"Fine Structure" of Hydrogen

We saw spectrum of H atom

$$E_n = -\frac{me^4}{2\hbar^2}\frac{1}{n^2} = \frac{-e^2}{2a_0}\frac{1}{n^2} \qquad a_0 = \frac{\hbar^2}{me^2}$$

And eigen functions

$$\psi_{n\ell m}(r,\theta,\phi) = R_{n\ell}(r)\,Y_{\ell m}(\theta,\phi)$$

$$\psi_{100} = 1/\sqrt{\pi a_0^3}\; e^{-r/a_0}$$

Actually $m \to \mu$ reduced mass to allow for fact that nucleus is not fixed at origin.

"Fine structure" corrections $O(\alpha^2)$ $\qquad \alpha = \frac{e^2}{\hbar c} = 1/137$

Two origins → relativistic correction
→ spin orbit coupling

FSH-2

We used $p^2/2m$ for kinetic energy, but really

$$\sqrt{p^2c^2+m^2c^4} - mc^2$$

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

$$= mc^2\left\{1+ p^2/2mc^2 - 1/8\left(p^2/m^2c^2\right)^2 + \dots\right\} - mc^2$$

$$= p^2/2m - p^4/8m^3c^2$$

Use first order perturbation theory to evaluate

$$E_{n1} = -1/8m^3c^2 \langle \psi_{no}|\hat{p}^4|\psi_{no}\rangle$$

A little trick is to write this as $\langle \psi_{no}|\hat{p}^2\ \hat{p}^2|\psi_{no}\rangle$

and use $\hat{p}^2|\psi_{no}\rangle = 2m\,(E_{no}-V)|\psi_{no}\rangle$

from the Schroedinger Eqn.

Then

$$E_{n1} = \frac{-1}{2mc^2}\langle \psi_{no}|(E_{no}-V)^2|\psi_{no}\rangle$$

$$= \frac{-1}{2mc^2}\left[E_{no}^2 + 2E_{no}e^2\langle\psi_{no}|\tfrac{1}{r}|\psi_{no}\rangle + e^4\langle\psi_{no}|1/r^2|\psi_{no}\rangle\right]$$

FSH-3

These are some algebra to evaluate.

$$\langle \frac{1}{r} \rangle = 1/n^2 a \qquad \Leftarrow \text{Easy}$$

$$\langle 1/r^2 \rangle = 1/(\ell + 1/2)\, n^3 a^2 \qquad \Leftarrow \text{Hard!}$$

Derivation of $\langle 1/r \rangle$:

Thus

$$E_{n_1} = -\frac{1}{2mc^2}\left\{ E_{n_0}^2 + 2E_{n_0}\frac{e^2}{n^2 a} + e^4/(l+1/2)\,n^3 a^2 \right\}$$

is the relativistic correction to H atom levels E_{n_0}.

Note there is now an l dependence.

This can be rewritten as

$$E_{n_1} = -E_{n_0}^2/2mc^2\left[\frac{4n}{l+1/2} - 3\right]$$

Q: What seems bogus about this calculation?!

A: We used nondegenerate perturbation theory!

This was actually okay because the matrix elements of this particular perturbation between different degenerate H atom levels are zero, so matrix of V is diagonal.

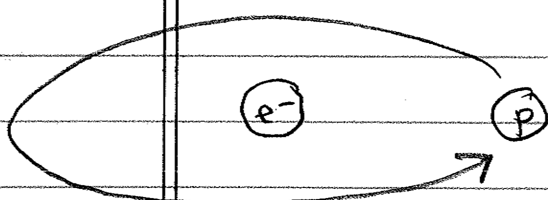
FSM-5

Spin-orbit coupling

Q: Does anyone know what this is

A: e^- circulating $\boxed{\text{orbiting}}$ around nucleus is moving through $\vec{E}$ field of proton. From its point of view (its rest frame) there is a $\vec{B}$ field to which its $\boxed{\text{spin}}$ couples

$$V = -\bar{\mu} \cdot \bar{B}$$



Rest frame of e^- has p circling around

$\vec{B}$ at center of current loop is a standard EM problem

$B = \mu_0 I / 2r$ (MKS) $\qquad 2\pi I / rc^2$ (CGS)

$I = e/T$ ← period

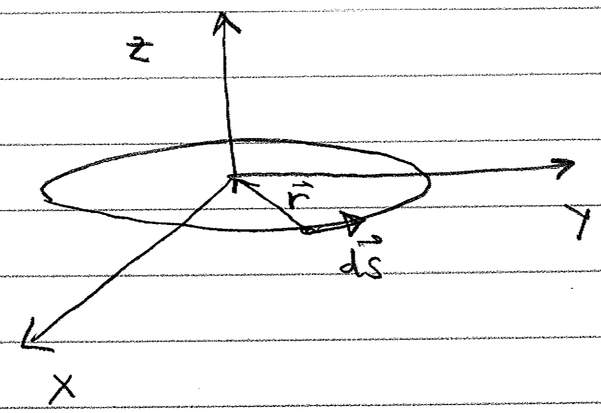
$$L = mrv = 2\pi m r^2 / T$$

so $I = e\, L / 2\pi m r^2 \qquad \frac{\mu_0}{4\pi} \to 1$

FSM-5'

