

H-atom: RK4

In this problem, you will solve the hydrogen atom problem using RK4.

- **The Equations**

The radial Schrödinger equation for the central potential $V(r)$ is given by

$$\left[\frac{d^2}{dr^2} + \frac{2}{r} \right] R(r) + \frac{2\mu}{\hbar^2} \left[E + V(r) - \frac{l(l+1)\hbar^2}{2\mu r^2} \right] R(r) = 0.$$

Here, μ is the reduced mass of the system, l is the orbital-angular momentum quantum number, and $R(r)$ is the radial wave function. The above equation, in atomic units, for the ground state ($l=0$) of the hydrogen atom can be written as

$$\left[\frac{d^2}{dr^2} + \frac{2}{r} \right] R + 2 \left[E_0 + \frac{1}{r} \right] R = 0.$$

Write a Fortran program to solve the above equation using RK4 to find E_0 with following starting values: $R(r = 0.0005) = 0.000001$, $R'(r = 0.0005) = -1000.0$. The r grid will be from 0.0005 unit to 5 unit with 10000 points.

The code will be for a range of E values, $-0.6 \leq E \leq -0.4$, with $\Delta E=0.01$. For finding the correct value of E , plot $R(r)$ and the radial distribution function, $|rR(r)|^2$, against r and check their convergence with respect to E .