

# Hydrogen atom

The hydrogen atom eigenfunction  $\psi_{nlm}(r, \theta, \phi)$  is the product of a radial eigenfunction  $R_{nl}(r)$  and a spherical harmonic eigenfunction  $Y_{lm}(\theta, \phi)$ .

$$\psi_{nlm}(r, \theta, \phi) = R_{nl}(r)Y_{lm}(\theta, \phi)$$

Quantum number  $n$  is the principal quantum number.

$$n = 1, 2, 3, \dots$$

Quantum number  $l$  is the angular momentum quantum number.

$$l = 0, 1, \dots, n - 1$$

Quantum number  $m$  is the magnetic quantum number.

$$m = -l, \dots, 0, \dots, l$$

The normalized radial eigenfunction  $R_{nl}(r)$  is computed from the following formula.

$$R_{nl}(r) = \frac{2}{n^2} \left( \frac{(n-l-1)!}{(n+l)!} \right)^{1/2} \left( \frac{2r}{na_0} \right)^l L_{n-l-1}^{2l+1} \left( \frac{2r}{na_0} \right) \exp \left( -\frac{r}{na_0} \right) a_0^{-3/2}$$

Symbol  $a_0$  is the Bohr radius.

$$a_0 = \frac{4\pi\epsilon_0\hbar^2}{e^2\mu} \approx 0.529 \times 10^{-10} \text{ meter}$$

Symbol  $\mu$  is the reduced mass of the electron.

$$\mu = \frac{m_e m_p}{m_e + m_p}$$

Symbol  $L$  is a Laguerre polynomial computed from the following formula.

$$L_n^m(x) = (n+m)! \sum_{k=0}^n \frac{(-x)^k}{(n-k)!(m+k)!k!}$$

The normalized spherical harmonic eigenfunction  $Y_{lm}(\theta, \phi)$  is computed from the following formula.

$$Y_{lm}(\theta, \phi) = (-1)^m \left( \frac{2l+1}{4\pi} \right)^{1/2} \left( \frac{(l-m)!}{(l+m)!} \right)^{1/2} P_l^m(\cos \theta) \exp(im\phi)$$

Symbol  $P$  is a Legendre polynomial which can be computed using Rodrigues's formula.

$$P_n^m(x) = \frac{1}{2^n n!} (1-x^2)^{m/2} \frac{d^{n+m}}{dx^{n+m}} (x^2-1)^n$$

The eigenfunction  $\psi_n \equiv \psi_{nlm}(r, \theta, \phi)$  solves Schrodinger's equation.

$$\hat{H}\psi_n = E_n\psi_n$$

Symbol  $\hat{H}$  is the Hamiltonian operator for the hydrogen atom.

$$\hat{H}\psi_n = -\frac{\hbar^2}{2\mu}\nabla^2\psi_n - \frac{e^2}{4\pi\epsilon_0 r}\psi_n$$

Symbol  $\nabla^2$  is the Laplacian operator in spherical coordinates.

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

Symbol  $E_n$  is the energy eigenvalue.

$$E_n = -\frac{\mu}{2n^2}\left(\frac{e^2}{4\pi\epsilon_0\hbar}\right)^2 \approx -\frac{1}{n^2} \times 13.6 \text{ eV}$$