(11). Lamb Shift Calculation for 1s Orbital

This is done to illustrate the method. In this case

$$\psi(1s) = \frac{2}{a^{3/2}} e^{-r/a} \quad -(1)$$

where $a = \frac{4\pi\epsilon_0 \hbar^2}{me^2} = 5.29177 \times 10^{-11}$ m.

Eq (1) is a solution of:

$$\left(-\frac{\hbar^2 \nabla^2}{2m} - \frac{e^2}{4\pi\epsilon_0 r}\right)\psi_0 = E\psi_0 \quad -(2)$$

The effect of the vacuum is to change eq. (2) to:

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

In general ψ are different from ψ_0. Eq (3) is expressed as:

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

by using:

$$-\frac{\hbar^2\nabla^2}{2m}\left(\frac{\alpha}{4\pi} + \frac{\alpha^2}{16\pi^2}\right)\psi = \frac{e^2}{4\pi\epsilon_0 r_{vac}}\psi \quad -(5)$$

If:

$$\alpha^2 << \alpha \quad -(6)$$

eq. (5) is

2) The effect of the vacuum from eq. (4) is to smear the electron over a small region of space, this smearing reduces the effectiveness of the Coulomb law and the energy of the orbital increases, (Atkins p. 221).

The mathematical problem is to find r_{vac} from eq (5) and use it in eq. (4). To do this, however, the wavefunction ϕ must be known. As a first approximation, the wavefunctions ϕ_0 of the unperturbed H atom are used in eq. (7):

$$\nabla^2 \phi_0 = -\frac{4mc}{\hbar} \frac{1}{r_{vac}} \phi_0 \quad -(8)$$

and this gives a first approximation to r_{vac} for each orbital.

For the 1s orbital, (eq. (1)):

$$\nabla^2 \phi_0 = \frac{\partial^2 \phi_0}{\partial r^2} + \frac{2}{r} \frac{\partial \phi_0}{\partial r} \quad -(9)$$

where:

$$\frac{\partial \phi_0}{\partial r} = -\frac{2}{a^{5/2}} e^{-r/a}, \quad -(10)$$

$$\frac{\partial^2 \phi_0}{\partial r^2} = \frac{2}{a^{7/2}} e^{-r/a}. \quad -(11)$$

so:

$$\nabla^2 \phi_0 = \frac{2}{a^{5/2}} \left(\frac{1}{a} - \frac{2}{r} \right) e^{-r/a} \quad -(12)$$

$$= -\frac{4mc}{\hbar} \frac{1}{r_{vac}} \cdot \frac{2}{a^{3/2}} e^{-r/a} \quad -(13)$$

from eq. (7).

$$\boxed{\begin{aligned}\frac{1}{r_{vac}} &= \frac{\hbar}{2mca}\left(\frac{1}{a}-\frac{2}{r}\right) \\ &= 0.1440\left(\frac{1}{a}-\frac{2}{r}\right)\end{aligned}} \quad -(14)$$

So:

$$\frac{1}{r}-\frac{1}{r_{vac}} = \frac{1}{r}+\frac{0.2880}{r}-\frac{0.1440}{a}$$

$$= \frac{1.2880}{r}-\frac{0.1440}{a}. \quad -(15)$$

i.e $$\boxed{\frac{1}{r} \rightarrow \frac{1.2880}{r}-\frac{0.1440}{a}} \quad -(16)$$

<u>in the first approximation</u>

The radial distribution function is:

$$f(r) = 4\pi r^2 \phi_0^2(1s) \quad -(17)$$

and its maximum is at

$$r = a \quad -(18)$$

At this point:

$$\frac{1}{r} \rightarrow \frac{1.1440}{r} \quad -(19)$$

<u>and the energy level is increased</u>.

4)

This calculation must now be repeated for:

$$\psi_0(2S) = \frac{1}{2\sqrt{2}\,a^{3/2}}\left(2 - \frac{r}{a}\right) e^{-r/(2a)} \quad -(20)$$

and

$$\psi_0(2p_z) = \frac{1}{4}\left(\frac{1}{2\pi a^3}\right)^{1/2} \frac{r}{a} \cos\theta \, e^{-r/(2a)} \quad -(21)$$

and the equivalent of eq. (19) found. The difference in the vacuum effects on eqns (20) and (21) gives a first approximation to the Lamb shift.