1)

85(12) : Summary of Lamb Shift Calculation

1s Orbital

$$\boxed{\phi(1s) = \frac{2}{a^{3/2}} e^{-r/a}} \quad \text{— (1)}$$

$$\boxed{\frac{1}{r_{vac}}(1s) = -\frac{\cancel{\ell}}{4mca}\left(\frac{1}{a} - \frac{2}{r}\right)}$$

$$= -0.0720\left(\frac{1}{a} - \frac{2}{r}\right) \quad \text{— (2)}$$

$$f(r) = 4\pi r^2 \phi^2, \quad r_{max} = a \quad \text{— (3)}$$

At r_{max} :

$$\boxed{\frac{1}{r_{vac}}(1s) = \frac{0.1440}{a}} \quad \text{— (4)}$$

2s Orbital

$$\boxed{\phi(2s) = \frac{1}{2\sqrt{2}\, a^{3/2}}\left(2 - \frac{r}{a}\right) e^{-r/(2a)}} \quad \text{— (5)}$$

$$\boxed{\frac{1}{r_{vac}}(2s) = \frac{\cancel{\ell}}{2mca}\left(\frac{2}{r} - \frac{5}{4a} + \frac{r}{8a^2}\right) \Big/ \left(2 - \frac{r}{a}\right)} \quad \text{— (6)}$$

If $f(r) = 4\pi r^2 \phi^2$ there is a maximum at $r = 1.1716\, a$ and a minimum at $r = 6.8284\, a$.

At $r = 6.8284\, a$:

$$\boxed{\frac{1}{r_{vac}}(2s) = \frac{0.02107}{a}} \quad \text{— (7)}$$

From a comparison of eqns. (4) and (7) it can be seen that the vacuum effect on 2s is much smaller than 1s.

2)

$2p_z$ Orbital

To calibrate properly with 1s and 2s:

$$\boxed{\psi(2p_z) = \frac{1}{4a^{3/2}}\frac{r}{a}e^{-r/(2a)}\cos\theta} \quad -(8)$$

This has a maximum at

$$\cos\theta = 1. \quad -(9)$$

At this point:

$$\boxed{\frac{1}{r_{vac}}(2p_z) = \frac{\hbar}{2mca}\left(\frac{5}{8a} - \frac{1}{r}\right)} \quad -(10)$$

The radial distribution function is maximized at

$$\theta = 0 \text{ or } \theta = \pi \text{ and } r = 2a. \quad -(11)$$

At this point:

$$\boxed{\frac{1}{r_{vac}}(2p_z) = \frac{0.018}{a}} \quad -(12)$$

It is seen that the vacuum has a larger effect on 2s than $2p_z$ as observed in ~~the~~ Lamb shift:

$$\frac{1}{r_{vac}}(2s) - \frac{1}{r_{vac}}(2p_z) = \frac{0.003}{a} \quad -(13)$$

$$\boxed{\Delta E_n \propto \frac{0.003}{a}} \quad -(14)$$

3)

To find the constant of proportionality in eq. (14) note that the H energy levels are, in wavenumbers:

$$\bar{\nu} = \frac{1}{4n^2}\frac{\alpha}{a} \text{ cm}^{-1} \quad -(15)$$

where α is the fine structure constant, and n is the main quantum number. For 2s and 2p, $n = 2$. So:

$$\boxed{\begin{aligned}\bar{\nu}(2s, 2p) &= \frac{1}{16}\frac{\alpha}{a} \text{ cm}^{-1} \\ &= 86,183 \text{ cm}^{-1}\end{aligned}} \quad -(16)$$

The experimentally observed Lamb shift is:

$$\boxed{\Delta\bar{\nu}(2s - 2p) = 0.0353 \text{ cm}^{-1}} \quad -(17)$$

So:

$$\boxed{\left(\frac{\Delta\bar{\nu}}{\bar{\nu}}\right)_{\text{expt.}} = 4.096 \times 10^{-7}} \quad -(18)$$

It can be seen that the Lamb shift is only one ten millionth of the unperturbed 2s = 2p energy level. Nevertheless, it does show the existence of vacuum electric and magnetic fields.

The basic method being used to calculate r_{vac} is:

$$\nabla^2 \longrightarrow \nabla^2\left(1 + \frac{\alpha}{4\pi}\right)^2 \quad -(19)$$

This means:

$$\boxed{\bar{\nu} \rightarrow \bar{\nu}\left(1 + \frac{\alpha}{4\pi}\right)^2} \quad -(20)$$

4)

To first order in α:

$$\bar{\nu} \rightarrow \bar{\nu}\left(1 + \frac{\alpha}{2\pi}\right)$$

so

$$\Delta\bar{\nu} = \frac{\alpha\bar{\nu}}{2\pi}, \quad \boxed{\frac{\Delta\bar{\nu}}{\bar{\nu}} = \frac{\alpha}{2\pi}} \quad -(21)$$

Therefore:

$$\Delta\Delta\bar{\nu}\,(2s - 2p) = \frac{0.003\,\alpha}{2\pi} \quad -(22)$$

<u>Normalization</u>

The $Y(0,0)$ spherical harmonic is normalized in a book such as P.W. Atkins, "Molecular Quantum Mechanics" (OUP, 1983, 2nd. ed.) to:

$$Y(0,0) = \frac{1}{(2\pi)^{1/2}} \quad -(23)$$

If this factor is included in the calculation then:

$$\boxed{\begin{aligned}\Delta\Delta\bar{\nu}\,(2s - 2p) &= \frac{0.003}{(2\pi)^{3/2}}\,\alpha \\ &= 1.433 \times 10^{-6}\end{aligned}} \quad -(24)$$

Comparing eqns. (18) and (24) it is seen that this first approximation produces the Lamb shift to the right order of magnitude and with no adjustable parameters or any QED method.

5) <u>Refinement of the Method</u>

The calculation has been carried out at chosen values of r, but in general:

$$\frac{1}{r_{vac}}(2s) - \frac{1}{r_{vac}}(2p)$$

$$= \frac{\hbar}{2mca}\left(\left(\frac{2}{r} - \frac{5}{4a} + \frac{r}{8a^2}\right) \Big/ \left(2 - \frac{r}{a}\right) + \frac{1}{r} - \frac{5}{8a}\right) \quad -(25)$$

and the Lamb shift is proportional to this. It is given by:

$$\boxed{\Delta\bar{\nu}(2s - 2p) = \frac{\hbar}{2mc} \cdot \frac{\alpha}{(2\pi)^{3/2}} a \left(\frac{\left(\frac{2}{r} - \frac{5}{4a} + \frac{r}{8a^2}\right)}{\left(2 - \frac{r}{a}\right)} + \frac{1}{r} - \frac{5}{8a}\right)}$$

$$-(26)$$

This can be made to fit the experimental result (18) to find the value of r that gives the right result.