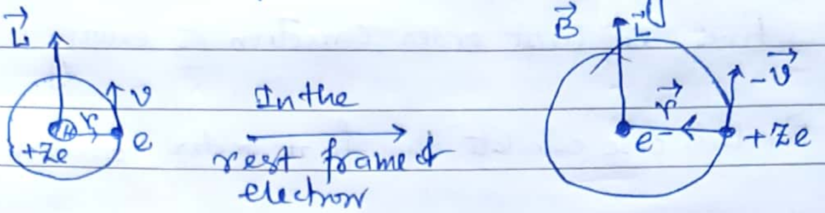
DR. Datta

E-Lecture-03 / PHS-201 A.

Application of perturbation theory: Fine Structure of H-atom.

The spin-orbit interaction between electron's spin moment and proton's orbital magnetic field ($\vec{B}$).

$$\vec{\mu}_s = -\frac{e\vec{S}}{2mc}$$



Magnetic field experienced by electron in the rest frame of electron by the proton

$$\vec{B} = -\frac{\vec{v}\times\vec{E}}{c} = -\frac{\vec{p}\times\vec{E}}{mc} = \frac{\vec{E}\times\vec{p}}{mc}$$

$$\vec{E} = -\vec{\nabla}\phi(r) = -\frac{1}{e}\vec{\nabla}V(r) = \frac{1}{e}\frac{\vec{r}}{r}\frac{dV}{dr}$$

$$\vec{B} = \frac{1}{emc}\frac{1}{r}\frac{dV}{dr}\vec{r}\times\vec{p} = \frac{1}{emc}\frac{1}{r}\frac{dV}{dr}\vec{L}$$

The spin-orbit coupling Hamiltonian is

$$H_{so} = -\vec{\mu}_s\cdot\vec{B} = \frac{e}{mc}\vec{S}\cdot\vec{B} = \frac{1}{m^2c^2r}\frac{dV}{dr}\vec{S}\cdot\vec{L}$$

This is calculated in the rest frame of electron. This frame is not inertial, for the electron accelarates in the circular orbits around the nucleus. For correct treatment we must transfrom in the rest frame of nucleus. Due to this $\frac{1}{2}$ factor comes.

$$H_{so} = \frac{1}{2m^2c^2}\left(\frac{1}{r}\frac{dV}{dr}\right)(\vec{S}\cdot\vec{L})$$

For H-atom $V(r) = -e^2/r \Rightarrow \frac{dV}{dr} = e^2/r^2$

$$H_{so} = \frac{e^2}{2m^2c^2}\left(\frac{1}{r^3}\right)\vec{S}\cdot\vec{L}$$

Total Hamiltonian

$$H = \frac{p^2}{2m} - \frac{e^2}{r} + \frac{e^2}{2m^2c^2r^3}(\vec{S}\cdot\vec{L}) = \hat{H}_0 + \hat{H}_{so}$$

Common eigenstate is $|n\,l\,j\,m_j\rangle$

[P.T.O]

$$E_{nljm_j} = E_n^{(0)} + \langle nljm_j | \hat{H}_{so} | nljm_j \rangle$$
$$= -\frac{e^2}{2a_0 n^2} + E_{so}^{(1)}$$

So $E_{so}^{(1)} = \langle nljm_j | \hat{H}_{so} | nljm_j \rangle$ | Now $\vec{L}\cdot\vec{S} = \frac{J^2 - L^2 - S^2}{2}$

$$= \frac{e^2\hbar^2}{4m^2c^2}\left[j(j+1) - l(l+1) - \frac{3}{4}\right] \underbrace{\langle nl | \frac{1}{r^3} | nl \rangle}_{\frac{2}{n^3 l(l+1)(2l+1)a_0^3}}$$

$$= \frac{e^2\hbar^2}{4m^2c^2}\left[\frac{j(j+1) - l(l+1) - 3/4}{n^3\, l(l+1)(2l+1)a_0^3}\right]$$

$$E_{so}^{(1)} = \frac{|E_n^{(0)}|\alpha^2}{n}\left[\frac{j(j+1) - l(l+1) - 3/4}{l(l+1)(2l+1)}\right]; \text{ where } \underset{\text{fine structure.}}{\alpha} = \frac{e^2}{\hbar c} = \frac{\hbar}{m_e c a_0}$$

