

Homework 8 Write-Up

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1. EXERCISE 8.10 COMETARY ORBITS

where

$$r = \sqrt{x^2 + y^2} \quad (3)$$

First we define all the parameters and constants, and change the DEs into first order DEs such that we are left with Equations 4, 5, 6, 7. This is so that we can use the 4th order Runge-Kutta method.

$$\frac{dx}{dt} = v_x \quad (4)$$

$$\frac{dv_x}{dt} = -GM \frac{x}{r^3} \quad (5)$$

$$\frac{dy}{dt} = v_y \quad (6)$$

$$\frac{dv_y}{dt} = -GM \frac{y}{r^3} \quad (7)$$

So, using the equations above and the Runge-Kutta code detailed in Newman, we can plot the x and y position of the comet. In my program, I made sure that my r vector was now a vector of four since there are four equations instead of the usual two. Because the path of the vector is super long, I found that I have to use approximately 2 billion seconds to plot the full path. With an 1,000,000 steps, I used an h-value of 2 thousand to accurately get the path.

Pseudo Code 8.10

```

{
  fx = vx
  fy = vy
  fvx = -GM(x/r^3)
  fvy = -GM(y/r^3)
}

r[0], r[1], r[2], r[3]
• plot x-points & y-points

Target accuracy:
while time < final time
{
  x1, y1 : runge-kutta w/ step size h * 2
  x2, y2 : runge-kutta w/ step size 2h * 1
  error_x = 1/30 (x1 - x2), error_y = 1/30 (y1 - y2)
  error_total = sqrt(error_x^2 + error_y^2)
  rho = h * delta / error_total (Epu. 8.53)
  if rho > 1:
    continue with t = t + 2h ← save calculated x & y values with good accuracy
  else:
    h' = h * rho^1/4 (bigger h)
    h' = h * rho^1/4 (smaller h)
    repeat
  ★ plot (x points, y points) → (scatter plot for part D)

```

FIG. 1: Pseudo code for Exercise 8.10 Newman.

This exercise helps us explore Newton's second law. We are asked to plot the orbit of a comet around the sun. Assuming the comet stays in one plane of orbit, we can show the motion of the orbit as a system of second-order DEs which we are given in Equation 1 and 2.

$$\frac{d^2x}{dt^2} = -GM \frac{x}{r^3} \quad (1)$$

$$\frac{d^2y}{dt^2} = -GM \frac{y}{r^3} \quad (2)$$

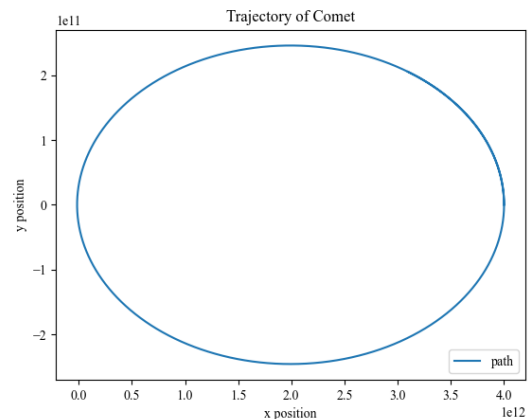


FIG. 2: Path of comet around the Sun.

I plotted the x-points and y-points and as expected, the path of the comet was elliptical as seen in Figure 2.

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The ellipse looks symmetrical and extends significantly along the x-axis. This code, however, took almost 30 seconds to run, which is not ideal.

For Part C, we are asked to repeat this calculation but with a target accuracy. We re-calculate the x-points and y-points by running the Runge-Kutta method with step size h twice and another time by running the Runge-Kutta method once with step size $2h$. Using these two estimates, we can get an error and target accuracy. We can use Equation 8 to see if we reached our target accuracy. When $p > 1$ we have reached the target accuracy. I used an "if" condition to keep the x and y points when it is within accuracy and to increase the h step size with Equation (8.52) from Newman. Otherwise, the h size decreases and re-runs the Runge-Kutta repeats with the same time value. I use a while $t < t_{final}$ condition to end collection of x and y when the time runs out. The resulting plot is seen in Figure 3.

$$\rho = \frac{30h\delta}{|x_1 - x_2|} \quad (8)$$

This method was much faster to run (a few seconds) and to the human eye it looks the same as the path shown in Figure 2.

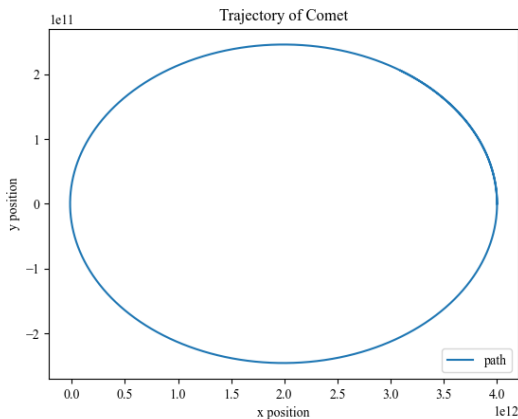


FIG. 3: Path of comet around the Sun.

We were asked to plot the x and y coordinates as a scatter plot to see where the comet slows and speeds. My plot in Figure 4 does not really show this...

