52 + 46.5 + 5 = 103.5

103.5/117

Homework 8 Write-Up

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(Dated: April 5, 2024)

1. EXERCISE 8.10 COMETARY ORBITS

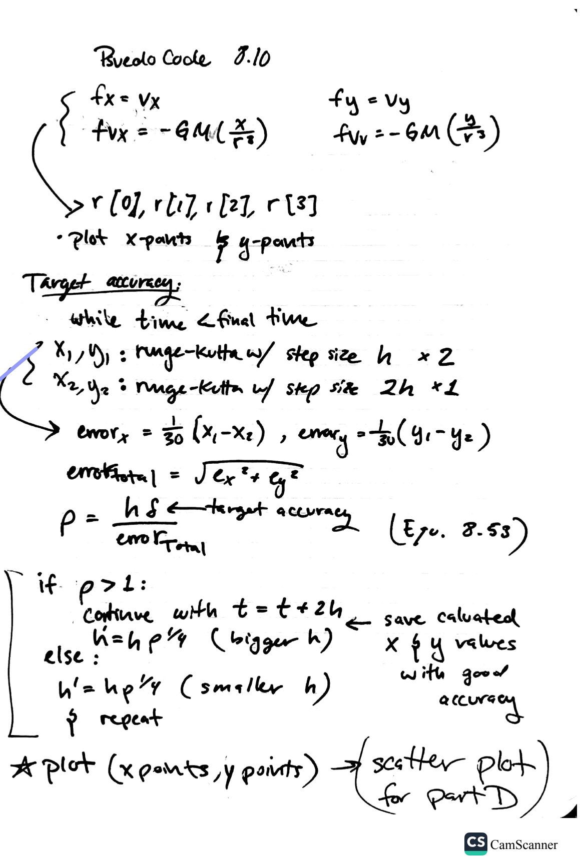

FIG. 1: Pseudo code for Exercise 8.10 Newman.

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.

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

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

where

$$r = \sqrt{x^2 + y^2} \tag{3}$$

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 4h order Runge-Kutta method.

$$\frac{d^x}{dt} = v_x \tag{4}$$

$$\frac{dv_x}{dt} = -GM\frac{y}{r^3} \tag{5}$$

$$\frac{dy}{dt} = v_y \tag{6}$$

$$\frac{dv_y}{dt} = -GM\frac{y}{r^3} \tag{7}$$

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.

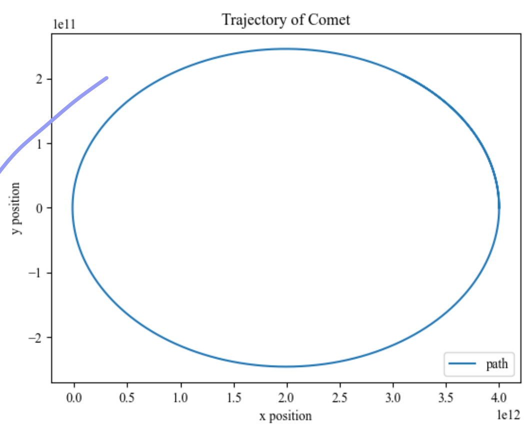

FIG. 2: Path of comet around the Sun.

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.

$$\rho = \frac{30h\delta}{|x1 - x2|} \tag{8}$$

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.

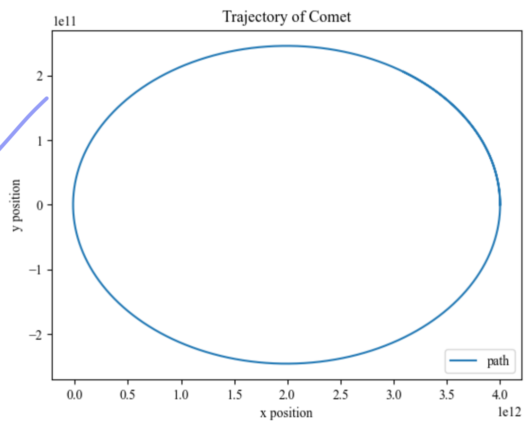

FIG. 3: Path of comet around the Sun.

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...

