

Hydrogen eigenfunctions

Verify

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

where \hat{H} is the Hamiltonian operator

$$\hat{H}\psi = -\frac{\hbar^2}{2\mu}\nabla^2\psi - \frac{\hbar^2}{\mu a_0 r}\psi$$

and E_n is the energy eigenvalue

$$E_n = -\frac{\hbar^2}{2n^2\mu a_0^2}$$

Symbol μ is the reduced electron mass

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

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 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

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

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, shown here for spherical coordinates.

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