Biot-Savart

$$\vec{dB} = \frac{\mu_0}{4\pi} I \frac{\vec{ds} \times \vec{r}}{r^3}$$

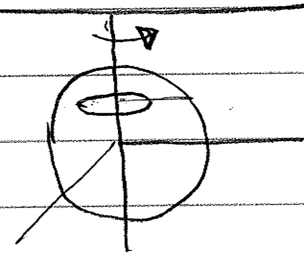


$$\vec{ds} \times \vec{r} = \underset{|ds|}{(r\,d\theta)}\,\underset{|\vec{r}|\sin\frac{\pi}{2}}{(r)}\,\hat{z}$$

$$\vec{B} = \int \vec{dB} = \int_0^{2\pi} \frac{\mu_0}{4\pi} I \frac{r^2 d\theta}{r^3}\hat{z}$$

$$= \frac{\mu_0 I}{2r}\hat{z}$$

Spinning Ball of charge



$$\mu = IA$$

$$\mu = \int_{-r}^{r} dz \int_0^{\sqrt{r^2-z^2}} d\rho\, 2\pi\rho\, \frac{Q}{\frac{4}{3}\pi r^3}\, \underbrace{\pi\rho^2}_{A}\, \frac{1}{T}$$

$2\pi\rho\, d\rho\, dz$ is volume of ring

charge density

$$= \frac{3\pi Q}{2Tr^3}\int_{-r}^{r} dz \int_0^{\sqrt{r^2-z^2}} \rho^3 d\rho = \frac{3\pi}{8Tr^3} Q \int_{-r}^{r} dz\, (r^2-z^2)^2$$

$$= \frac{3\pi Q}{8Tr^3}\left(r^4 z - \frac{2r^2z^3}{3} + \frac{z^5}{5}\right)\Big|_{-r}^{r} = \frac{3\pi}{4Tr^3} Q\left(1 - \frac{2}{3} + \frac{1}{5}\right) r^5 = \frac{2}{5}\frac{\pi r^2}{T} Q$$

FSH-5''

Sphere moment of Inertia (basically same calculation)

$$I = \frac{2}{5} M r^2$$

$$L = I\omega = I \frac{2\pi}{T}$$

$$\mu = Q \frac{2}{5} \pi \frac{r^2}{T} \qquad L = \frac{2}{5} M r^2 \frac{2\pi}{T}$$

We see that $\mu = \frac{Q}{2M} L$

Actually the right answer is

$$\mu = -\frac{e}{M} S$$

This factor of 2 is Landé g-factor

and was only explained by Dirac!

FSH-6

$$\vec{B} = \frac{\mu_0}{2r}\frac{eL}{2\pi m r^2} = \frac{\mu_0}{4\pi}\frac{e\vec{L}}{mr^3}$$

$$V = -\vec{\mu}\cdot\vec{B}$$

So need $\vec{\mu}$. If you do a classical spinning ball of charge you get

(see pages FSH-5′, 5″)

$$\vec{\mu} = \frac{Q}{2M}\vec{L}$$

Actual result is "Lande g-factor"

$$\vec{\mu} = -\frac{e}{M}\vec{S}$$

Explained by Dirac Eqn

So... $$V_{SO} = -\vec{\mu}\cdot\vec{B}$$

$$= \frac{e}{m}\vec{S}\cdot\frac{\mu_0}{4\pi}\frac{e\vec{L}}{mr^3}$$

$$= \frac{\mu_0 e^2}{4\pi}\frac{1}{m^2r^3}\vec{S}\cdot\vec{L}$$

One often writes this as

$$\vec{S}\cdot\vec{L} = \left[(\vec{L}+\vec{S})^2 - L^2 - S^2\right]\frac{1}{2} = \frac{1}{2}\left[J^2 - L^2 - \underset{\frac{1}{2}\left(\frac{1}{2}+1\right)}{S^2}\right]$$

FSH-7

$$V_{so} = \frac{\mu_o e^2}{8\pi} \frac{\hbar^2}{m^2 r^3} \left[j(j+1) - l(l+1) - 3/4 \right]$$

$$\left\langle \frac{1}{r^3} \right\rangle = \frac{1}{n^3 a^3} \ {}^1\!/_{l(l+1/2)(l+1)}$$

$$\left\langle \frac{1}{r} \right\rangle = \frac{1}{n^2} \frac{1}{a}$$

"Big Picture" Imagine you are a physicist in 1920's

QM is a new theory

You do these detailed calculations and they all

match up to expt!