

The Hydrogen atom 1.

Coulomb potential:

$$V(r) = -k \frac{e^2}{r} = -\frac{1}{4\pi\epsilon_0} \cdot \frac{e^2}{r}$$

Schrödinger equation

$$-\frac{\hbar^2}{2m} \cdot \underbrace{\left(\frac{\partial^2 \psi}{\partial x^2} + \frac{\partial^2 \psi}{\partial y^2} + \frac{\partial^2 \psi}{\partial z^2} \right)}_{\text{Laplace operator : } \Delta} + V\psi = E\psi$$

Laplace operator : Δ

$$-\frac{\hbar^2}{2m} \cdot \Delta\psi + V\psi = E\psi$$

In Cartesian coordinates:

$$\text{Nabla operator : } \nabla = \left(\frac{\partial}{\partial x}, \frac{\partial}{\partial y}, \frac{\partial}{\partial z} \right)$$

$$\text{Laplace operator : } \Delta = \nabla^2 = \left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} \right)$$

Laplace operator in spherical coordinates:

$$\Delta = \frac{1}{r^2} \cdot \frac{\partial}{\partial r} \left(r^2 \frac{\partial}{\partial r} \right) + \frac{1}{r^2 \sin \theta} \frac{\partial}{\partial \theta} \left(\sin \theta \frac{\partial}{\partial \theta} \right) + \frac{1}{r^2 \sin^2 \theta} \cdot \frac{\partial^2}{\partial \phi^2}$$

coordinates : (r, θ, ϕ)

The Hydrogen atom 2.

Separation of variables:

$$\Psi(r, \theta, \varphi) = R(r) \cdot f(\theta) \cdot g(\varphi)$$

Radial equation:

$$\frac{1}{r^2} \cdot \frac{d}{dr} \left(r^2 \frac{dR}{dr} \right) + \frac{2\mu}{\hbar^2} \left[E - V - \frac{\hbar^2}{2\mu} \cdot \frac{l(l+1)}{r^2} \right] R = 0$$

associated Laguerre equation

Polar or angular equation:

$$\frac{1}{\sin \theta} \cdot \frac{d}{d\theta} \left(\sin \theta \cdot \frac{df}{d\theta} \right) + \left[l(l+1) - \frac{m_l^2}{\sin^2 \theta} \right] f = 0$$

associated Legendre equation

Azimuthal equation:

$$\frac{d^2 g}{d\varphi^2} = -m_l^2 \cdot g$$

Quantum numbers:

principal: n ; $n = 1, 2, 3, \dots$

orbital angular momentum: l

$l = 0, 1, 2, \dots (n-1)$;

magnetic: m_l

$m_l = -l, \dots, -1, 0, +1, \dots, +l$; $-l \leq m_l \leq l$

The Hydrogen atom 3.

$$\begin{aligned}\Psi(r, \theta, \varphi) &= R(r) \cdot f(\theta) \cdot g(\varphi) = \\ &= R_{nl}(r) \cdot Y_{lm_l}(\theta, \varphi)\end{aligned}$$

$R_{nl}(r)$: radial wave functions

$$n=1, l=0: R_{10}(r) = \frac{2}{\sqrt{a_0^3}} \cdot e^{-\frac{r}{a_0}}$$

$$n=2, l=0: R_{20}(r) = \frac{1}{\sqrt{(2a_0)^3}} \cdot \left(2 - \frac{r}{a_0}\right) \cdot e^{-\frac{r}{2a_0}}$$

$$n=2, l=1: R_{21}(r) = \frac{1}{\sqrt{3(2a_0)^3}} \cdot \frac{r}{a_0} \cdot e^{-\frac{r}{2a_0}}$$

