Hydrogen Atom

Byungjoon Min October 26, 2018 From Coulomb's law, the potential energy is

$$V(r) = -\frac{e^2}{2\pi\epsilon_0}\frac{1}{r}.$$

Then, the radial equation of Schrödinger equation in the spherical coordinate, Then, we have radial and angular equations:

$$-\frac{\hbar^2}{2m}\frac{d^2u}{dr^2} + \left[-\frac{e^2}{4\pi\epsilon_0}\frac{1}{r} + \frac{\hbar^2}{2m}\frac{l(l+1)}{r^2}\right]u = Eu.$$
 (1)

Defining

$$\kappa = \frac{\sqrt{-2mE}}{\hbar}, \quad \rho = \kappa r, \quad \rho_0 = \frac{me^2}{2\pi\epsilon_0\hbar^2\kappa},$$

so that

$$\frac{d^2u}{d\rho^2} = \left[1 - \frac{\rho_0}{\rho} + \frac{l(l+1)}{\rho^2}\right]u.$$

Due to the asymptotic form of the solution as $\rho \to \infty$ and $\rho \to 0$, the solution should have the form:

$$u(\rho) = \rho^{l+1} e^{-\rho} v(\rho).$$

Finally, we have an equation with $v(\rho)$ as

$$\rho \frac{d^2 v}{d\rho^2} + 2(l+1-\rho)\frac{dv}{d\rho} + [\rho_0 - 2(l+1)]v = 0.$$

Trying a power series solution as

$$v(\rho) - \sum_{j=1}^{\infty} c_j \rho^j,$$

we have the following recursion folmula of the coefficients:

$$c_{j+1} = \left[\frac{2(j+l+1) - \rho_0}{(j+1)(j+2l+2)}\right] c_j.$$
 (2)

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Note that for large j,

$$c_{j+1} \approx \frac{2j}{j(j+1)} c_j = \frac{2}{j+1} c_j,$$

 $v(\rho) \approx c_0 \sum_{j=0}^{\infty} \frac{2^j}{j!} \rho^j = c_0 e^{2\rho}.$

In order to prevent divergence at large ρ (equivalently large r), the series must terminate at some maximal integer j_{max} . Therefore

$$c(j_{max} + l + 1) - \rho_0 = 0.$$

Defining principal quantum number n as $n = j_{max} + l + 1$, we have

$$\rho_0 = 2n,$$
$$E = -\frac{\hbar^2 \kappa^2}{2m}$$

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The eigenvalue of Hydrogen Atom is then

$$E_n = -\left[\frac{m}{2\hbar^2} \left(\frac{e^2}{4\pi\epsilon_0}\right)^2\right] \frac{1}{n^2} = \frac{E_1}{n^2}, \quad n = 1, 2, 3, \cdots.$$

And, the ground state is the case n = 1:

$$E_1 = -\left[\frac{m}{2\hbar^2} \left(\frac{e^2}{4\pi\epsilon_0}\right)^2\right] = -13.6eV.$$

In general, the wave function of hydrogen atom can be represented with an associated Laguerre polynomial,

$$\psi_{nlm} = \sqrt{\left(\frac{2}{na}\right)^3 \frac{(n-l-1)!}{2n[(n+1)!]^3}} e^{-r/na} \left(\frac{2r}{na}\right)^l \left[L_{n-l-1}^{2l+1}(2r/na)\right] Y_l^m(\theta,\phi).$$
(3)

The difference between two states in hydrogen atom is

$$\Delta E = E_i - E_f = -13.6eV\left(\frac{1}{n_i^2} - \frac{1}{n_f^2}\right).$$

The energy of a photon is

$$E = \hbar\omega = h\nu = \frac{hc}{\lambda},$$
$$\frac{1}{\lambda} = R\left(\frac{1}{n_f^2} - \frac{1}{n_i^2}\right),$$

where
$$R = \frac{m}{4\pi c \hbar^3} \left(\frac{e^2}{4\pi\epsilon_0}\right)^2 = 1.097 \times 10^7 m^{-1}.$$