3(1): Variation of the H_1 Hamiltonian

The complete hamiltonian being considered is:

$$\hat{H}\psi = \frac{e}{4m^2c^2}\left(\underset{\sim}{r}\cdot\underline{p} + i\underline{\sigma}\cdot\underline{L}\right)\frac{\phi}{r^2}\left(\underset{\sim}{r}\cdot\underline{p} + i\underline{\sigma}\cdot\underline{L}\right)\psi \quad -(1)$$

and the H_1 hamiltonian is:

$$\hat{H}_1\psi = \frac{e}{4m^2c^2}\underset{\sim}{r}\cdot\underline{p}\left(\frac{\phi}{r^2}\underset{\sim}{r}\cdot\underline{p}\,\psi\right) \quad -(2)$$

$$= -\frac{ie\hbar}{4m^2c^2}\, r\frac{\partial}{\partial r}\left(\frac{\phi}{r^2}\underset{\sim}{r}\cdot\underline{p}\,\psi\right)$$

In note 252(4) this was evaluated by regarding $\underset{\sim}{r}\cdot\underline{p}$ as a function. In this note the hamiltonian is evaluated by regarding $\underset{\sim}{r}\cdot\underline{p}$ as an operator, so:

$$H_1\psi = -\frac{ie\hbar}{4m^2c^2}\, r\frac{\partial}{\partial r}\left(\frac{\phi}{r^2}\left(-i\hbar r\frac{\partial}{\partial r}\right)\psi\right) \quad -(3)$$

$$= \frac{-e\hbar^2}{4m^2c^2}\, r\frac{\partial}{\partial r}\left(\left(\frac{\phi}{r}\frac{\partial}{\partial r}\right)\psi\right)$$

$$= -\frac{e\hbar^2}{4m^2c^2}\, r\frac{\partial}{\partial r}\left(\frac{\phi}{r}\frac{\partial\psi}{\partial r}\right)$$

Now note that $\partial\psi/\partial r$ is a function of r:

$$\frac{\partial\psi}{\partial r} = f(r) \quad -(4)$$

So

$$\frac{\partial}{\partial r}\left(\frac{\phi}{r} f(r)\right) = \left(\frac{\partial}{\partial r}\left(\frac{\phi}{r}\right)\right) f(r) + \frac{\phi}{r}\frac{\partial f(r)}{\partial r} \quad -(5)$$

using the Leibnitz Theorem. Therefore:

$$\hat{H}_1 \psi = -\frac{e\hbar^2}{4m^2c^2} r\left[\left(\frac{\partial}{\partial r}\left(\frac{\phi}{r}\right)\right)\frac{\partial \psi}{\partial r} + \frac{\phi}{r}\frac{\partial^2 \psi}{\partial r^2}\right] \quad -(6)$$

where

$$\frac{\phi}{r} = -\frac{e}{4\pi \epsilon_0 r^2} \quad -(7)$$

and

$$\frac{\partial}{\partial r}\left(\frac{\phi}{r}\right) = \frac{e}{2\pi \epsilon_0 r^3} \quad -(8)$$

So:

$$\hat{H}_1 \psi = -\frac{e\hbar^2 r}{4m^2c^2}\left[\frac{e}{2\pi \epsilon_0 r^3}\frac{\partial \psi}{\partial r} - \frac{e}{4\pi \epsilon_0 r^2}\frac{\partial^2 \psi}{\partial r^2}\right]$$

$$= \frac{-e^2\hbar^2}{16\pi \epsilon_0 m^2 c^2}\left[\frac{2}{r^2}\frac{\partial \psi}{\partial r} - \frac{1}{r}\frac{\partial^2 \psi}{\partial r^2}\right] \quad -(9)$$

The expectation values of energy are: $-(10)$

$$E_1 = -\frac{e^2\hbar^2}{16\pi \epsilon_0 m^2c^2}\int \psi^*\left(\frac{2}{r^2}\frac{\partial \psi}{\partial r} - \frac{1}{r}\frac{\partial^2 \psi}{\partial r^2}\right) d\tau$$

ere

$$d\tau = r^2 \sin\theta \, dr \, d\theta \, d\phi \quad -(11)$$

ese can be worked out for the hydrogenic orbitals by
puter algebra.