H atom: one proton, one electron - two body problem

\[ \hat{H} \psi = E \psi \]

Spherical polar coordinates \((x, y, z) \rightarrow (r, \theta, \Phi)\)

\[ E_n = -2.178 \times 10^{-18} J \left(\frac{Z^2}{n^2}\right) \]

Only depends on \(n\)

\[ \psi(r, \theta, \Phi) = \psi_{\text{radial}} \psi_{\text{angular}} \]

- \(n\) principal Quantum Number
- \(l\) the angular momentum quantum number
- \(m_l\) the magnetic quantum number

Electron around a point charge of \(Z\)

\(Z = 1\) for a H atom

\[ E = -E_0 \frac{Z^2}{n^2} \]

\[ E = -2.17 \times 10^{-18} J \frac{Z^2}{n^2} \]

\[ E = -1300 \text{ kJ/mol} \frac{Z^2}{n^2} \]

The wave functions are three dimensional so they should have 3 quantum numbers. Where are the other two?

Since we are dealing with a sphere only the first one involves distance, \(r\), the radius. The others involve angles.

Number of nodes = \((n-1)\)
The wave functions are three dimensional so they should have 3 quantum numbers. Where are the other two?

The second is the azimuthal quantum number, \( l \). It indexes the shape of the orbital, its angular properties.

principal quantum number \( n = 1, 2, 3 \ldots \)

azimuthal quantum number: \( l = 0, 1, 2, \ldots (n-1) \)

s orbitals have no angular dependence. Their \( l \) value is 0. But p orbitals have a angular dependence their \( l \) value is 1.

The quantum numbers

- \( n \) principal q.n. indexes energy
- \( l \) azimuthal q.n. indexes shape
- \( m \) magnetic q.n. tells us which particular orbital.

The magnetic quantum number \( m \) tells us which particular orbital.

\[ m = \pm l \]

The magnetic quantum number \( m_l \) tells us which particular orbital.
The magnetic quantum number $m_l$ tells us which particular orbital.

$m_l = (-l \ldots -1, 0, 1 \ldots l)$

The quantum numbers
- $n$ principal q.n. indexes energy
- $l$ azimuthal q.n. indexes shape
- $m_l$ magnetic q.n. indexes orientation

$n = 1, 2, 3 \ldots$
$l = 0, 1, 2, \ldots n-1$
$m_l = -l \ldots -1, 0, 1 \ldots l$

The $d$ orbitals
- $3d$ (n=3, $l=2$, $m_l = 2$)
- $3dz^2$ (n=3, $l=2$, $m_l = 0$)
- $3dx^2-y^2$ (n=3, $l=2$, $m_l = -2$)
- $3dxy$ (n=3, $l=2$, $m_l = 1$)
- $3dxz$ (n=3, $l=2$, $m_l = -1$)
- $3dyz$ (n=3, $l=2$, $m_l = 1$)

The $s$ orbitals $l = 0$
- $1s$ (n=1, $l=0$, $m_l = 0$)

The $p$ orbitals $l = 1$
- $2p_x$ (n=2, $l=1$)
- $2p_y$ (n=2, $l=1$)
- $2p_z$ (n=2, $l=1$)

The $d$ orbitals $l = 2$
- $3d$ (n=3, $l=2$, $m_l = 2$)
- $3dz^2$ (n=3, $l=2$, $m_l = 0$)
- $3dx^2-y^2$ (n=3, $l=2$, $m_l = -2$)
- $3dxy$ (n=3, $l=2$, $m_l = 1$)
- $3dxz$ (n=3, $l=2$, $m_l = -1$)
- $3dyz$ (n=3, $l=2$, $m_l = 1$)
\[ \psi(r, \theta, \Phi) = \psi_{\text{radial}} \psi_{\text{angular}} \]

Radial Wavefunction (only depends on \( r \))
\[ \psi_{n=1} = \frac{1}{\sqrt{\pi}} \left( \frac{Z}{a_0} \right)^{\frac{3}{2}} e^{-r/a_0} \]
\[ \psi_{n=2} = \frac{1}{4 \sqrt{2} \pi} \left( \frac{Z}{a_0} \right)^{\frac{3}{2}} (2 - \sigma) e^{-2r/a_0} \]
\[ \psi_{n=2} = \frac{1}{4 \sqrt{2} \pi} \left( \frac{Z}{a_0} \right)^{\frac{3}{2}} (2 - \sigma^3) \sin \theta \cos \phi \]
\[ \psi_{n=3} = \frac{1}{8 \sqrt{6 \pi}} \left( \frac{Z}{a_0} \right)^{\frac{3}{2}} 2 \sigma e^{-3r/a_0} (3 \sin^2 \theta - 1) \]

