1) 85(7): Rough Calculation in Non-Relativistic H

The method of obtaining the g factor in paper 18

$$p^\mu \to p^\mu \left(1 + \frac{\alpha}{4\pi} \right) \quad -(1)$$

which is equivalent to

$$\gamma^\mu \to \gamma^\mu \left(1 + \frac{\alpha}{4\pi} \right). \quad -(2)$$

Here

$$p^\mu = \left(\frac{E_n}{c}, \underline{p} \right). \quad -(3)$$

Use

$$p^\mu = i\hbar \partial^\mu \quad -(4)$$

where

$$\partial^\mu = \left(\frac{1}{c}\frac{\partial}{\partial t}, -\underline{\nabla} \right), \quad -(5)$$

so

$$\underline{p} = -i\hbar \underline{\nabla}. \quad -(6)$$

This means:

$$\underline{\nabla} \to \underline{\nabla} \left(1 + \frac{\alpha}{4\pi} \right) \quad -(7)$$

$$\nabla^2 \to \nabla^2 \left(1 + \frac{\alpha}{4\pi} \right)^2 \quad -(8)$$

The Schrödinger equation for the H atom is:

$$\left(-\frac{\hbar^2 \nabla^2}{2m} - \frac{e^2}{4\pi\epsilon_0 r} \right) \psi = E\psi \quad -(9)$$

which goes to:

$$\boxed{\left(-\frac{\hbar^2 \nabla^2}{2m} \left(1 + \frac{\alpha}{4\pi} \right)^2 - \frac{e^2}{4\pi\epsilon_0 r} \right) \psi = E\psi}$$

It is convenient to adapt the rule:

$$\hbar \rightarrow \hbar\left(1 + \frac{\alpha}{4\pi}\right) \qquad (11)$$

to find the effect of $\alpha / 4\pi$ on the H-like orbitals. The radial wavefunctions are given by Atkins on pp. 72 ff. They are defined as follows for H:

$$a := \frac{4\pi \epsilon_0 \hbar^2}{m e^2}, \quad \rho = \left(\frac{2}{na}\right) r \qquad (12)$$

n	l	$R_{nl}(r)$
1	0 (1s)	$(1/a)^{3/2}\, 2 \exp(-\rho/2)$
2	0 (2s)	$(1/a)^{3/2} (1/(2\sqrt{2}))(2-\rho) \exp(-\rho/2)$
	1 (2p)	$(1/a)^{3/2} (1/2\sqrt{6})\, \rho \exp(-\rho/2)$
3	0 (3s)	$(1/a)^{3/2} (1/(9\sqrt{3}))(6 - 6\rho + \rho^2) \exp(-\rho/2)$
	1 (3p)	$(1/a)^{3/2} (1/(9\sqrt{6}))(4-\rho)\rho \exp(-\rho/2)$
	2 (3d)	$(1/a)^{3/2} (1/(9\sqrt{30}))\rho^2 \exp(-\rho/2)$

The energy levels of the H atom are:

$$E_n = -\frac{m e^4}{32\pi^2 \epsilon_0^2 \hbar^2} \frac{1}{n^2} \qquad (13)$$

and the complete wavefunctions are:

$$\psi_{n l m_l}(r, \theta, \phi) = R_{nl}(r)\, Y_{l m_l}(\theta, \phi)$$

(14)

3) It is seen that:

$$\rho \to \rho\left(1+\frac{\alpha}{4\pi}\right)^{-2} \quad -(15)$$

$$E_n \to E_n\left(1+\frac{\alpha}{4\pi}\right)^{-2} \quad -(16)$$

i.e

$$E_n \to E_n\left(1-\frac{\alpha}{4\pi}+\frac{3\alpha^2}{16\pi^2}-\frac{\alpha^3}{16\pi^3}+\cdots\right) \quad -(17)$$

$$\rho \to \rho\left(1-\frac{\alpha}{4\pi}+\frac{3\alpha^2}{16\pi^2}-\frac{\alpha^3}{16\pi^3}+\cdots\right) \quad -(18)$$

