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Time: 01pm

MPHYCC10 – 13

Quantum mechanical relativity correction:

Relativistic effect is equally important as it produces energy shift comparable to spin-orbit interaction (In Hydrogen atom)

$$H = K + V \quad \ldots \quad (1)$$

K = relativistic kinetic energy, V = potential energy

$$K = (p^2c^2 + m_0^2c^4)^{1/2} - m_0c^2$$

P = momentum, m_0 = rest mass of electron.

H = Hamiltonian

$$H = (p^2c^2 + m_0^2c^4)^{1/2} - m_0c^2 + V$$

$$= m_0c^2\left[1 + \frac{p^2}{m_0^2c^2}\right]^{1/2} - m_0c^2 + V$$

$$= m_0c^2\left[1 + \frac{1}{2}\frac{p^2}{m_0^2c^2} - \frac{1}{8}\frac{p^4}{m_0^4c^4} + \cdots\right] - m_0c^2 + V$$

$$= m_0c^2 + \frac{p^2}{2m_0} - \frac{p^4}{8m_0^3c^2} + \cdots - m_0c^2 + V$$

$$H = \frac{p^2}{2m_0} - \frac{p^4}{8m_0^3c^2} + \cdots + V \quad \ldots \quad (2)$$

Change in Hamiltonian due to relativity $= \dfrac{-p^4}{8m_0^3c^2}$ = perturbation term.

$$p = -i\hbar\frac{\partial}{\partial q} = -\frac{ih}{2\pi}\frac{\partial}{\partial q}$$

Then the Hamiltonian operator can be written as

$$H = \frac{-1}{8m_0^3c^2}\left(-\frac{ih}{2\pi}\frac{\partial}{\partial q}\right)^4 = -\frac{1}{8m_0^3c^2}\frac{h^4}{16\pi^4}\nabla^4.$$

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If ψ_0 = unperturbed wave function of the hydrogen atom then first order energy shift due to relativity

$$\Delta E_r = -\int \psi_0^* \left[\frac{h^4/16\pi^4}{8m_0^3c^2}\right]\nabla^4\psi_0\, d\tau.$$

$$\Delta E_r = -\frac{R_\infty \alpha^2 Z^4 hc}{n^3}\left[\frac{1}{l+\frac{1}{2}} - \frac{3}{4n}\right]$$

The relativistic term shift $\Delta T_r = -\frac{\Delta E_r}{hc} = \frac{R_\infty \alpha^2 Z^4}{n^3}\left[\frac{1}{l+\frac{1}{2}} - \frac{3}{4n}\right]$

Hydrogen fine structure :→

First order perturbation corrections due to different effect combine linearly. Hence net term shift due to spin orbit interaction and the relativistic effect in a hydrogen like atom is

$$\Delta T = \Delta T_{l,s} + \Delta T_r$$

$$= -\frac{R_\infty \alpha^2 Z^4}{2n^3 l(l+\frac{1}{2})(l+1)}\left[j(j+1) - l(l+1) - s(s+1)\right] + \frac{R_\infty \alpha^2 Z^4}{n^3}\left[\frac{1}{l+\frac{1}{2}} - \frac{3}{4n}\right]$$

$$= \frac{R_\infty \alpha^2 Z^4}{n^3}\left[\frac{1}{l+\frac{1}{2}} - \frac{j(j+1) - l(l+1) - s(s+1)}{2l(l+\frac{1}{2})(l+1)} - \frac{3}{4n}\right] \quad \text{--- (1)}$$

$s = \frac{1}{2}$, $J = l+\frac{1}{2}$ & $J = l - \frac{1}{2}$ we will have

$$\left.\begin{aligned} j(j+1) - l(l+1) - s(s+1) &= l \quad \text{for } J = l+\tfrac{1}{2} \ \& \ s = \tfrac{1}{2} \\ &= -(l+1) \quad \text{for } J = l - \tfrac{1}{2} \ \& \ s = \tfrac{1}{2} \end{aligned}\right] \text{--- (2)}$$

using (2) in (1) the net term shifts corresponding to $j = l+\frac{1}{2}$ & $J = l - \frac{1}{2}$

$$\Delta T = \frac{R_\infty \alpha^2 Z^4}{n^3}\left[\frac{1}{l+1} - \frac{3}{4n}\right] \quad \text{--- (3)}$$