Angular Wavefunction (only depends on \( \Phi \) and \( \Theta \))
\[ \sigma = Z/a_0 \text{ function of } r \]
\[ a_0 = \frac{\alpha_0^2}{\pi m c^2} = 5.29 \times 10^{-11} \text{ m (0.529\text{\textbar}) Bohr radius} \]

Radial Wavefunction depends only on \( r \)
\[ \psi_{1s} \sim e^{-r/a_0} \]
\[ \psi_{2s} \sim (2 - \sigma) e^{-r/a_0} = (2 - \sigma) e^{-2r/2a_0} \]
\[ \psi_{3s} \sim (27 - 18\sigma + 2\sigma^2) e^{-r/3a_0} \]

Sample
Exponential increase and exponential decay
\[ 10^0 = 1 \quad 10^0 = 1 \]
\[ 10^1 = 10 \quad 10^{-1} = 0.1 \]
\[ 10^2 = 100 \quad 10^{-2} = 0.01 \]

Radial wave functions and distributions for the hydrogen atom, \( n \leq n \leq 5 \).
Radial Wavefunction (only depends on $r$)

Angular Wavefunction (only depends on $\Phi$ and $\Theta$)

Angular Wavefunction

$p_z \sim \cos \theta$
$p_x \sim \sin \theta \cos \phi$
$p_y \sim \sin \theta \sin \phi$

d_{z^2} \sim (3\cos^2\theta - 1)

d_{x^2-y^2} \sim \sin^2 \theta \cos 2\phi$

d_{xy} \sim \sin^2 \theta \sin 2\phi$

d_{xz} \sim \sin \theta \cos \theta \cos \phi$

d_{yz} \sim \sin \theta \cos \theta \sin \phi$

Radial Wavefunction:

$$\psi_n = \frac{1}{\sqrt{\pi}} \left( \frac{Z}{a_0} \right)^{1/2} e^{-Zr/a_0}$$

Angular Wavefunction:

$$\psi_l = \frac{1}{\sqrt{4\pi \lambda}} \left( \frac{Z}{a_0} \right)^{1/2} \left( 2 - \frac{m}{l} \right)^{1/2} \sigma^{l-1/2} \sin \theta \cos \phi$$

$$\psi_{l \pm 1} = \frac{1}{\sqrt{4\pi \lambda}} \left( \frac{Z}{a_0} \right)^{1/2} \left( 2 - \frac{m}{l} \right)^{1/2} \sigma^{l-1/2} \sin \phi \cos \theta$$

$$\psi_{l \pm 2} = \frac{1}{\sqrt{4\pi \lambda}} \left( \frac{Z}{a_0} \right)^{1/2} \left( 2 - \frac{m}{l} \right)^{1/2} \sigma^{l-1/2} \sin \theta \sin \phi$$

$$\psi_{l \pm 3} = \frac{1}{\sqrt{8\pi \lambda}} \left( \frac{Z}{a_0} \right)^{1/2} \left( 2 - \frac{m}{l} \right)^{1/2} \sigma^{l-1/2} (3\cos^2 \theta - 1)$$

$\sigma = Z/r/a_0$, function of $r$

$$a_0 = \frac{\hbar^2}{m e^2} = 5.29 \times 10^{-11} m (0.529 \text{ Bohr radius})$$

Energy Levels:

- $E_n = -\frac{\hbar^2}{2m} \frac{1}{a_0^2}$
- $p$ orbitals $l=1$
  - $m_l = \pm 1, 0$
- $d$ orbitals $l=2$
  - $m_l = \pm 2, \pm 1, 0$
- $f$ orbitals $l=3$
  - $m_l = \pm 3, \pm 2, \pm 1, 0$
- $s$ orbitals $l=0$
  - $m_l = 0$
- $p$ orbitals $l=1$
  - $m_l = \pm 1$
- $d$ orbitals $l=2$
  - $m_l = \pm 2, \pm 1, 0, -1$