CBE 310
Molecular Concepts and Applications

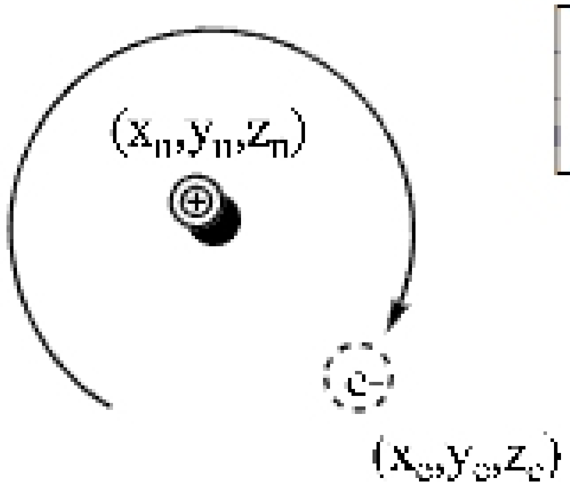
Hydrogen Atom and Angular Momentum

09 24 2014

Reading: Chapter 4 of Lowe
Chapter 13 of Atkins
(Rotational and Vibrational Spectra)

HW#4 Due next Wednesday 10/1

Schrödinger's solution to Hydrogen Atom

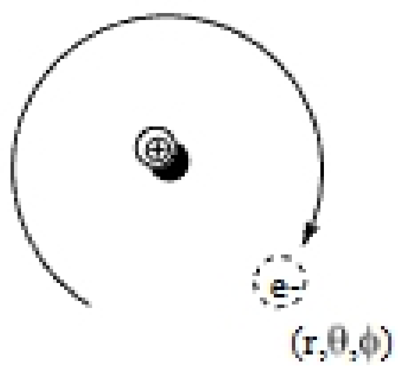


$$\left[\frac{-h^2}{8\pi M_n}\left(\frac{\partial^2}{\partial x_n^2}+\frac{\partial^2}{\partial y_n^2}+\frac{\partial^2}{\partial z_n^2}\right)-\frac{h^2}{8\pi m_e}\left(\frac{\partial^2}{\partial x_e^2}+\frac{\partial^2}{\partial y_e^2}+\frac{\partial^2}{\partial z_e^2}\right)-\frac{Ze^2}{4\pi\varepsilon_0\sqrt{(x_n-x_e)^2+(y_n-y_e)^2+(z_n-z_e)^2}}\right]$$

1) Move to Center of mass Coordinate system

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

Becomes:



2) Because the potential is only a function of r, the problem has spherical symmetry, move to spherical cooordinates

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

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

Schrödinger's solution to Hydrogen Atom

We begin the solution of this problem by making the assumption that $\psi(r,\theta,\varphi,)$ can be expressed as the product of functions each of a single variable:

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

Φ solution = Particle in a ring solution

$$\frac{1}{\Phi}\frac{\partial^2}{\partial\phi^2}\Phi = \text{constant} \equiv -m^2$$

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

Θ, R solution ==> Follow logic of Harmonic oscillator solution

The solutions to the equation in Θ and R are obtained in a manner analogous to the solutions to the harmonic oscillator:

(1) Transform into a modified coordinate system to simplify the resulting solutions
(2) Write the solutions as power series and generate a recursion relation
(3) Choose the appropriate functions, when terms misbehave.
(4) Have the series terminate to keep it from blowing up.
(5) The get a known class of polynomials as the solutions