To first order in α:

$$E_n(2s) \to \frac{\alpha}{4\pi} E_n(2s) \quad -(19)$$

$$E_n(2p) \to \frac{\alpha}{4\pi} E_n(2p) \quad -(20)$$

There is no $2s(1/2)$ and $2p(1/2)$ a this level because there is no S quantum number. A Lamb shift can be introduced empirically if it is assumed that:

$$E_n(2s) - E_n(2p) = 1060\ M_Z$$

i.e

$$\boxed{\frac{1}{4\pi}(\alpha_1-\alpha_2)E_n = 1060\ M_Z} \quad -(21)$$

More accurately:

$$\left(\langle\alpha_{2s}\rangle - \langle\alpha_{2p}\rangle\right)E_n = 1060\ M_Z$$

$$-(22)$$

+) This result is the simplest way of understanding the Lamb shift. The electromagnetic field has been quantized as a collection of harmonic oscillators. A harmonic oscillation is never completely at rest because it has zero point energy. In the absence of photons there is a mean $A_\mu^{(vac)}$ due to the fluctuating electric and magnetic fields of the vacuum. An electron (in this case of the H atom) experiences this fluctuation and instead of moving smoothly it jitterbugs (zitterbewegung). As it spins it wobbles and g is increased:

$$g \rightarrow g\left(1+\frac{\alpha}{4\pi}\right)^2 = 2\left(1+\frac{\alpha}{4\pi}\right)^2 \quad -(23)$$

This jitterbugging smears the electron over a small region of space, and this effect is greater for 2s because the electron spends more time closer to the nucleus in 2s than in 2p. The energy of the 2s rises more than in 2p.

Spin-Orbit Coupling in H, Schrödinger Level

On the Schrödinger level the effect of half integral spin is introduced by considering a spin quantum number s. In H, the 2p(1/2) state is:

$$2p_{1/2}: n=2,\ \ell=1,\ j=1/2,\ s=1/2$$

and:

$$2s_{1/2}: n=2,\ \ell=0,\ j=1/2,\ s=1/2$$

) From angular momentum theory:

$$j^2 = |\underline{l} + \underline{s}|^2 = l^2 + s^2 + 2\underline{l}\cdot\underline{s} \quad -(24)$$

and:

$$j = l+s,\ l+s-1,\ \ldots,\ |l-s| \quad -(25)$$

This means that for H, every term with $l > 0$ is a doublet with two values of j.

There is an orbital magnetic moment:

$$\underline{m} = \gamma_e \underline{L},\quad \gamma_e = -\frac{e}{2m} \quad -(26)$$

and a spin magnetic moment:

$$\underline{m}_s = g\gamma_e \underline{S} \quad -(27)$$

where:

$$g = 2\left(1+\frac{\alpha}{4\pi}\right)^2 \quad -(28)$$

The Dirac equation is used to take account of the Thomas precession to give the spin-orbit interaction hamiltonian:

$$H_{so} = \xi(r)\,\underline{S}\cdot\underline{L} = -\frac{e}{2m_e^2c^2}\left(1+\frac{\alpha}{4\pi}\right)^2\frac{1}{r}\frac{d\phi}{dr} \quad -(29)$$

where we have used eq. (28).

Without the Thomas precession, the result is twice that of eq. (29). The Thomas precession is a relativistic effect that reduces the magnetic moment of interaction to $\frac{1}{2}g\gamma_e\underline{S}$.

The spin-orbit coupling constant in wavenumbers is:

$$\zeta_{nl} = \frac{\hbar}{2\pi c}\left(1+\frac{\alpha}{4\pi}\right)^2 \int_0^\infty \xi(r) R_{nl}^2(r)\, r^2\, dr, \qquad -(30)$$

$$= \alpha^2\left(1+\frac{\alpha}{4\pi}\right)^2 \frac{R_\infty}{n^3 l(l+1/2)(l+1)} \qquad -(31)$$

where R_∞ is

$$R_\infty = \frac{m e^4}{8\epsilon_0^2 h^3 c} \qquad -(32)$$

is the Rydberg constant for hydrogen.

