Lecture 27: H Atom cont.

H atom

\[ \left[ -\frac{\hbar^2}{2m} \nabla^2 + V(r) \right] \psi_{n\ell m}(r, \Theta, \Phi) = E_n \psi_{n\ell m}(r, \Theta, \Phi) \]

\[ V(r) = -\frac{e^2}{4\pi \varepsilon_0} \frac{1}{r} \]

Full wave function

\[ \psi_{n\ell m} = \frac{U_{n\ell}}{r} Y_{\ell m}(\Theta, \Phi) \]

\[ \int_0^\infty (U_{n\ell})^2 r^2 \, dr = 1 \]

\[ \alpha = \sqrt{\frac{-2mE_n}{\hbar^2}} \]

\[ \rho = \frac{1}{2\pi} r \]

\[ p_\alpha = \frac{me^2}{2\pi \varepsilon_0 \hbar^2} \]

\[ U_{n\ell}(r) = U(r) = \rho^{l+1} e^{-\rho} V(\rho) \]

\[ V(\rho) = \sum_{j=0}^{\infty} a_j \rho^j \]

Plug into Sch. eq. and find

\[ a_{j+1} = \left[ \frac{2(2j+1) - p_\alpha}{(j+1)(j+2 \ell + 2)} \right] a_j \]

Consider large j limit

\[ a_{j+1} \sim \frac{2}{\ell} a_j \]

\[ a_j \sim \frac{2^j}{\ell^j} A \]
IF series does not terminate
\[ V(p) = A \sum_{j \geq 0} \frac{\epsilon_j}{j!} = Ae^{-p} \]
so \[ U(p) = \rho^{-1} e^{p2} \]
\[ \Rightarrow \text{Series must terminate for some } j_{\text{max}} \]

\[ a \cdot j_{\text{max}+1} = 0 \]

\[ 2(j_{\text{max}} + l+1) - p_c = 0 \]

or \[ p_c = 2n \]

Define principal quantum number \[ n = j_{\text{max}} + l + 1 \]

\[ p_c = 2n = \frac{m e^2}{(2\pi \varepsilon_0 \hbar c)^2} \]

and \[ -\frac{\hbar c}{2m} = E \]

\[ E_n = -\frac{m}{2\hbar^2} \left( \frac{e^2}{4\pi \varepsilon_0} \right)^2 \frac{1}{n^2} \]

\[ n = 1, 2, 3, \ldots \] Bohr formula

\[ E_n = E_1 / n^2 \]

\[ E_1 = -\frac{mc^2}{2} \left( \frac{e^2}{4\pi \varepsilon_0 \hbar c} \right)^2 \]

multiply and divide by \( c^2 \) 2

\[ mc^2 = 0.511 \text{ MeV} = 0.511 \times 10^6 \text{ eV} \]

\[ V = \frac{e^2}{4\pi \varepsilon_0} \frac{1}{r} = \frac{e^2}{4\pi \varepsilon_0} \text{ has units energy} - \text{length} \]
\[ h \alpha = \text{units energy - length also} \]

So \[ \alpha = \frac{e^2}{4\pi \varepsilon_0 \hbar \c} \approx 1/137.036 \]

is dimensionless. Fine structure constant sets strength of E-M interaction.

\[ E_1 = -\frac{mc^2}{2} \alpha^2 = -13.6 \text{ eV} \]

Need to add 13.6 eV to H atom to ionize the electron.

\[ \alpha = \frac{1}{ac} \quad \text{(4)} \]

\[ \alpha = \frac{4\pi \varepsilon_0 \hbar^2}{mc^2} = \frac{\hbar c}{\sqrt{\alpha mc^2}} = \frac{5.29 \times 10^{-11} \text{ Fm}}{0.529 \times 10^{-10} \text{ m}} \]

\[ \hbar c = 197.33 \text{ MeV - Fm} \]

\[ mc^2 = 0.511 \text{ MeV} \]

\[ P = \frac{r}{an} \quad \text{N}_n e^{-P} \]

Thus a called Bohr radius and is a called Bohr radius size of atoms.

