langle \phi | V | \phi \rangle$$

$\langle \phi | V | \phi \rangle = ?$

Virial Theorem

$$2\langle \phi | T | \phi \rangle = \langle \phi | \vec{r} \cdot \vec{\nabla} V | \phi \rangle$$

$$\vec{\nabla} \hat{V} = -Z\alpha \nabla \frac{1}{r} = Z\alpha \frac{\vec{r}}{r^3}$$

$$\vec{r} \cdot \vec{\nabla} V = \frac{Z\alpha}{r}$$

$$\underbrace{2\langle \phi | T | \phi \rangle}_{-2\langle V \rangle} = -\langle \phi | V | \phi \rangle \quad 2\langle V \rangle$$

$$2\langle \phi | \overbrace{T + V_0}^{H_0} | \phi \rangle = \langle \phi | V | \phi \rangle$$

$$2\langle \phi | H_0 | \phi \rangle = \langle \phi | V | \phi \rangle$$

$$\langle \phi | V | \phi \rangle = 2E_n^0$$

$$\boxed{\langle \phi | H_0 V | \phi \rangle = 2E_n^{0\,2}}$$

3) $\langle \phi_0 | V H_0 | \rangle = \langle \phi_0 | H_0 V | \phi \rangle$

4) $\boxed{\langle \phi | V^2 | \phi \rangle} = -Z^2\alpha^2 \langle \phi | \frac{1}{r^2} | \phi \rangle =$

$$= \boxed{\frac{\alpha^4 m^2}{n^3(n+\frac{1}{2})}}$$

$$E_n^0 = -\frac{Z^2\alpha^2 m}{2n^2}$$

Combining 1) 2) 3) 4) Terms

$$\Delta_{kin} = -\frac{1}{2m}\Big(\underbrace{E_n^{0\,2} - 4E_n^{0\,2}}_{-3E_n^{0\,2}} + \frac{\alpha^4 m^2}{n^3(\ell+\frac{1}{2})} \Big) =$$

$$= -\frac{Z^4}{2m}\Big(-\frac{3\alpha^4 m^2}{4n^4} + \frac{\alpha^4 m^2}{n^3(\ell+\frac{1}{2})} \Big) =$$

$$= \frac{Z^4\alpha^4 m}{2n^4}\Big(\frac{3}{4} - \frac{n}{(\ell+\frac{1}{2})} \Big)$$

Fine Structure Constant

$$\Delta_{FS} = \Delta_{kin} + \Delta_{LS} =$$

$$\frac{Z^4\alpha^4 m}{4n^3 \ell(\ell+1)(\ell+\frac{1}{2})} \begin{pmatrix} \ell \\ -(1+\ell) \end{pmatrix} + \frac{Z^4\alpha^4 m}{2n^4}\Big(\frac{3}{4} - \frac{n}{(\ell+\frac{1}{2})} \Big)$$

$$= \frac{Z^4\alpha^4 m}{2n^4}\underbrace{\left(\frac{n}{2\ell(\ell+1)(\ell+\frac{1}{2})}\begin{pmatrix}\ell \\ -(1+\ell)\end{pmatrix} + \frac{3}{4} - \frac{n}{(\ell+\frac{1}{2})}\right)}_{\text{Term}}$$

a) if $j = \ell + \frac{1}{2}$ $\quad \ell = j - \frac{1}{2}$

$$\text{Term}^a = \left(\frac{n}{2(j-\frac{1}{2})(j+\frac{1}{2})j}\left(j-\frac{1}{2}\right) + \frac{3}{4} - \frac{n}{j}\right)$$

$$= \left(\frac{n}{2(j+\frac{1}{2})j} + \frac{3}{4} - \frac{n}{j}\right) = \left(\frac{3}{4} - n\left(\frac{\overset{2j}{2(j+\frac{1}{2})} - 1}{2j(j+\frac{1}{2})}\right)\right)$$

$$= \left(\frac{3}{4} - \frac{2n}{2j+1}\right)$$

b) if $j = \ell - \frac{1}{2}$ $\quad \ell = j + \frac{1}{2}$

$$\text{Term}^b = \left(\frac{-n\,(j+\frac{3}{2})}{2(j+\frac{1}{2})(j+\frac{3}{2})(j+1)} + \frac{3}{4} - \frac{n}{j+1}\right) =$$

$$= \left(\frac{-n}{2(j+\frac{1}{2})(j+1)} - \frac{n}{j+1} + \frac{3}{4}\right) = \left(\frac{-n\overset{2(j+1)}{(2j+1+1)}}{(2j+1)(j+1)} + \frac{3}{4}\right)$$

$$= \frac{3}{4} - \frac{2n}{2j+1} \longrightarrow$$ The same as $\text{Term}^{(a)}$

$\Rightarrow$ Therefore

$$\boxed{\Delta_{FS} = \frac{Z^4\alpha^4 m}{2n^4}\left(\frac{3}{4} - \frac{2n}{2j+1}\right)}$$

Splitting Depends on j

$2P_{\frac{1}{2}}$ $\quad 2P_{\frac{3}{2}}$ — Split $\qquad E_n = -\frac{Z^2\alpha^2 m}{2n^2}$

$2S_{\frac{1}{2}}$ $\quad 2P_{\frac{1}{2}}$ — not splitting

$\Rightarrow$ Fine Structure of Hydrogen Atom

$$\Delta_{FS} = \frac{\alpha^4 m}{2n^4}\left(\frac{3}{4} - \frac{2n}{2j+1}\right) \qquad \begin{matrix} j = \ell + \frac{1}{2} \\ j = \ell - \frac{1}{2}\end{matrix}$$

$\ell < n-1$

— Splitting between $j = \frac{1}{2}$ $\quad j = \frac{3}{2}$

$$\Delta_{FS}^{\frac{1}{2}} = \frac{\alpha^4 m}{2n^4}\left(\frac{3}{4} - n\right)$$

$$\Delta_{FS}^{\frac{3}{2}} = \frac{\alpha^4 m}{\ldots}\left(\frac{3}{\ldots} - \frac{n}{\ldots}\right)$$

$$\Delta_{FS} = -\frac{\alpha^4 m}{2n^3}\left(\frac{}{4} - \frac{}{2}\right)$$

$$\Delta_{FS}^{j=\frac{3}{2}} - \Delta_{FS}^{j=\frac{1}{2}} = \frac{\alpha^4 m}{2n^3}\,\frac{1}{2} = \frac{\alpha^4 m}{4n^3}$$

$\Rightarrow$ Splitting starts to appear at $n=2$

For $n=2$ $\quad \Delta_{FS}^{\frac{3}{2}-\frac{1}{2}} = \frac{\alpha^4 m}{32} = 4.528\times10^{-5}\,eV$

$\Rightarrow$ Excitation of $n=1 \to n=2$

$$\frac{\alpha^2 m}{2}\left(1-\frac{1}{4}\right) = \frac{3\alpha^2 m}{8} = 10.2\,eV$$

$\Rightarrow$ Energy Shift for $n=1$

$$\Delta_{FS}^{j=\frac{1}{2}}(n=1) = \frac{\alpha^4 m}{2}\left(\frac{3}{4}-1\right) = -\frac{\alpha^4 m}{2}\,\frac{1}{4} = -\frac{\alpha^4 m}{8}$$

$$\Delta_{FS}(n=1) = 1.13\times10^{-5}\,eV$$

$$E_g = -\frac{\alpha^2 m}{2} = 13.6\,eV$$