For $n = 2$, $l = 1$ (2p electron):

$$n^3 l(l+1/2)(l+1) = 24 \qquad -(33)$$

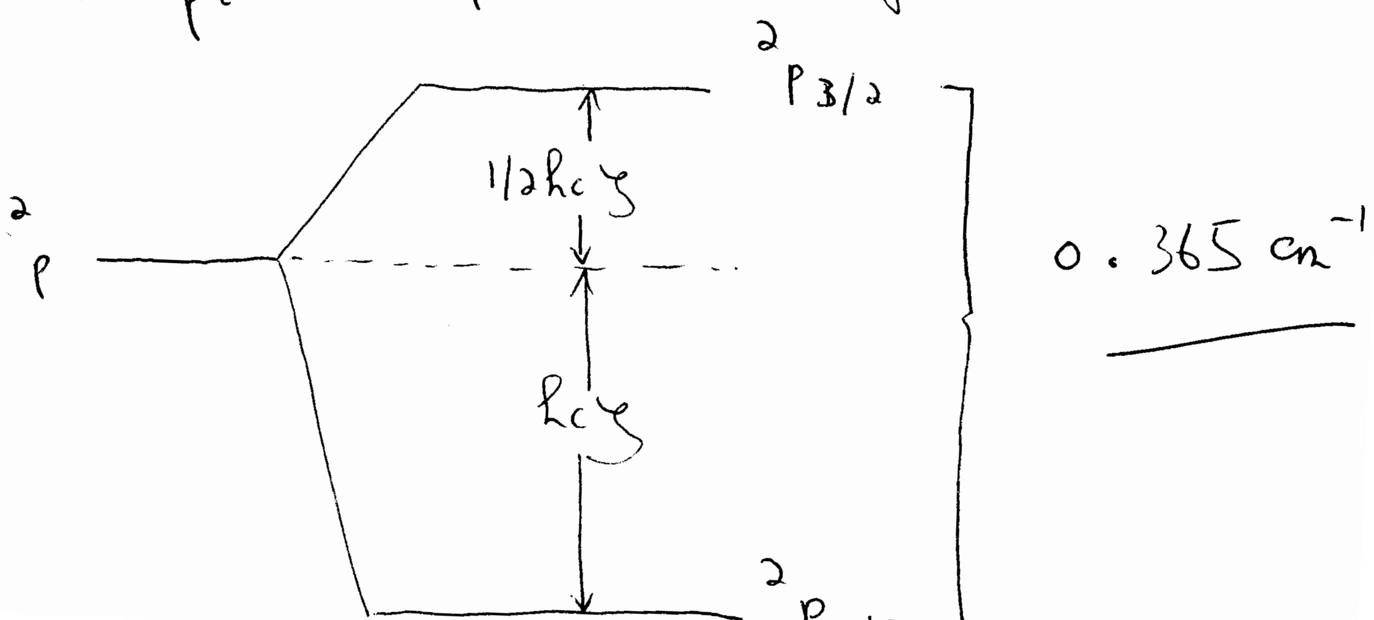
and:

$$\boxed{\zeta_{nl} = \alpha^2\left(1+\frac{\alpha}{2\pi}\right)^2 \frac{R_\infty}{24}} \qquad -(34)$$

where

$$R_\infty = 1.097373 \times 10^5\ \text{cm}^{-1}.$$

So the spin orbit splitting is as follows:



7) The interaction energy is:

$$E_{so} = \langle nls; jm_j | H_{so} | nls; jm_j \rangle \quad -(35)$$

where:

$$H_{so} = \xi(r)\, \underline{l} \cdot \underline{s}. \quad -(36)$$

We have:

$$\underline{l} \cdot \underline{s} | nls; jm_j \rangle = \frac{1}{2}\left(j^2 - l^2 - s^2\right) | nls; jm_j \rangle \quad -(37)$$

$$= \frac{1}{2}\hbar^2 \left(j(j+1) - l(l+1) - s(s+1) \right) | nls; jm_j \rangle \quad -(37)$$

