Flow Chart 7

a) Write down the Schrödinger equation for this problem and convert it from a second-order equation to two first-order ones, as in Example 8.9. Write a program, or modify the one from Example 8.9, to find the energies of the ground state and the first two excited states for these equations when m is the electron mass, $V_0 = 50\,\text{eV}$, and $a = 10^{-11}\,\text{m}$. Note that in theory the wavefunction goes all the way out to $x = \pm\infty$, but you can get good answers by using a large but finite interval. Try using $x = -10a$ to $+10a$, with the wavefunction $\psi = 0$ at both boundaries. (In effect, you are putting the harmonic oscillator in a box with impenetrable walls.) The wavefunction is real everywhere, so you don't need to use complex variables, and you can use evenly spaced points for the solution—there is no need to use an adaptive method for this problem.

The quantum harmonic oscillator is known to have energy states that are equally spaced. Check that this is true, to the precision of your calculation, for your answers. (Hint: The ground state has energy in the range 100 to 200 eV.)

Background info

$$V(x) = \frac{V_0 x^2}{a^2} \quad \text{where } V_0 \text{ \& } a \text{ are constants}$$

$m =$ electron mass, $V_0 = 50\,eV$ $\quad a = 10^{-11}\,m.$ $\quad x = -10a$ to $10a$

w/ $\psi = 0$

a) Convert from secon order equation to two first orders.

Schrödinger equation for this problem:

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + \frac{V_0 x^2}{a^2}(\psi(x)) = E\psi(x)$$

$$\frac{d\psi}{dx} = \phi, \quad \frac{d\phi}{dx} = \frac{2m}{\hbar^2}\left[\frac{a^2}{V_0 x^2} - E\right]\psi$$

Flow Chart for Code for 8.14

Define constants

↓

Define the given Potential Function

↓

Outside of code, convert the time-independent Shrödinger equation from second-order equation to two first-order ones.

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Define the first-order equations

Create a function to calculate the wavefunction for the particular energy

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Use fourth-order Runge-Kutta method

↓

Use secant method to find the energies

↓

Print the ground state energy as well as the first & second excited state energy

Exercise 8.10: Cometary orbits

Eqns. part (a)

$$\frac{d^2x}{dt^2} = -GM\frac{x}{r^3} \qquad \frac{d^2y}{dt^2} = -GM\frac{y}{r^3}$$

$$\frac{dx}{dt} = v_x \quad \frac{dv_x}{dt} = -GM\frac{x}{r^3} \qquad \frac{dy}{dt} = v_y \quad \frac{dv_y}{dt} = -GM\frac{y}{r^3}$$

$$r = \sqrt{x^2+y^2}$$

part (b)

$M = 1.9891 \times 10^{30}$ kg

$G = 6.67408 \times 10^{-11} \frac{N\,m^2}{kg^2}$

$x = 4$ billion kilometers $\qquad \sqrt{\frac{g}{l}}$

$y = 0$

$v_x = 0 \qquad v_y = 500\ ms^{-1}$

b) target accuracy of $\delta = 1$ km. per year

$\varepsilon = ch^5 = \frac{1}{30}(x_1 - x_2) \Rightarrow$ make equal to $\delta = 1$ km

$$h' = h\left(\frac{30h\delta}{|x_1 - x_2|}\right)^{1/4} = h\rho^{1/4}$$

1st step: 2 steps of h start at time t

$$x(t+2h) = x_1 + 2ch^5$$

2: One step of size 2h

$$x(t+2h) = x_2 + 32ch^5$$

For coordinates of a point in a two-dimensional space, use $\sqrt{\epsilon_x^2 + \epsilon_y^2}$

For each variable

$$\epsilon = \frac{1}{30}(x_1 - x_2) \qquad \epsilon = \frac{1}{30}(y_1 - y_2)$$

Flow Chart for 8.10

Part (a)

First, turn the two second-order equations into four first-order equations (done above)

↓

Define constants & initial conditions

↓

To know what fixed step size h to use so that it accurately calculates at least two full orbits of the comet, I can calculate the period of the comet's orbit using Kepler's third law, and then multiply it time 2 (2 full orbits)

↓

Define the four first-order equations

↓

Create empty lists to store the x and y points

↓

For loop to integrate the equations using the fourth-order Runge-Kutta method and append the current values to their respective lists

↓

Plot the comet's trajectory

Part (b & c)

First, turn the two second-order equations into four first-order equations (done above)

Define constants, initial conditions and δ

To know what fixed step size h to use so that it accurately calculates at least two full orbits of the comet, I can calculate the period of the comet's orbit using Kepler's third law, and then multiply it time 2 (2 full orbits) & use an initial value of h

Define the four first-order equations

Create empty lists to store the t, x and y points

A while loop integrate the equations using the fourth-order Runge-Kutta method and calculate the error in the position estimate

Plot the comet's trajectory with the adaptable step size & add dots to the plot at each Runge-Kutta step.