Lecture 3

Hydrogen atom continued

$$K = \left(\frac{me^2}{4\pi\varepsilon_0\hbar^2}\right)\frac{1}{n} \equiv \frac{1}{a_0}\frac{1}{n}$$

$$a_0 \equiv \frac{4\pi\varepsilon_0\hbar^2}{me^2} = 0.529 \times 10^{-10}\,m \quad \text{Bohr radius}$$

$$\rho = \frac{r}{a_0 n}$$

Put everything together:

$$\psi_{nlm}(r,\vartheta,\phi) = R_{nl}(r)\,Y_l^m(\vartheta,\phi)$$

$$R_{nl}(r) = \frac{1}{r}\rho^{l+1}e^{-\rho}\underbrace{v(\rho)}_{\text{polynomial of degree } j_{max} = n-l-1 \text{ with coeff.}}$$

$$c_{j+1} = \frac{2(j+l+1-n)}{(j+1)(j+2l+2)}c_j$$

Ground state: $n=1$, $l=0$, $m=0$

$$E_1 = -\left[\frac{m}{2\hbar^2}\left(\frac{e^2}{4\pi\varepsilon_0}\right)^2\right] = -\underbrace{13.6\,eV}_{\text{binding energy of the H atom}}$$

Wavefunction of the ground state:

$$\psi_{100}(r,\theta,\phi) = R_{10}(r)\, Y_0^0(\theta,\phi)$$

$c_0 = \text{const}$; $c_1 = 0$

$$\Downarrow$$

$$R_{10}(r) = \frac{c_0}{a_0}\, e^{-\frac{r}{a_0}}$$

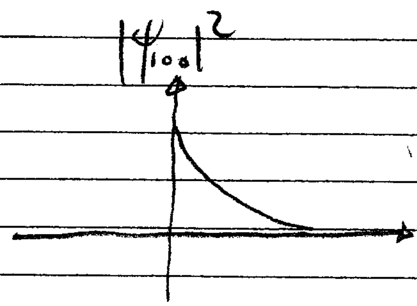
using $\int_0^\infty |R_{10}|^2 r^2 dr = 1 \Rightarrow c_0 = \frac{2}{\sqrt{a_0}}$

$$Y_0^0 = \frac{1}{\sqrt{4\pi}}$$

$$\Downarrow$$

$$\psi_{100}(r,\theta,\phi) = \frac{1}{\sqrt{\pi a_0^3}}\, e^{-\frac{r}{a_0}}$$

Probability distribution $|\psi_{100}|^2 = \frac{1}{\pi a_0^3}\, e^{-\frac{2r}{a_0}}$



s-orbital

For every n

$$l = 0, 1, 2, \ldots, n-1$$

For each l, $(2l+1)$ values of m

$$\Downarrow$$

degeneracy of level $E_n = \sum_{l=0}^{n-1} (2l+1) = n^2$

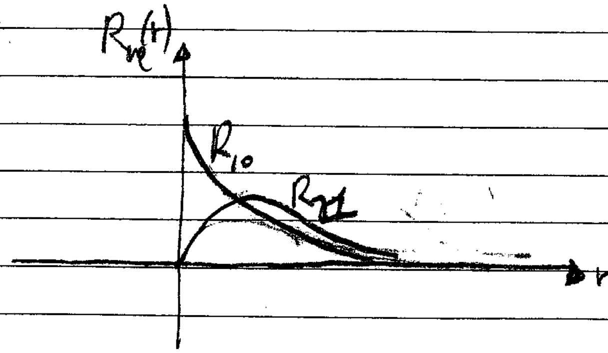
In general

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

$\downarrow$ associated Laguerre polynomial

Energies depend only on n

$$\int \psi^*_{nlm}\, \psi_{n'l'm'}\, r^2 \sin\theta\, dr\, d\theta\, d\phi = \delta_{nn'}\delta_{ll'}\delta_{mm'}$$



The energy spectrum

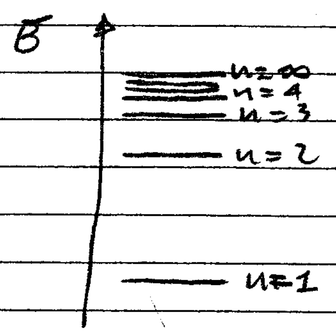
transition energy due to a photon excitation

$$E_\gamma = E_i - E_f = -13.6\,eV\left(\frac{1}{n_i^2} - \frac{1}{n_f^2}\right)$$

$$E_\gamma = h\nu \qquad \nu = \frac{c}{\lambda}$$

$$\frac{1}{\lambda} = R\left(\frac{1}{n_f^2} - \frac{1}{n_i^2}\right) \rightarrow \text{Ry formula}$$

$$R \equiv \frac{m}{4\pi c\hbar^3}\left(\frac{e^2}{4\pi\epsilon_0}\right)^2 = 1.097\times10^7\,m^{-1} = \text{Ry constant}$$



l and m are related to the angular momentum

$$L_x = yp_z - zp_y\,,\quad L_y = zp_x - xp_z\,,\quad L_z = xp_y - yp_x$$

$$L^2 = L_x^2 + L_y^2 + L_z^2$$

$$(\vec{L})_z \rightarrow \hbar m$$

$$[L^2, \vec{L}] = 0 \qquad L^2 \rightarrow \hbar^2 l(l+1)$$

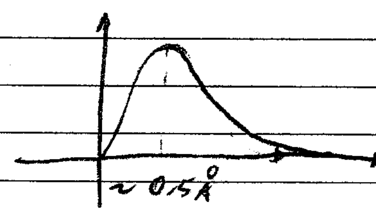
Eigenfunctions of L^2, L_z = spherical harmonics $Y_l^m(\theta,\phi)$

Note on H atom

Probability that an electron is found in a thin spherical shell of radius r and thickness dr

$$|\psi_{100}(r,\theta,\varphi)|^2 \underbrace{dV}_{r^2 dr\, d\Omega} = r^2 dr \int_0^{\pi} d\theta \int_0^{2\pi} d\varphi \sin\theta\, |\psi_{100}|^2 =$$

$$= \frac{4}{a_0^3}\, r^2 e^{-\frac{2r}{a_0}} dr$$



$$\langle r \rangle_{n\ell} = \frac{1}{2} a_0 \left[3n^2 - \ell(\ell+1)\right]$$

$n=1,\ \ell=0 \qquad \langle r \rangle = \frac{3}{2} a_0$