Hydrogen eigenfunctions

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.

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

Quantum number l is the angular momentum quantum number.

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

Quantum number m is the magnetic quantum number.

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

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.

$$a_0 = \frac{4\pi\varepsilon_0\hbar^2}{e^2\mu} \approx 0.529\times10^{-10}\,\text{meter}$$

Symbol μ 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.

$$\hat{H}\psi_n = -\frac{\hbar^2}{2\mu}\nabla^2\psi_n - \frac{e^2}{4\pi\varepsilon_0 r}\psi_n$$

Symbol ∇^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.

$$E_n = -\frac{\mu}{2n^2}\left(\frac{e^2}{4\pi\varepsilon_0\hbar}\right)^2 \approx -\frac{1}{n^2} \times 13.6\,\mathrm{eV}$$