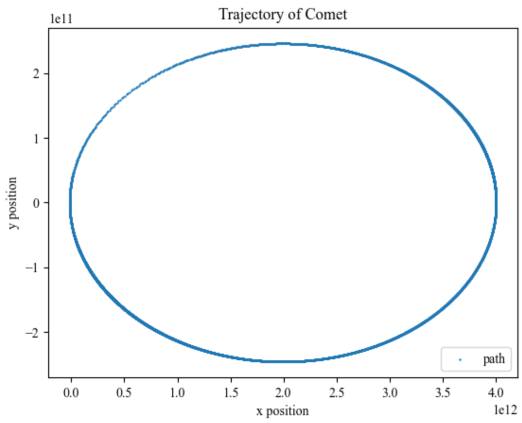

FIG. 4: Path of comet around the Sun.

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.

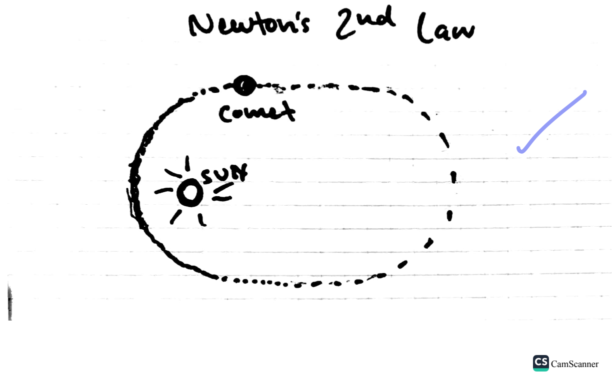

FIG. 5: Theoretical path of comet around the Sun.

Nice!

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.

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

expand on derivation to 1st order

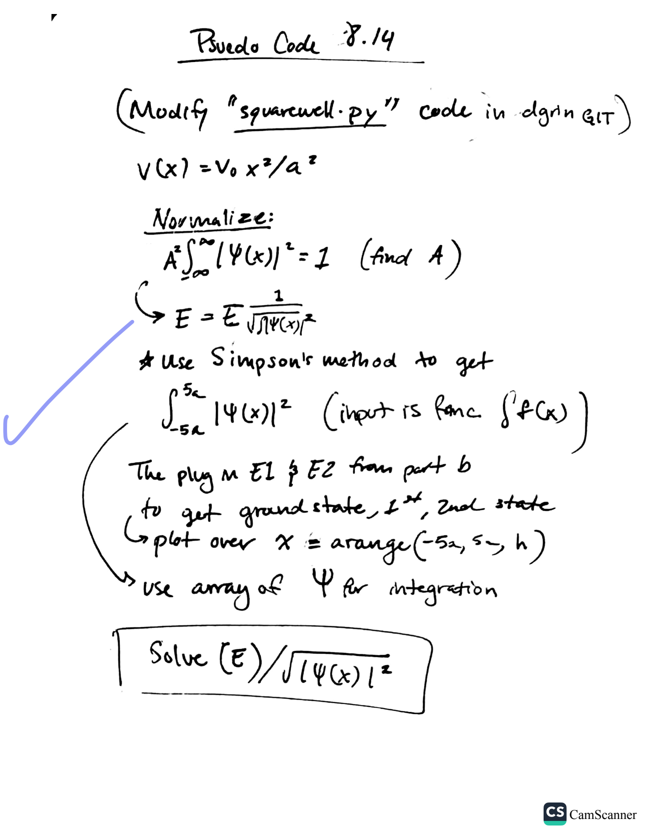

FIG. 6: Pseudo code for Exercise 8.14 Newman.

First, we find the energy states when the potential is Equation 10. Because it is a quantum harmonic oscillator, the energy states are equally states; 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.

$$V(x) = V_0 x^2/a^2 \tag{10}$$

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.

$$V(x) = V_0 x^4/a^4 \tag{11}$$

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.

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

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.

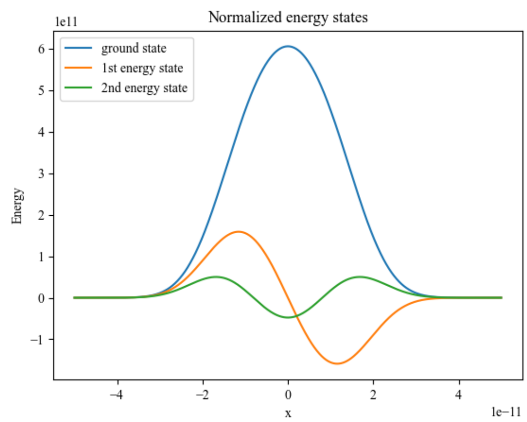

FIG. 7: Energy levels with normalized wavefunctions.

3. SURVEY QUESTIONS .5

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 weeks assignment was too long.

