

Assignment on numerical simulation of Hydrogen atom

Hydrogenic atom wave function is $\psi(r, \theta, \phi) = N \frac{u}{r} Y_{lm}(\theta, \phi)$

1. The effective 1-D equation for u is a dimensionless form is

$$\left(\frac{d^2}{d\rho^2} - \frac{l(l+1)}{\rho^2} + \frac{2Z}{\rho} - 2\gamma \right) u = 0$$

Where $\rho = \frac{r}{a}$, $\gamma = -\frac{E}{\frac{e^2}{a}}$, $a = \frac{\hbar^2}{me^2}$ = Bohr Radius

Use Shooting method to find out the eigenvalues (γ) and normalized eigenvectors in 1s, 2s, 3s, 3p and 3d states (Take $Z=1$)

2. Repeat the above problem for 1s state with $Z=1, 2, 4$ and superpose the plots of the normalized eigenvectors

2. Instead of Coulombic potential if a Screened coulomb potential $V(r) = -\frac{e^2}{r} \exp(-\frac{r}{b})$ is used then the The effective 1-D equation for u is a dimensionless form is

$$\left(\frac{d^2}{d\rho^2} - \frac{l(l+1)}{\rho^2} + \frac{2 \exp(-\frac{r}{\lambda})}{\rho} - 2\gamma \right) u = 0$$

Where $b = \lambda a$

a) Find 1s, 2s, 3s states for $\lambda = 10, 20, 50$

b) compare the eigenvalues of 3s, 3p and 3d states with $\lambda = 10$