Relativistic correction

K.E of electron $T = \sqrt{p^2c^2 + m^2c^4} - mc^2$
$$\simeq \frac{p^2}{2m} - \frac{p^4}{8m^3c^2} + \cdots\cdots$$

$$H = \frac{p^2}{2m} - \frac{p^4}{8m^3c^2} - \frac{e^2}{r} = \hat{H}_0 + \hat{H}_R$$

where $\hat{H}_0 = \frac{p^2}{2m} - \frac{e^2}{r}$ and $\hat{H}_R = -\frac{\hat{p}^4}{8m^3c^2}$

Now $E_R^{(1)} = \langle nljm_j | \hat{H}_R | nljm_j \rangle$
$$= -\frac{1}{8m^3c^2}\langle nljm_j | \hat{p}^4 | nljm_j \rangle$$
$$= \frac{\alpha^4 m^4 c^4}{n^4}\left(\frac{8n}{2l+1} - 3\right)$$
$$E_R^{(1)} = -\frac{\alpha^2 |E_n^0|}{4n^2}\left(\frac{8n}{2l+1} - 3\right)$$

For H-like atom $E_n = Z^2\left(E_n^{(0)} + E_R^{(1)}\right)$
$$\therefore E_n = Z^2 E_n^{(0)}\left[1 + \frac{\alpha^2}{n}\left(\frac{2}{2l+1} - \frac{3}{4n}\right)\right]$$

[P.T.O]

So the fine structure $E_{FS}^{(1)} = E_{so}^{(1)} + E_{R}^{(1)}$

$$E_{FS}^{(1)} = \frac{\alpha^4 mc^2}{2n^3}\left[\frac{j(j+1) - l(l+1) - 3/4}{l(l+1)(2l+1)}\right] - \frac{\alpha^4 mc^2}{8n^4}\left[\frac{8n}{2l+1} - 3\right].$$

Here values of $j = l \pm \frac{1}{2}$

for $j = l + \frac{1}{2}$, or, $l = j - \frac{1}{2}$

$$E_{FS}^{(1)} = \frac{\alpha^4 mc^2}{8n^4}\left[3 - \frac{4n}{j+\frac{1}{2}}\right]$$

if $j = l - \frac{1}{2}$, or, $l = j + \frac{1}{2}$

$$E_{FS}^{(1)} = \frac{\alpha^4 mc^2}{8n^4}\left[3 - \frac{4n}{j+\frac{1}{2}}\right]$$

Hence $E_{FS}^{(1)} = E_{so}^{(1)} + E_{R}^{(1)}$

$$= \frac{\alpha^4 mc^2}{8n^4}\left[3 - \frac{4n}{j+\frac{1}{2}}\right]$$

$$E_{FS}^{(1)} = \frac{\alpha^2 E_n^{(0)}}{4n^2}\left[\frac{4n}{j+\frac{1}{2}} - 3\right]; \quad \text{where } E_n^{(0)} = -\frac{\alpha^2 mc^2}{2n^2}$$

Now: $\hat{H} = \hat{H}_0 + \hat{H}_{FS}$

$$= \hat{H}_0 + \hat{H}_{so} + \hat{H}_R$$

$$= \left(\frac{p^2}{2m} - \frac{e^2}{r}\right) + \left(\frac{e^2}{2m^2c^2r^3}\vec{S}\cdot\vec{L} - \frac{p^4}{8m^3c^2}\right)$$

$$E_{nj} = E_n^{(0)} + E_{FS}^{(1)} = E_n^{(0)}\left(1 + \frac{\alpha^2}{4n^2}\left(\frac{4n}{j+\frac{1}{2}} - 3\right)\right)$$

Now, in addition to the fine structure there is another effect called hyperfine structure.

This arises due to interaction between magnetic moment of electron and nucleus.

[P.T.O]

$$\vec{\mu}_p = g_p \frac{e}{2m_p} \vec{S}_p \; ; \quad \vec{\mu}_e = -\frac{e}{m_e} \vec{S}_e$$

g_p: gyromagnetic ratio of proton.

