85(10): Defining the Lamb Shift Calculation in H, Schrödinger Equation

First recall that the fully relativistic problem is:

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

$$i\gamma^\mu \partial_\mu \psi = \frac{4\pi}{r_{vac}} \psi \quad -(2)$$

as in previous notes for paper 85. The method is to solve these two equations simultaneously. In the non-relativistic approximation the Schrödinger equation is used:

$$\boxed{\left(-\frac{\hbar^2 \nabla^2}{2m} \left(1 + \frac{\alpha}{4\pi}\right)^2 - \frac{e^2}{4\pi\epsilon_0 r} \right) \psi = E\psi} \quad -(3)$$

So eqn. (2) becomes:

$$-\frac{\hbar^2 \nabla^2}{2m} \left(\frac{\alpha}{2\pi} + \frac{\alpha^2}{16\pi^2} \right) \psi = \frac{e^2}{4\pi\epsilon_0 r_{vac}} \psi \quad -(4)$$

If:

$$\alpha^2 \ll \alpha \quad -(5)$$

eq. (4) is

$$\boxed{\nabla^2 \psi = -\left(\frac{4mc}{\hbar}\right) \frac{1}{r_{vac}} \psi} \quad -(6)$$

2) If the H radial orbitals are used in eq. (6) then r_{vac} can be calculated for each orbital.

In spherical polar coordinates:

$$\nabla^2 \psi = \frac{\partial^2 \psi}{\partial r^2} + \frac{2}{r}\frac{\partial \psi}{\partial r} \quad —(7)$$

<u>1s Orbital</u>

$$\psi(1s) = 2\left(\frac{1}{a}\right)^{3/2} \exp\left(-\frac{\rho}{2}\right) \quad —(8)$$

where:

$$\frac{1}{a} = \frac{me^2}{4\pi\epsilon_0 \hbar^2}, \quad \rho = \frac{2r}{na}, \quad n = 1 \quad —(9)$$

and

$$m = \text{reduced mass}. \quad —(10)$$

<u>2s Orbital</u>

$$\psi(2s) = \left(\frac{1}{a}\right)^{3/2} \left(\frac{2-\rho}{2\sqrt{2}}\right) \exp\left(-\frac{\rho}{2}\right)$$

$$\rho = \frac{2r}{na}, \quad n = 2 \quad —(11)$$

<u>2p Orbital</u>

$$\psi(2p) = \left(\frac{1}{a}\right)^{3/2} \left(\frac{1}{2\sqrt{6}}\right) \exp\left(-\frac{\rho}{2}\right)$$

$$—(12)$$

It is seen from eqns (6) to (12) that r_{vac}

3) is different for each orbital and it is a function of r, the radial coordinate. Therefore the average r_{vac} can be found and denoted $\langle r_{vac} \rangle$.

The Lamb shift in joules is: —(13)

$$\Delta E_{Lamb} = \frac{e^2}{4\pi \epsilon_0} \left(\frac{1}{\langle r_{vac}^2 \rangle_{2s}^{1/2}} - \frac{1}{\langle r_{vac}^2 \rangle_{2p}^{1/2}} \right)$$

The Lamb shift in hertz (s^{-1}) is: —(14)

$$\Delta E_{Lamb} (\text{hertz}) = \frac{e^2}{4\pi \epsilon_0 \hbar} \left(\frac{1}{\langle r_{vac}^2 \rangle_{2s}^{1/2}} - \frac{1}{\langle r_{vac}^2 \rangle_{2p}^{1/2}} \right)$$

The Lamb shift in wavenumbers (cm^{-1}) is: —(15)

$$\Delta E_{Lamb} (\text{wavenumbers}) = \frac{e^2}{4\pi \epsilon_0 \hbar c} \left(\frac{1}{\langle r_{vac}^2 \rangle_{2s}^{1/2}} - \frac{1}{\langle r_{vac}^2 \rangle_{2p}^{1/2}} \right)$$

where:

$$\alpha = \frac{e^2}{4\pi \epsilon_0 \hbar c} \qquad -(16)$$

is the fine structure constant.

We have:

$$\omega = 2\pi f = 2\pi \bar{\nu} c \qquad -(17)$$

$$\boxed{\Delta \bar{\nu} (\text{Lamb}) = 0.00729735(34) \left(\frac{1}{\langle r_{vac}^2 \rangle_{2s}^{1/2}} - \frac{1}{\langle r_{vac}^2 \rangle_{2p}^{1/2}} \right) cm^{-1}} \qquad -(18)$$

4)

Experimental Lamb shift

$$\Delta f\,(2s-2p) = 1.060 \text{ GHz}$$

$$= \frac{1.060}{30} \text{ cm}^{-1}$$

$$= 0.0353 \text{ cm}^{-1}; \quad -(19)$$

so:

$$\frac{1}{\langle r_{vac}^2 \rangle_{2s}^{1/2}} - \frac{1}{\langle r_{vac}^2 \rangle_{2p}^{1/2}} = \frac{0.0353}{0.007297(34)} \text{ cm}^{-1}$$

$$= 4.837 \text{ cm}^{-1} \quad -(20)$$

The shift in energy due to this shift is:

$$\Delta E\,(\text{lamb}) = \frac{e^2}{(4\pi\epsilon_0)\,4.837} \text{ joules} \quad -(21)$$

We denote:

$$\boxed{\langle \Delta \bar{\nu} \rangle_{vac} = 4.837 \text{ cm}^{-1}} \quad -(22)$$

which occurs in ~~the~~ far infra-red.

The next step is to work out $\langle r_{vac}^2 \rangle_{2s}^{1/2}$ and $\langle r_{vac}^2 \rangle_{2p}^{1/2}$ analytically from eqns. (6) to (12), bearing in mind that this is a non-relativistic approximation, but in H a very good one.

5)

It is known that in the absence of α,

$$E_n(2s) = E_n(2p). \quad — (23)$$

The absence of α can be regarded mathematically as:

$$\alpha \to 0, \quad \Delta E_{Lamb} \to 0 \quad — (24)$$

so:

$$\langle \Delta \bar{\nu} \rangle_{vac} \to \frac{0}{0} \quad — (25)$$

from eq. (16), so $\langle r_{vac}^2 \rangle_{2s}^{1/2}$ and $\langle r_{vac}^2 \rangle_{2p}^{1/2}$ become indeterminate.

In eq. (6):

$$m = 9.10953 \times 10^{-31} \text{ kgm}$$
$$c = 2.997925 \times 10^{8} \text{ ms}^{-1}$$
$$h = 6.62618 \times 10^{-34} \text{ Js}$$

Atkins' values

Compton wavelength of electron $(\lambda_c) = \frac{h}{mc} = 2.426 \times 10^{-12}$ m,

so: $\frac{mc}{h} = \frac{2\pi}{\lambda_c}$ and:

$$\boxed{\nabla^2 \phi = - \frac{8\pi}{\lambda_c} \frac{1}{r_{vac}} \phi}$$

We have

$$\lambda_c = 2.426 \times 10^{-10} \text{ cm}$$

From eq. (20), this is affected by:

$$\Delta \lambda_c = \frac{2.426 \times 10^{-10}}{4.837} \sim 0.50 \times 10^{-10} \text{ cm}$$

$$\boxed{\sim 0.005 \text{ Å}}$$