

Hydrogen atom 1

The Hamiltonian is

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

where μ is the reduced electron mass

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

Symbol ∇^2 is the Laplacian operator

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

We seek eigenfunctions $\psi(\mathbf{r})$ that solve the eigenvalue equation

$$H\psi(\mathbf{r}) = E\psi(\mathbf{r})$$

The eigenfunctions are

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

and the eigenvalues are

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

The allowed quantum numbers are

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

$$l = 0, 1, 2, \dots, n-1$$

$$m = 0, \pm 1, \pm 2, \dots, \pm l$$

For $R_{nl}(r)$ we have

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

where a_0 is the Bohr radius

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

and 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

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

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

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

Eigenmath script