

Hydrogen eigenfunctions

Verify

$$H\psi_{nlm}(r, \theta, \phi) = E_n\psi_{nlm}(r, \theta, \phi)$$

where H is the Hamiltonian operator

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

and E_n is the energy eigenvalue

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

Hydrogen eigenfunctions ψ_{nlm} are formed as

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

Radial eigenfunction R_{nl} is formed as

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

Symbol a_0 is the Bohr radius

$$a_0 = \frac{4\pi\epsilon_0\hbar^2}{e^2\mu}$$

Symbol μ is the reduced electron mass

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

Symbol L_n^m is the Laguerre polynomial

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

Symbol Y_{lm} is the spherical harmonic

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

Legendre polynomial $P_l^m(\cos\theta)$ is formed as (see arxiv.org/abs/1805.12125)

$$P_l^m(\cos\theta) = \begin{cases} \left(\frac{\sin\theta}{2} \right)^m \sum_{k=0}^{l-m} (-1)^k \frac{(l+m+k)!}{(l-m-k)!(m+k)!k!} \left(\frac{1-\cos\theta}{2} \right)^k, & m \geq 0 \\ (-1)^m \frac{(l+m)!}{(l-m)!} P_l^{|m|}(\cos\theta), & m < 0 \end{cases}$$

Symbol ∇^2 is the Laplacian operator in spherical coordinates.

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