So:

$$\boxed{E_{so} = \alpha^2 \left(1 + \frac{\alpha}{4\pi}\right)^2 hcR_\infty \left(\frac{j(j+1) - l(l+1) - s(s+1)}{2n^3 l(l+1/2)(l+1)} \right)} \quad -(38)$$

and:

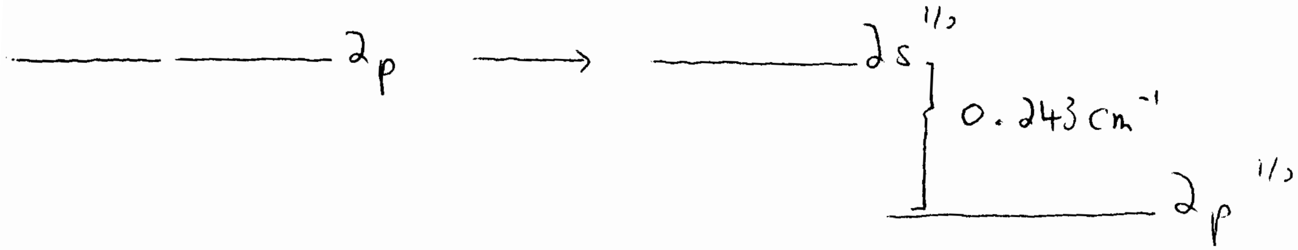
$$E_{so}(2p^{1/2}) = -\frac{hcR_\infty \alpha^2}{12}\left(1 + \frac{\alpha}{4\pi}\right)^2 \quad -(39a)$$

$$E_{so}(2s^{1/2}) = 0. \quad -(39b)$$

Thus

$$\boxed{E_{so}(2s^{1/2}) - E_{so}(2p^{1/2}) = \frac{hcR_\infty \alpha^2}{12}\left(1 + \frac{\alpha}{4\pi}\right)^2}$$

This means:



due to spin-orbit coupling.

This is of the same order of magnitude as the Lamb shift, which is 1060 MHz. We use:

$$1\ \text{cm}^{-1} = 30{,}000\ \text{MHz} = 30\ \text{GHz}$$

so:

$$1060\ \text{MHz} = 0.0353\ \text{cm}^{-1}$$

i.e the Lamb shift is about ten times smaller than the spin-orbit shift from the Schrödinger equation for H. As shown in note 85(6), the Dirac equation of H shows that $^2S_{1/2}$ and $^2P_{1/2}$ are degenerate, the reason why the Schrödinger equation gives $0.243\ \text{cm}^{-1}$ energy difference is that the Schrödinger equation is not correctly relativistic.

The only source of energy difference between $2s^{1/2}$ and $2p^{1/2}$ in H is the Lamb shift.

1)

This is why eqn. (7) of 85(6) is used:

$$\left(i\gamma^\mu\left(1+\frac{\alpha}{4\pi}\right)\partial_\mu - \frac{mc}{\hbar} - \frac{\alpha}{r}\right)\psi = 0 \quad -(41)$$

This is correctly relativistic from the beginning, and automatically accounts for the Thomas precession. In the absence of vacuum perturbation (jitterbuggers) of the electron:

$$\left(i\gamma^\mu\partial_\mu - \frac{mc}{\hbar} - \frac{\alpha}{r}\right)\psi_0 = 0 \quad -(42)$$

Eq. (42) is the Dirac equation of H that produces the result:

$$\boxed{En\left({}^2S^{1/2}\right) = En\left({}^2P^{1/2}\right)} \quad -(43)$$

<u>even in</u> the <u>presence</u> of <u>spin-orbit coupling</u>.

