5(11b): Vacuum Shift for $2p_z$ Orbital

The $2p_z$ orbital is the required normalization is

$$\phi_0(2p_z) = \frac{1}{4a^{3/2}} \frac{r}{a} e^{-r/(2a)} \cos\theta \quad -(1)$$

(Atlas page 76). This has a maximum at

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

for the radial distribution function. At this maximum point:

$$\frac{d\phi_0}{dr} = \frac{1}{4a^{5/2}}\left(1 - \frac{r}{2a}\right) e^{-r/(2a)} \quad -(3)$$

and

$$\frac{d^2\phi_0}{dr^2} = -\frac{e^{-r/(2a_0)}}{16a^{7/2}} \quad -(4)$$

So:

$$\nabla^2\phi = -\frac{e^{-r/(2a)}}{16a^{7/2}} + \frac{2}{4a^{5/2}r}\left(1 - \frac{r}{2a}\right) e^{-r/(2a)}$$

$$= -\frac{4mc}{\hbar} \frac{1}{r_{vac}} \frac{1}{4a^{3/2}} \frac{r}{a} e^{-r/(2a)} \quad -(5)$$

i.e.

$$-\frac{1}{16a^2} + \frac{1}{2ra}\left(1 - \frac{r}{2a}\right) = -\frac{mc}{\hbar}\frac{1}{r_{vac}} \quad -(6)$$

$$\boxed{\frac{1}{r_{vac}} = \frac{\hbar}{mc}\left(\frac{5}{16a^2} - \frac{1}{2ra}\right)} \quad -(7)$$

At the maximum

$$r = 2a \quad -(8)$$

$$\boxed{\frac{1}{r_{vac}} = +\frac{0.018}{r}} \quad -(9)$$

So:

$$\boxed{\begin{aligned} \frac{1}{r_{vac}}(2s) &= +\frac{0.0211}{a} \\ \frac{1}{r_{vac}}(2p_z) &= +\frac{0.018}{a} \end{aligned}} \quad \text{— (10)}$$

It is seen that this is qualitatively the right result, because the energy increase in the 2s orbital is more than that in the $2p_z$ orbital. In both cases the energy increase has been calculated at the point where the radial distribution function is a maximum. These are the points where the electron is most likely to be.

For the 1s electron:

$$\boxed{\frac{1}{r_{vac}}(1s) = \frac{0.2880}{a}} \quad \text{— (11)}$$

Here:

$$a = \frac{4\pi\epsilon_0\hbar^2}{me^2} = 5.292 \times 10^{-11}\,m \quad \text{— (12)}$$

The Lamb shift is proportional to:

$$\boxed{\Delta\left(\frac{1}{r_{vac}}\right) = \frac{0.003}{a}} \quad \text{— (13)}$$

In the unperturbed condition, the energy level of the 2s and 2p states are the same:

3)

$$E_n = \frac{m e^4}{128 \pi^2 \epsilon_0^2 \hbar^2} \text{ joules} \quad -(14)$$

i.e.

$$\bar{\nu} = \frac{1}{16} \frac{\alpha}{a} \quad -(15)$$

where α is the fine structure constant. It is s- that:

$$\bar{\nu}(2s - 2p) = \frac{1}{16} \times \frac{0.007297}{5.29177 \times 10^{-9}} \text{ cm}^{-1}$$

$$= \frac{0.007297}{16 \times 5.29177} \times 10^{9} \text{ cm}^{-1} \quad -(16)$$

$$\bar{\nu} = 8.6183 \times 10^{4} \text{ cm}^{-1} \quad -(17)$$

The experimental Lamb shift is

$$\Delta \bar{\nu} = 0.0353 \text{ cm}^{-1} \quad -(18)$$

So:

$$\boxed{\frac{\Delta \bar{\nu}}{\bar{\nu}} = 4.096 \times 10^{-7}} \quad -(19)$$

From eqns. (15) and (13) it is seen that

$$\left(\frac{\Delta \bar{\nu}}{\bar{\nu}}\right)_{max} = \frac{0.003 \alpha}{16} = 1.368 \times 10^{-6}$$

So in this first approximation:

$$\boxed{\frac{\Delta \bar{\nu}}{\bar{\nu}} < 1.368 \times 10^{-6}} \quad -(20)$$