

## 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

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

Here,  $\mu$  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

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

Write a 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 its convergence with respect to  $E$ .

