

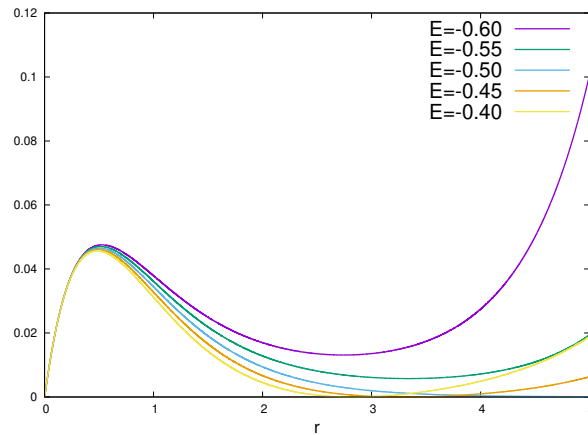
1. The radial Schrödinger equation for the central potential $V(r)$ is given by

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

Here, 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

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

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 . At the E where both $R(r)$ and $|rR(r)|^2$ behave properly against r , that will be the answer. You will submit one zip file, q1.zip, containing the following files: the code, and 5 different output files containing the data for $R(r)$ and $|rR(r)|^2$ vs r . The figure below shows the plot of $|rR(r)|^2$ vs r for 5 different energies. You will show the results for $E = -0.60, -0.55, -0.50, -0.45$ and -0.40 .



2. The energy of the simple harmonic oscillator is $E = \frac{p^2}{2m} + \frac{1}{2}kx^2$. Here m is the mass, k is the spring force constant, and $p = m\dot{x}$ is the momentum. Let us set $m = k=1$, so the angular frequency, ω , and period, T , are given by $\omega = \sqrt{\frac{k}{m}} = 1$, and $T = \frac{2\pi}{\omega} = 2\pi$. Hence, $2E = p^2 + x^2$ is a constant, and a plot of p vs x will be a circle of radius $\sqrt{2E}$. We will solve the Newton's equation of motion $\ddot{x} = -x$ which will be written as two first order differential equations

$$\dot{x} = p \text{ and } \dot{p} = -x. \quad (1)$$

Numerically integrate these equations using the Euler and RK4 methods.

- Use initial conditions, $x = 1$ and $p = 0$. Hence $2E = 1$. Use a time step $h = 0.02T$. Use 200 time steps in total. Plot $2E$ vs t/period , x vs p and x vs t/period .

In the figure below, results obtained using Euler's, RK2 and RK4 methods are shown. **But you need to show the results only for Euler's and RK4 methods.** You will submit a zip file, q2.zip, containing the code(s), and six output files, 3 for each method.

