CBE 310 Molecular Concepts and Applications

09 26 2014

ANNOUNCEMENTS:

Reading chapters 1-5 and 7 of Lowe, we will be going over material in 4, 5 and 7 in a somewhat piecemeal and back and forth manner. (Chapter 8,9,10 in Atkins cover 1-7 in Lowe)

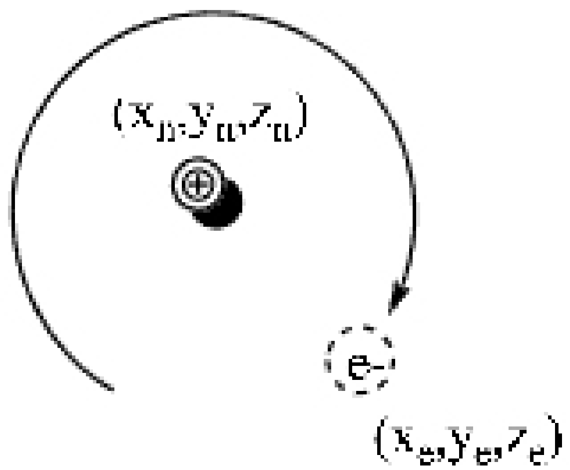
Chapter 13 in Atkins on Spectroscopy

This is going to be as far as we go.

1) A little more about the Hydrogen Atom Solutions
   p_x and p_y, Nodal positions, Energies
2) Rovibratinal Spectroscopy of HCL
3) More parts to the problem: Stern-Gerlach Experiment
3) Electron Spin
4) Spectroscopy: How do light and matter interact?
5) Atoms beyond hydrogen additional components of the wave function

Schrödinger's solution to Hydrogen Atom

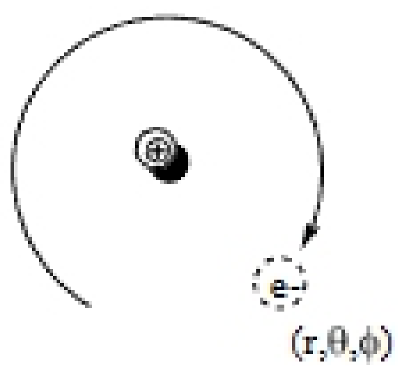
the Hamiltonian:



$$\left[\frac{-h^2}{8\pi\mu}\left(\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}+\frac{\partial^2}{\partial z^2}\right)-\frac{Ze^2}{4\pi\varepsilon_0\sqrt{x^2+y^2+z^2}}\right]$$

Becomes:

$$\left[\frac{-h^2}{8\pi\mu}\nabla^2-\frac{Ze^2}{4\pi\varepsilon_0 r}\right]\psi(r,\theta,\phi)=E\psi(r,\theta,\phi)$$



Notice that potential is only a function of r, that is it has spherical symmetry.

$$\nabla^2=\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right)+\frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right)+\frac{1}{r^2\sin^2\theta}\frac{\partial^2}{\partial\phi^2}$$

Schrödinger's Solution to Hydrogen Atom

We begin the solution of this problem by making the assumption that ψ(r,θ,φ,) can be expressed as the product of functions each of a single variable:

$$\psi(r,\theta,\varphi) = R(r)\Theta(\theta)\Phi(\varphi)$$

Because the individual dimensions are independent (we can separate them) they must have constant values or else we would not be dealing with eigen value equation

$$\frac{\partial^2}{\partial\phi^2}\Phi = -m^2\Phi$$

Φ Solutions are easy (particle in a ring)

$$\frac{1}{R}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right)R + \left(\frac{Ze^2}{4\pi\varepsilon_0 r} + E\right)\frac{8\pi r^2\mu}{h^2} = \beta$$

R Solutions are hard
(solve as in harmonic oscillator)

$$\frac{\sin\theta}{\Theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\Theta\right) - \frac{m^2}{\sin^2\theta} = -\beta$$

Θ Solutions are hard
(solve as in harmonic oscillator)