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$$\Delta T' = \frac{R_\infty \alpha^2 Z^4}{n^3}\left[\frac{1}{l+1} - \frac{3}{4n}\right] \quad \text{--- (4)}$$

$$\Delta T'' = \frac{R_\infty \alpha^2 Z^4}{n^3}\left[\frac{1}{l} - \frac{3}{4n}\right] \quad \text{--- (5)} \quad J = l+\frac{1}{2} \text{ \& } J = l-\frac{1}{2}$$

then eqn (4) & (5) can be represented by single eqn

$$\Delta T = \frac{R_\infty \alpha^2 Z^4}{n^3}\left[\frac{1}{J+\frac{1}{2}} - \frac{3}{4n}\right]$$

R_∞ = Rydberg's constant for heavy nucleus $= 1.097\times10^7\ m^{-1}$, $\alpha = \frac{1}{137}$

$Z = 1$ for Hydrogen atom.

$$\boxed{\Delta T = \frac{584}{n^3}\left[\frac{1}{k} - \frac{3}{4n}\right] m^{-1} = \frac{5.84}{n^3}\left[\frac{1}{k} - \frac{3}{4n}\right] cm^{-1}}$$ Sommerfeld Formula.

$$\boxed{\Delta T = \frac{584}{n^3}\left[\frac{1}{J+\frac{1}{2}} - \frac{3}{4n}\right] m^{-1} = \frac{5.84}{n^3}\left[\frac{1}{J+\frac{1}{2}} - \frac{3}{4n}\right] cm^{-1}}$$ Dirac formula

Bohr level n	Sommerfeld levels k	$\Delta T\ (cm^{-1})$	Dirac levels l	$J = l \pm \frac{1}{2}$	$\Delta T\ (cm^{-1})$
1	1	1.46	0	$\frac{1}{2}$	1.46
2	2	0.091	1	$\frac{3}{2}, \frac{1}{2}$	0.091, 0.456
	1	0.456	0	$\frac{1}{2}$	0.456
3	3	0.018	2	$\frac{5}{2}, \frac{3}{2}$	0.018, 0.054
	2	0.054	1	$\frac{3}{2}, \frac{1}{2}$	0.054, 0.162
	1	0.162	0	$\frac{1}{2}$	0.162