Now magnetic field due to magnetic dipole of moment $\vec{\mu}$ is

$$\vec{B} = \frac{\mu_0}{4\pi r^3}\left[3(\vec{\mu}\cdot\hat{r})\hat{r} - \vec{\mu}\right] + \underbrace{\frac{2\mu_0}{3}\vec{\mu}\,\delta^{(3)}(\vec{r})}$$

We are not familiar with this term, but this can be derived considering dipole as spining charged shell where taking radius $R \to 0$ and charge $(q) \to \infty$.

Now the hyperfine Hamiltonian of electron in the proton's magnetic field is

$$\hat{H}_{HF} = -\vec{\mu}_e \cdot \vec{B}$$

$$\Rightarrow \hat{H}_{HF} = \frac{\mu_0 g_p e^2}{8\pi m_p m_e}\left[\frac{3(\vec{S}_p\cdot\hat{r})(\vec{S}_e\cdot\hat{r}) - \vec{S}_p\cdot\vec{S}_e}{r^3}\right] + \frac{\mu_0 g_p e^2}{3 m_p m_e}\vec{S}_p\cdot\vec{S}_e\,\delta^{(3)}(\vec{r})$$

$$E^{(1)}_{HF} = \frac{\mu_0 g_p e^2}{8\pi m_p m_e}\left\langle\frac{3(\vec{S}_p\cdot\hat{r})(\vec{S}_e\cdot\hat{r}) - \vec{S}_p\cdot\vec{S}_e}{r^3}\right\rangle + \frac{\mu_0 g_p e^2}{3 m_p m_e}\langle\vec{S}_p\cdot\vec{S}_e\rangle\,|\psi(0)|^2$$

If we evaluate $E^{(1)}_{HF}$ in the ground state ~~the~~ $(l=0)$ then the first term vanish; the contribution from second term is

$$E^{(1)}_{HF} = \frac{\mu_0 g_p e^2}{3\pi m_p m_e a^3}\langle\vec{S}_p\cdot\vec{S}_e\rangle \; ; \quad \text{As } |\psi(0)|^2 = \frac{1}{\pi a^3}.$$

Where $\vec{S}_p\cdot\vec{S}_e = \dfrac{S^2 - S_p^2 - S_e^2}{2}$ where $S_e^2 = S_p^2 = \dfrac{3\hbar^2}{4}$ and

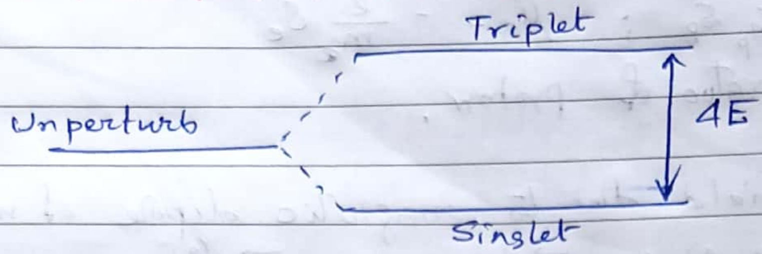
$$S^2 = \begin{cases} 2\hbar^2 ; & s=1 \text{ (triplet)} \\ 0\hbar^2 ; & s=0 \text{ (singlet)}. \end{cases}$$

$$E^{(1)}_{HF} = \frac{4 g_p \hbar^4}{3 m_p m_e^2 c^2 a^4}\begin{cases} +\frac{1}{4} ; & \text{triplet} \\ \frac{3}{4} ; & \text{singlet} \end{cases}$$

The spin-spin coupling breaks the degeneracy for ground state and ~~shifting~~ lifting the triplet state and depressing the singlet. The energy gap

$$\Delta E = \frac{4 g_p \hbar^4}{3 m_p m_e^2 c^2 a^4} = 5.88 \times 10^{-6}\,\text{eV}.$$

[P.T.O]



The frequency of emitted photon from triplet to singlet is $\nu = \frac{E}{h} = 1420$ MHz.
and wavelength $\lambda = \frac{c}{\nu} = 21$ cm, which is in microwave region. This famous 21 cm line → the most of the information we possess about intersteller hydrozen cloud had its origin in radio astronomy by study this 21 cm line.

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