Ground state \( n=1 = j_{\text{max}} + l + 1 \)

\[ l = j_{\text{max}} = 0 \quad V(r) = a_o \quad \text{a const} \]

\[ U_{\text{le}} = a_o r^{l+1} e^{-P} = a_o r e^{-\frac{r}{a}} \]

\[ U_{10} = \frac{a_o}{a} r e^{-\frac{r}{a}} \]

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\[ \psi_{100}(r, \theta, \phi) = \frac{U_{10}(r)}{r} Y^0_0(\theta, \phi) \]

Normalized ground state:
\[ \psi_{100} = \frac{1}{\sqrt{4\pi}} e^{-r/a} \]

2nd energy level:
\[ E_2 = \frac{E_1}{2} = \frac{-13.6}{4} = -3.4 \text{ eV} \]

Two choices:
\[ \ell + 1 = 2 \]

(a) \( \ell = 1 \), \( j_{max} = 0 \)
P wave or \( P \) state

(b) \( \ell = 0 \), \( j_{max} = 1 \)
2nd \( S \) state

Note:

Old spectroscopic notation:

Look at \( \ell = 0 \), \( j_{max} = 1 \)
\[ a_1 = \left[ \frac{2(0+0+1) - p_c}{1(2)} \right] a_0 \]
\[ j = 0, \ell = 0 \]
\[ p_c = 2n = 4 \]
\[ a_1 = -a_0 \text{ and } a_2 = 0 \]

\[ U_{20}(r) = \rho e^{-\rho} a_0 [1 - \rho] \]

In general, wave func. is exp. times poly. 4
associated Laguerre polynomial

\[ L^p_{q-p}(x) = (-1)^p \left( \frac{d}{dx} \right)^p L^q(x) \]

and

\[ L^q(x) = e^x \left( \frac{d}{dx} \right)^q (e^{-x} x^q) \]

\[ \Psi_{n\ell m} = \left[ \frac{(2\pi)^3}{(n\pi)^2} \right]^{\frac{1}{2}} \frac{(n-\ell-1)!}{2n[(n+\ell+1)^{3/2}]} \frac{e^{-r/a}}{(2\ell)!} L^{n-\ell-1}(2\ell) \Psi^m_\ell(x, y) \]

\[ P = \frac{r}{na} \]

\[ R_{\ell m}(r) = \frac{U_{\ell m}(r)}{r} \]

\[ \sum_{\ell m} |R_{\ell m}|^2 = 1 \]

\[ R_{10} = 2a^{-3/2} e^{-r/2a} \quad \text{ground state} \]

\[ R_{20} = \frac{1}{\sqrt{2}a^{3/2}} e^{-r/2a} \left[ 1 - \frac{r}{2a} \right] \quad 2s \text{ state} \]

\[ R_{21} = \frac{1}{(2+\ell^2) a^{3/2}} \frac{r}{a} e^{-r/2a} \quad 2p \text{ state} \]

Spectrum of Hydrogen

Consider a transition from \( E_i = \frac{E_1}{i^2} \)

\[ E_f = \frac{E_1}{f^2} \]
The atom can emit a photon of energy
\[ E_Y = E_i - E_f = -13.6 \text{ eV} \left( \frac{1}{n_i^2} - \frac{1}{n_f^2} \right) \]
and the energy of the photon is related to its frequency
\[ E_Y = h \nu \]
Plank's Formula
\[ \frac{1}{\lambda} = R \left( \frac{1}{n_i^2} - \frac{1}{n_f^2} \right) \]
\[ R = \text{Rydberg constant} = \frac{m}{4\pi^2 \hbar^3} \left( \frac{e^2}{4\pi \epsilon_0} \right)^2 \]
\[ R = 1.097 \times 10^7 \text{ m}^{-1} \]

Transitions to \( n_f = 1 \) are in ultraviolet and are called Lyman Series.

Transitions to \( n_f = 2 \) are called Balmer Series.