Electrons in an Infinite Square Well

$$E = \frac{p^2}{2m} = \frac{\hbar^2 k^2}{2m} = \frac{h^2}{32m}\left(\frac{n_x^2}{a^2} + \frac{n_y^2}{b^2} + \frac{n_z^2}{c^2}\right)$$

$$a = 1 \;\; Angstrom = 10^{-10}\, m$$

$$b = 1 \;\; Angstrom = 10^{-10}\, m$$

$$c = 2 \;\; Angstrom = 2 \times 10^{-10}\, m$$

$$E \approx 6 \;\; eV(n_x^2 + n_y^2 + \frac{1}{4} n_z^2)$$

0 0 1 = 1.5 eV

1 0 0 = 6 eV

0 1 0 = 6 eV

0 0 2 = 6 eV

1 0 1 = 7.5 eV

0 1 1 = 7.5 eV

1 1 1 = 13.5 eV

1 0 2 = 12 eV

0 1 2 = 12 eV

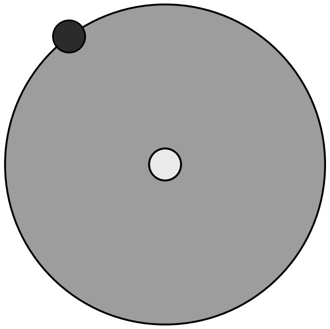
States for which energies are the same are degenerate

Quantum Mechanics of Atoms

- Solve the SE for a Coulomb potential U~1/r
- Simplest case is hydrogen atom
- Initial motivation from atomic spectra
- Rydberg formula

$$\frac{1}{\lambda} = R\left(\frac{1}{n_2^2} - \frac{1}{n_1^2}\right)$$

$$R(hydrogen) = 1.1 \times 10^7 m^{-1}$$



Hydrogen Atom

$$U = -\frac{keZe}{r},\ \ k = \frac{1}{4\pi\varepsilon_0},\ \ e = 1.6\times 10^{-19}\ \ eV,\ \ Z = atomic\ \ number$$

$$F = -\frac{dU}{dr} = \frac{kZe^2}{r^2} = \frac{mv^2}{r}\ \ equation\ \ for\ \ force$$

$$K = \frac{1}{2}mv^2 = \frac{1}{2}\frac{kZe^2}{r},\ \ equation\ \ for\ \ kinetic\ \ energy$$

$$E = K + U = \frac{1}{2}\frac{kZe^2}{r} - \frac{keZe}{r} = -\frac{1}{2}\frac{kZe^2}{r}$$

Chapter 37, Notes 1

Physics 2403, Fall 2000

Chapter 37: Notes 1

Nils Bohr proposed an *ad hoc* quantization condition on the angular momentum of an orbital electron in a hydrogen atom. The condition is that allowed values of angular momentum are quantized in units of nh/(2π), where n is a positive integer.

1. Write down the equation for angular momentum for an electron in a circular orbit as a function of the electron mass, the electron velocity and the orbital radius.
2. Now express the same angular momentum as a function of the energy of the electron and as many other quantities as you need.
3. Set this orbital angular momentum equal to nh/(2π). Now solve the equation you determined in part 2 above for the energy E.
4. Find the energy difference for two energy levels, one with quantum number n_1 and the other with quantum number n_2.
5. Write this energy difference in a similar form to the Rydberg equation. Remember that E=hf=hc/λ. In other words, 1/λ = ΔE/hc, where ΔE is the difference that you worked out in part 4 above. What combination of fundamental constants such as h,c,e, etc. form the Rydberg constant? How different are the numerical values between these constants and the Rydberg constant.

Bohr’s Condition

- Bohr proposed quantization of angular momentum in about 1912, a decade before deBroglie’s wave hypothesis
- Using a wave model for electrons, angular momentum quantization is required for wave continuity
- Show that $2\pi r=n\lambda=nh/p$ is equivalent to the Bohr quantization condition on angular momentum

Bohr Orbit Radius

What is the radius of the first Bohr orbit?

Bohr Orbit Radius

What is the radius of the first Bohr orbit?

$$\lambda = 2\pi a_0$$

$$a_0 = \frac{\lambda}{2\pi} = \frac{\hbar}{p} = \frac{\hbar}{\sqrt{2mE}}$$

$$E = -\frac{k^2 e^4 m}{2\hbar^2}$$

$$a_0 = \frac{\hbar^2}{ke^2 m} = 0.529 \quad Angstroms$$

SE in 3-dimensional spherical coordinates

$$-\frac{\hbar^2}{2m}\nabla^2\varphi + U(r)\varphi = E\varphi$$

$$-\frac{\hbar^2}{2mr^2}\left[\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right)+\left[\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right)+\frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2}\right]\right]\varphi + U(r)\varphi = E\varphi$$

Solve PDE by separation of variables

Radial Equation

- Potential energy U(r) depends on radius alone in the absence of a magnetic field
- Hydrogen atom is energy-degenerate with respect to both azimuthal angle and polar angle dependence

Hydrogen Atom Wave Functions

$$\varphi_{100} = \frac{1}{\sqrt{4\pi}} \frac{2}{a_0^{3/2}} e^{-r/a_0}$$

$$\varphi_{200} = \frac{1}{\sqrt{4\pi}} \frac{2}{(2a_0)^{3/2}} \left(1 - \frac{r}{2a_0}\right) e^{-r/(2a_0)}$$

$$\varphi_{211} = -\frac{1}{\sqrt{8\pi}} \frac{1}{(2a_0)^{3/2}} \sin\theta e^{i\phi} \left(\frac{r}{a_0}\right) e^{-r/(2a_0)}$$

$$\varphi_{210} = \frac{1}{\sqrt{4\pi}} \frac{1}{(2a_0)^{3/2}} \cos\theta \left(\frac{r}{a_0}\right) e^{-r/(2a_0)}$$