So to a first approximation one may take the orbitals of H from eq. (41), and perturb them with

$$p^\mu = i\hbar\partial^\mu \rightarrow i\hbar\partial^\mu\left(1+\frac{\alpha}{4\pi}\right) \quad -(44)$$

i.e.

$$\hbar \rightarrow \hbar\left(1+\frac{\alpha}{4\pi}\right) \quad -(45)$$

10)

In this case the unperturbed Dirac equation (41) gives the result (43) from:

$$E = mc^2\left(1 + \frac{\alpha^2}{((j+1/2)^2 - \alpha^2)^{1/2} + n')^2}\right)^{1/2} \quad -(46)$$

Where:

$$\alpha = \frac{e^2}{4\pi\epsilon_0 \hbar c} \quad -(47)$$

Here:

$$\left.\begin{aligned} j &= \frac{1}{2}, \frac{3}{2}, \frac{5}{2}; \quad n' = 0, 1, 2 \\ n\,(\text{non-relativistic}) &= j + 1/2 + n' \end{aligned}\right\} \quad -(48)$$

In the absence of the vacuum potential pairs of states with the same j but opposite parity are degenerate. This is because $(j + 1/2)^2$ appears in eq. (46).

The Lamb shift lifts this degeneracy. Eq. (46) means that:

$$E(2S^{1/2}) = E(2P^{1/2}) \quad -(49)$$

because:

$$\left.\begin{aligned} j(2S^{1/2}) &= j(2P^{1/2}) = 1/2 \\ n' &= n - (j + 1/2) = 1 \end{aligned}\right\} \quad -(50)$$

To introduce the Lamb shift, note that:

$$p^\mu p_\mu = m^2c^2 \quad -(51)$$

$$\rightarrow m^2c^2\left(1 + \frac{\alpha}{4\pi}\right)^2 \quad -(52)$$

This means that the energy levels in eq. (46)

e changed to:

$$E \rightarrow E\left(1+\frac{\alpha}{4\pi}\right)^2 \quad - (53)$$

$$= E\left(1+\frac{\alpha}{2\pi}+\frac{\alpha^2}{16\pi^2}\right)$$

To first order:

$$\Delta E = \frac{\alpha}{2\pi} E \quad - (54)$$

This is twice the results (19) and (20) from the Schrödinger equation.

However, at this level of approximation there is again no Lamb shift, because eq. (54) perturbs eq. (46) by the same amount for $^2S_{1/2}$ and $^2P_{1/2}$. This is due to the fact that eq. (46) is an approximate solution of the equation (41).

To proceed we may use the relativistic version of eq. (21):

$$\frac{1}{2\pi}(\alpha_1-\alpha_2)E_n = 1060 \text{ MHz} \quad - (55)$$

A better method is to use:

12)

$$\frac{\alpha}{4\pi} i\gamma^\mu \partial_\mu \psi = \frac{\alpha}{r_{vac}} \psi \quad -(56)$$

So:

$$\left(i\gamma^\mu \partial_\mu - \frac{mc}{\hbar} + \alpha\left(\frac{1}{r_{vac}} - \frac{1}{r}\right)\right)\psi = 0 \quad -(57)$$

Eq. (56) is:

$$i\gamma^\mu \partial_\mu \psi = \frac{4\pi}{r_{vac}} \psi \quad -(58)$$

so:

$$\left\langle \frac{4\pi}{r_{vac}} \right\rangle = \overline{\psi} \frac{4\pi}{r_{vac}} \psi \quad -(59)$$

In the first approximation:

$$\left\langle \frac{4\pi}{r_{vac}} \right\rangle = \overline{\psi_0} \frac{4\pi}{r_{vac}} \psi_0 \quad -(60)$$

for the unperturbed ψ_0 of eq. (42). Given the eigenfunctions ψ_0, the expectation value $\langle 4\pi / r_{vac} \rangle$ is found analytically from eq. (60). This is different for $^2S_{1/2}$ and $^2P_{1/2}$, because the perturbation caused by $1/\langle r_{vac} \rangle$ in eq. (57) is different for each state. Finally iterate to the right result using advanced computer methods.