Spring 2000 # 9



Consider the proton to be a spherical shell of charge with radius $R$ (use $R \ll a_0$, the Bohr radius)

→ The Hamiltonian for the Hydrogen atom with a point-like nucleus is:

$$H_0 \psi = -\frac{\hbar^2}{2m} \nabla^2 \psi - \frac{e^2}{r} \psi = E_0 \psi$$ (Gaussian units)

However, if the proton were a shell of charge, its potential would be

$$V_p(r) = \begin{cases} e/R & r < R \\ e/r & r > R \end{cases}$$

Thus the new Hamiltonian would be:

$$H \psi = -\frac{\hbar^2}{2m} \nabla^2 \psi - \left(\frac{e^2}{R}\right) \psi = E \psi \qquad \text{for } r < R$$

The Hamiltonian would be unchanged for $r > R$

Then for $H = H_0 + H' \Rightarrow H' = H - H_0$

$$H' = -\frac{e^2}{R} + \frac{e^2}{r} = -e^2\left(\frac{1}{R} - \frac{1}{r}\right) \qquad r < R$$

the 1st order correction to the energy is given by

$\langle \psi | H' | \psi \rangle$ $\quad \psi$ = unperturbed eigenstate

Recall $\psi_{ground} = R_{10} Y_{00} = 2 a^{-3/2} e^{-r/a} \frac{1}{\sqrt{4\pi}}$

So

$$\langle \psi | H' | \psi \rangle = \int_0^{2\pi}\int_0^{\pi}\int_0^{R} \frac{-e^2}{\pi} a^{-3} e^{-2r/a} \left(\frac{1}{R} - \frac{1}{r}\right) r^2 \sin\theta \, dr \, d\theta \, d\varphi$$

Now, since $r \ll a$, $e^{-2r/a} \approx 1$, also $\int_0^{2\pi}\int_0^{\pi} \sin\theta \, d\theta \, d\varphi = 4\pi$

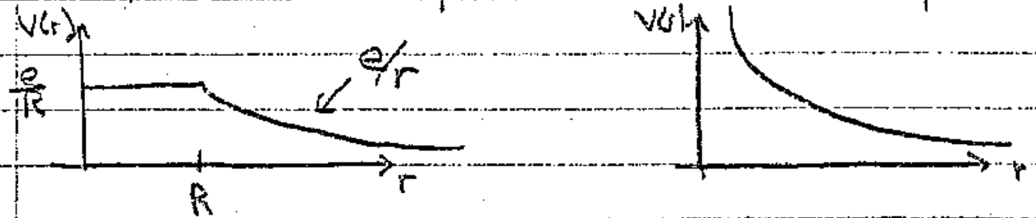
$$\langle \psi | H' | \psi \rangle = -4 e^2 a^{-3} \int_0^R \left(\frac{r^2}{R} - r\right) dr$$

$$= -4 e^2 a^{-3} \left[\frac{R^3}{3R} - \frac{R^2}{2}\right] = -4\pi e^2 a^{-3} \left[\frac{2R^2 - 3R^2}{6}\right]$$

$$\boxed{\langle \psi | H' | \psi \rangle = \frac{2}{3} e^2 a^{-3} R^2}$$

b) Does the sign of the result make physical sense?

Yes, if one compares the different potentials one sees:




Shell proton                Point proton

In the case of the shell proton, the potential will interact more weakly with the electron's wave function for $r < R$ than it would for the point proton. This would make the atom easier to dissociate, as the result to (a) indicates.

c) Estimate the magnitude of this correction in eV units.

$$\Delta E = \frac{2}{3} e^2 R^2 a^{-3}$$

now use $a = \frac{\hbar}{mc\alpha}$, $R \approx 10^{-5}\,\text{Å}$, $e^2 = \alpha\hbar c$, $m = 0.511 \times 10^6\ \frac{eV}{c^2}$

$$\Delta E = \frac{2}{3} \alpha\hbar c\ (10^{-5}\,\text{Å})^2\ \frac{m^3 c^3 \alpha^3}{\hbar^3}$$

$$\Delta E = \frac{2}{3} (10^{-10}) (\text{Å})^2 \frac{\alpha^4 m^3 c^4}{\hbar^2}$$

$\frac{2}{3} \approx 1$   $m \approx 10^6\ \frac{eV}{c^2}$   $\alpha \approx 10^{-2}$

$$\Delta E \approx \frac{(10^{-10})(10^{-8})(10^{18})(\text{Å})^2 (eV)^3}{\hbar^2 c^2}$$

now use $\hbar c \approx 1974\ eV \cdot \text{Å} \approx 10^3\, eV \cdot \text{Å}$

$$\boxed{\Delta E = 10^{-6}\ eV}$$