8.10

52/66

Computational Physics/Astrophysics, Winter 2024:

Grading Rubrics [1]

Haverford College, Prof. Daniel Grin

For coding assignments, roughly 56 points will be available per problem. Partial credit available on all non-1 items.

remember plt.show() -1

2 1. Does the program complete without crashing in a reasonable time frame? (+4 points)

plt.savefig causes error -1

2 2. Does the program use the exact program files given (if given), and produce an answer in the specified format? (+2 points)

3 3. Does the code follow the problem specifications (i.e numerical method; output requested etc.) (+3 points)

5 4. Is the algorithm appropriate for the problem? If a specific algorithm was requested in the prompt, was it used? (+5 points)

4 5. If relevant, were proper parameters/choices made for a numerically converged answer? (+4 points)

4 6. Is the output answer correct? (+4 points).

2 7. Is the code readable? (+3 points)

. 5.1. Are variables named reasonably?

. 5.2. Are the user-functions and imports used?

[1] Inspired by rubric of D. Narayanan, U. Florida, and C. Cooksey, U. Hawaii

. 5.3. Are units explained (if necessary)? units? -1

. 5.4. Are algorithms found on the internet/book/etc. properly attributed?

3 8. Is the code well documented? (+3 points)

. 6.1. Is the code author named?

. 6.2. Are the functions described and ambiguous variables defined?

. 6.3. Is the code functionality (i.e. can I run it easily enough?) documented?

9. Write-up (up to 28 points)

5 . Is the problem-solving approach clearly indicated through a flow-chart, pseudo-code, or other appropriate schematic? (+5 points)

✓ . Is a clear, legible LaTeX type-set write up handed in?

3 . Are key figures and numbers from the problem given? (+ 3 points)

4 . Do figures and or tables have captions/legends/units clearly indicated. (+ 4 points)

2 . Do figures have a sufficient number of points to infer the claimed/desired trends? (+ 3 points) too many points in scatter plot, cannot see the results -1

2 . Is a brief explanation of physical context given? (+2 points)

1 . If relevant, are helpful analytic scalings or known solutions given? (+1 point)

3 . Is the algorithm used explicitly stated and justified? (+3 points)

2 . When relevant, are numerical errors/convergence justified/shown/explained? (+2 points)

2 . Are 3-4 key equations listed (preferably the ones solved in the programming assignment) and algorithms named? (+2 points)

1 . Are collaborators clearly acknowledged? (+1 point)

2 . Are any outside references appropriately cited? (+2 point)

8.14

46.5/56

Computational Physics/Astrophysics, Winter 2024:

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Haverford College, Prof. Daniel Grin

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plt.savefig causes error -1

1 2. Does the program use the exact program files given (if given), and produce an answer in the specified format? (+2 points)

remember plt.show() -1

1 3. Does the code follow the problem specifications (i.e numerical method; output requested etc.) (+3 points) (a+b)

Missing first two energy level outputs -2

5 4. Is the algorithm appropriate for the problem? If a specific algorithm was requested in the prompt, was it used? (+5 points)

4 5. If relevant, were proper parameters/choices made for a numerically converged answer? (+4 points)

3 6. Is the output answer correct? (+4 points).

normalization error -1

2.5 7. Is the code readable? (+3 points)

. 5.1. Are variables named reasonably?

. 5.2. Are the user-functions and imports used?

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[1] Inspired by rubric of D. Narayanan, U. Florida, and C. Cooksey, U. Hawaii

. 5.3. Are units explained (if necessary)? missing some units -0.5

. 5.4. Are algorithms found on the internet/book/etc. properly attributed?

3 8. Is the code well documented? (+3 points)

. 6.1. Is the code author named?

. 6.2. Are the functions described and ambiguous variables defined?

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3 . Do figures have a sufficient number of points to infer the claimed/desired trends? (+ 3 points)

0 . Is a brief explanation of physical context given? (+2 points) Explain the difference between the harmonic and anharmonic solution -2

0 . If relevant, are helpful analytic scalings or known solutions given? (+1 point) compare to known solu -1

3 . Is the algorithm used explicitly stated and justified? (+3 points)

2 . When relevant, are numerical errors/convergence justified/shown/explained? (+2 points)

1 . Are 3-4 key equations listed (preferably the ones solved in the programming assignment) and algorithms named? (+2 points)

expand on deriv to 1st order -1

1 . Are collaborators clearly acknowledged? (+1 point)

2 . Are any outside references appropriately cited? (+2 point)