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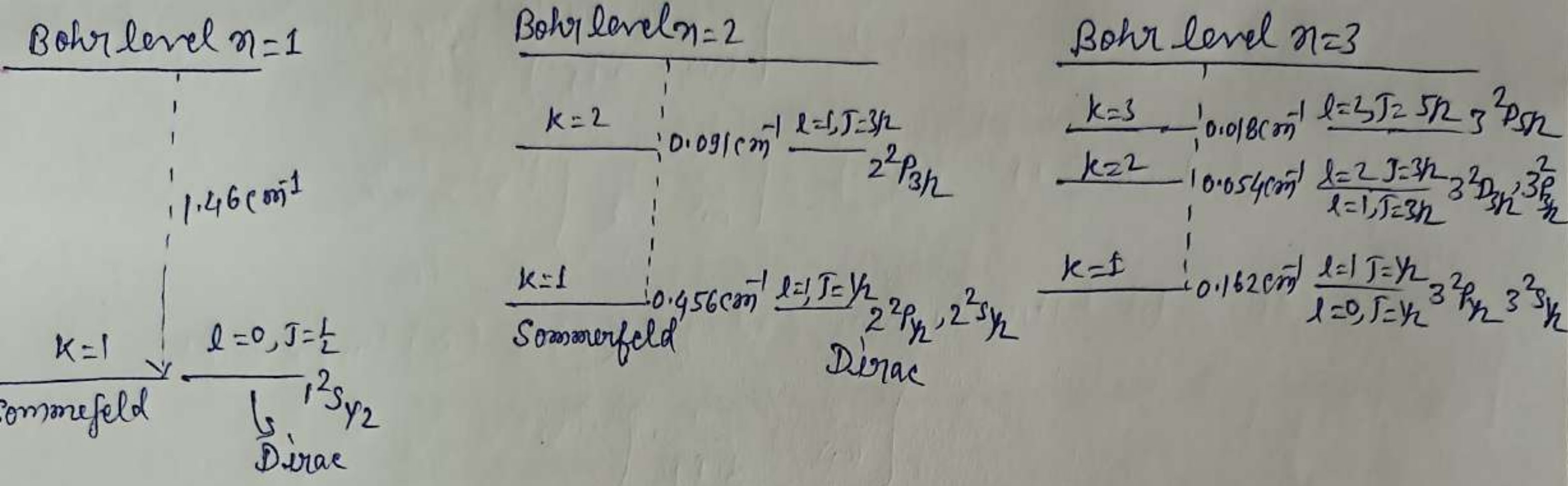
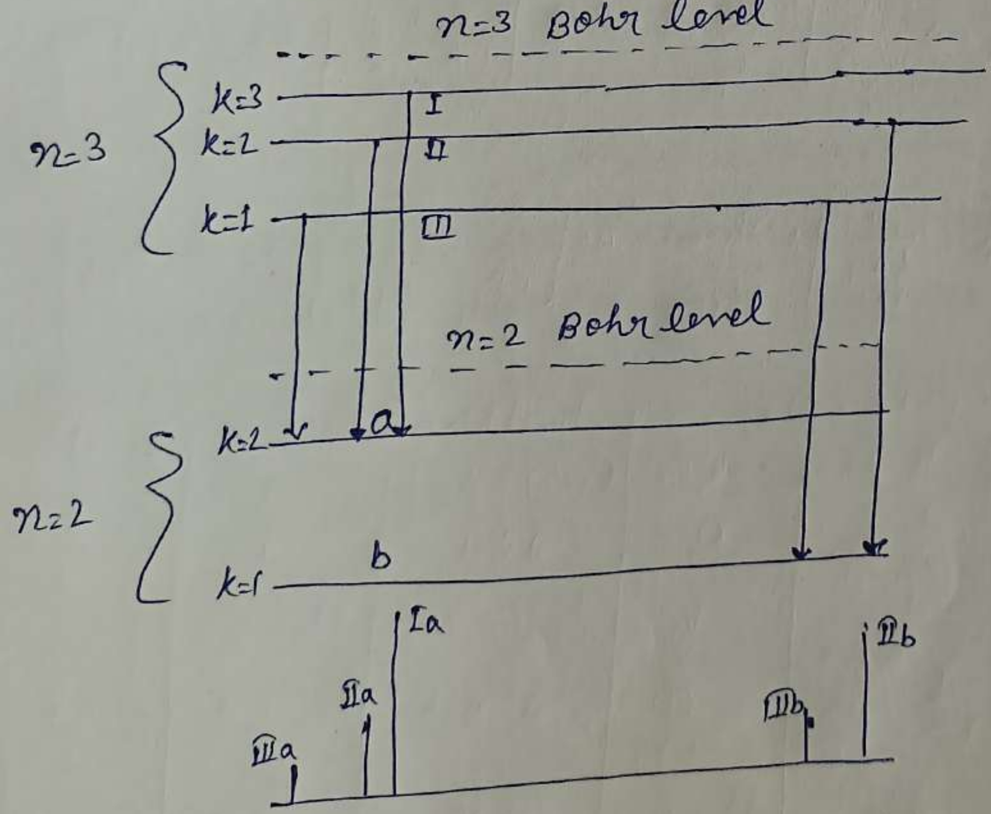


According to Dirac theory most levels are really double

Fine structure of Hα line ($3 \to n=2$) on the basis of Dirac theory



The selection rule for the dipole transitions are

$\Delta l = \pm 1$

$\Delta J = 0, \pm 1$

but $J=0 \not\leftrightarrow J=0$

Theoretically deduced structure of Hα line has general agreement with Hansen's observations. Still it is away from perfect agreement