

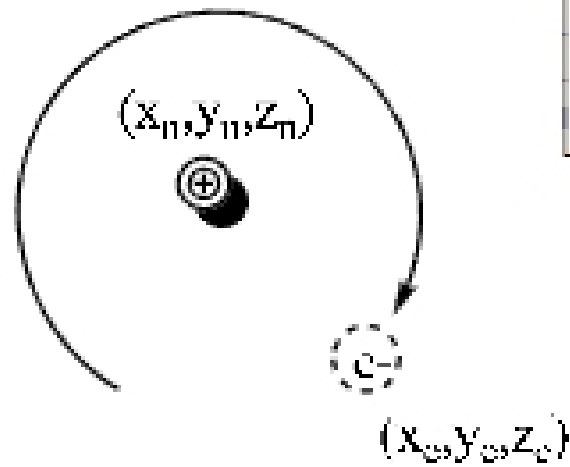
CBE 310
Molecular Concepts and Applications
Hydrogen Atom and Angular Momentum

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

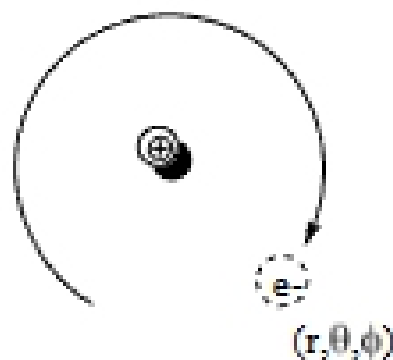


$$\left[\frac{-h^2}{8\pi M_n} \left(\frac{\partial^2}{\partial x_n^2} + \frac{\partial^2}{\partial y_n^2} + \frac{\partial^2}{\partial z_n^2} \right) - \frac{h^2}{8\pi m_e} \left(\frac{\partial^2}{\partial x_e^2} + \frac{\partial^2}{\partial y_e^2} + \frac{\partial^2}{\partial z_e^2} \right) - \frac{Ze^2}{4\pi\epsilon_0 \sqrt{(x_e - x_n)^2 + (y_e - y_n)^2 + (z_e - z_n)^2}} \right]$$

1) Move to Center of mass Coordinate system

$$\left[\frac{-h^2}{8\pi\mu} \left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} \right) - \frac{Ze^2}{4\pi\epsilon_0 \sqrt{x^2 + y^2 + z^2}} \right]$$

Becomes:



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

$$\left[\frac{-h^2}{8\pi\mu} \nabla^2 - \frac{Ze^2}{4\pi\epsilon_0 r} \right] \psi(r, \theta, \phi) = E \psi(r, \theta, \phi)$$

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

Schrödinger's solution to Hydrogen Atom

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

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

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 $\implies$
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