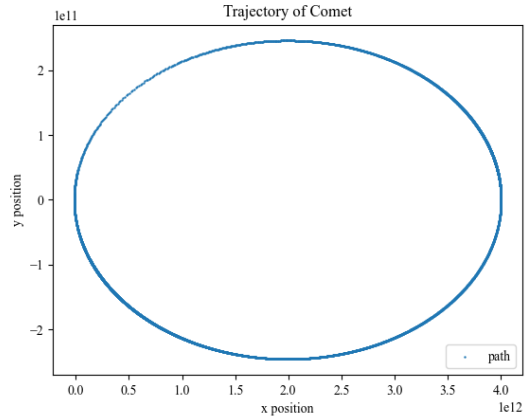


FIG. 4: Path of comet around the Sun.

The expected result would look more like Figure 5, where the comet speeds up near the gravity of the Sun and slows when further away shown by the wider spaced points.

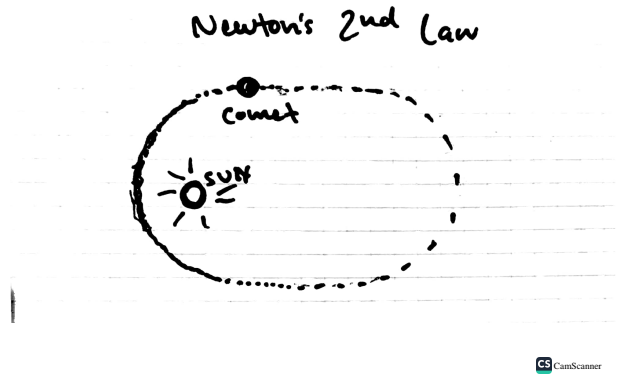


FIG. 5: Theoretical path of comet around the Sun.

2. EXERCISE 8.14 QUANTUM OSCILLATOR

In this exercise, we calculate the energy levels with Schrodinger's equation (9). I modified the code "squarewell.py" in Dr. Grin's GIT which uses Runge-Kutta to calculate energy levels from wavefunctions and input energies.

$$-\frac{\hbar^2}{2m}\nabla^2\psi + V(x)\psi = E\psi \quad (9)$$

Pseudo Code 8.14

(Modify "squarewell.py" code in dgrin & IT)

$$V(x) = V_0 x^2/a^2$$

Normalize:

$$A^2 \int_{-\infty}^{\infty} |\Psi(x)|^2 = 1 \quad (\text{find } A)$$

$$\rightarrow E = E \frac{1}{\sqrt{\int |\Psi(x)|^2}}$$

* Use Simpson's method to get

$$\int_{-5a}^{5a} |\Psi(x)|^2 \quad (\text{input is func } f(x))$$

The plug in E1 & E2 from part b
to get ground state, 1st, 2nd state
→ plot over x = a range (-5a, 5a, h)

→ use array of Ψ for integration

$$\text{Solve } (E) / \sqrt{\int |\Psi(x)|^2}$$

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FIG. 6: Pseudo code for Exercise 8.14 Newman.

First, we find the energy states when the potential is Equation 10. Because it is a quantum harmonic oscillator, the energy states are equally spaced; knowing this and messing around with inputs we find that the ground state and first two energy levels are 178.38eV, 414.08eV, and 690.12eV respectively.

$$V(x) = V_0 x^2/a^2 \quad (10)$$

When the potential is Equation 10, the same energy states are 205.31eV, 735.69eV, and 1443.57eV. From this you can see that is an anharmonic oscillator.

$$V(x) = V_0 x^4/a^4 \quad (11)$$

Finally, we are asked to modify our code to normalize the wavefunction of the anharmonic oscillator using Equation 12. I collected the wavefunctions into an array and ran a Simpson method program to solve the integral, where the input is the wavefunction. Instead of infinite limits, we were told to use the interval from -5a to 5a. I divide the energy by the square-root of Equation 12 - Please refer to Figure 7 for the calculations leading to this conclusion.

$$x = \int_{-\infty}^{\infty} |\Psi(x)|^2 \quad (12)$$

I plotted the normalized energies over the x interval. The general shapes of the levels look right, but I'm not convinced this is actually normalized... but I'm not sure what is wrong.

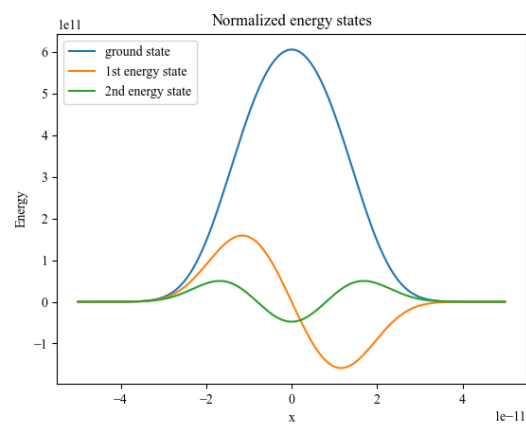


FIG. 7: Energy levels with normalized wavefunctions.

3. SURVEY QUESTIONS

The homework this week took approximately 12 hours. Part C of Exercise 8.10 and Part C of Exercise 8.14 was really difficult for me and I'm still not sure of how where in my code I messed up. I think this week's assignment was too long.