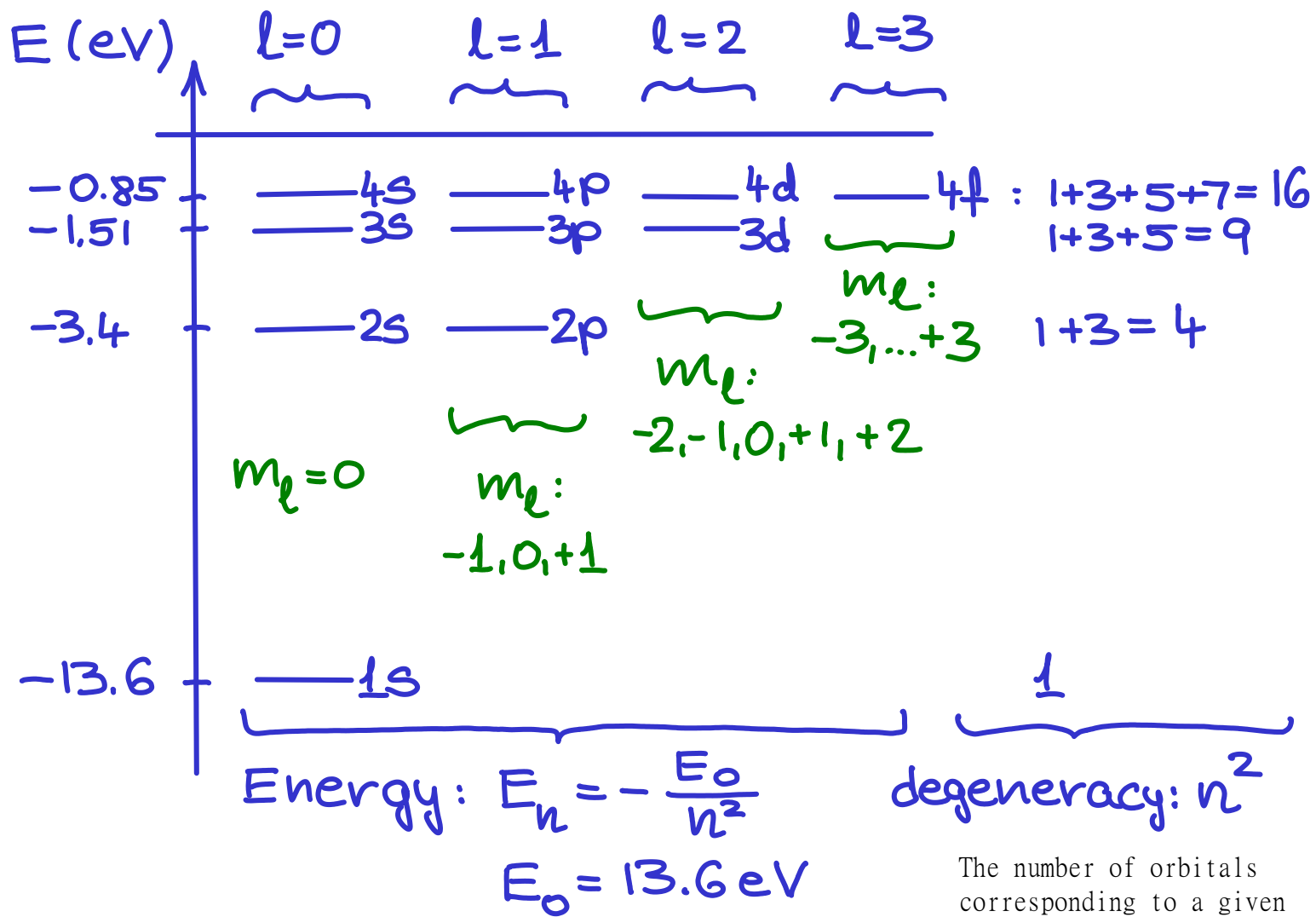
$Y_{lm_l}(\theta, \varphi)$: spherical harmonics

$$l=0, m_l=0: Y_{00} = \frac{1}{\sqrt{4\pi}}$$

$$l=1, m_l=0: Y_{10} = \sqrt{\frac{3}{4\pi}} \cdot \cos\theta$$

$$l=1, m_l=\pm 1: Y_{1\pm 1} = \mp \sqrt{\frac{3}{8\pi}} \cdot \sin\theta \cdot e^{\pm i\varphi}$$

The Hydrogen atom 4.



The number of orbitals corresponding to a given principle quantum number n is n^2

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



$l = 0, 1, 2, 3, 4, 5, \dots$

$s, p, d, f, g, h, \dots$

(label)