PHYS304 HW7

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Haverford College
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Advice — don't forget \left(around big equations, and to put commas inside equations, etc

1. EXERCISE 8.10: COMETARY ORBITS

An adaptive size method can be useful for a system with the brief but fast-moving period of time. For example, in a rare occasion of a comet travelling very fast for a fly-by and for a brief period of time when their orbit brings them close to the Sun. For the large periods of time when the comet is moving slowly we can use long time-steps, so that the program runs quickly, but short time-steps are crucial for the case like this.

The differential equation obeyed by a comet can be derived from Newton's second law according to the force between the Sun, with mass M at the origin, and a comet of mass m with position vector r, which is $\frac{GMm}{r^2}$ in direction $-r/r$ (i.e., the direction towards the Sun), resulting in the equation,

$$m\frac{d^2 r}{dt^2} = -(\frac{GMm}{r^2})\frac{r}{r} \tag{1}$$

By canceling the m and taking the x component, and similarly for the other two coordinates. We can throw out one of the coordinates because the comet stays in a single plane as it orbits. If we orient our axes so that this plane is perpendicular to the z-axis, we can forget about the z coordinate and we are left with just two second-order equations to solve,

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

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

a) First we turn these two second-order equations into four first-order equations by defining the equation given for the comet and creating arrays for variable sets which we will use in the step.

b) For this part, we are asked to write a program to solve the equations using the fourth-order Runge–Kutta method with a fixed step size. With the mass of the sun and Newton's gravitational constant G as initial conditions, we take a comet at coordinates $x = 4$ billion kilometers and $y = 0$ (close to the orbit of Neptune) with initial velocity of $v_x = 0$ and $v_x = 500$ ms^{-1}. In order to have the accuracy of the trajectory to calculate at least two full orbits, we need a smaller value of h, thus a large number of N points. I use a fixed step size h of 0.00033 (165/500000, for N = 500000) to plot y against x, showing the trajectory of the comet in 1.

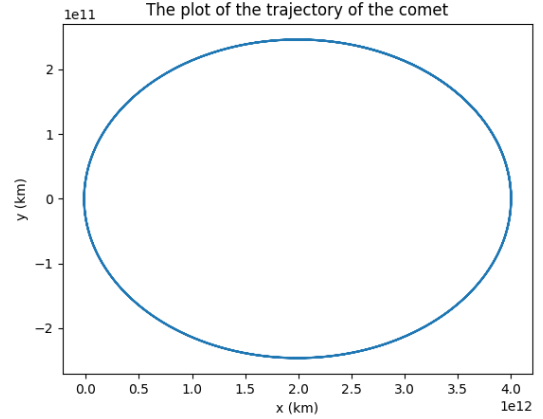According to the graph, we can see that successive orbits of the comet lie on top of one another on the plot

FIG. 1: The plot of the trajectory of the comet with a fixed step size h = 0.00033.

which is a good indicator of an accurate calculation since orbits are periodic. The calculation takes about just more than a minute to run.

c) I make a copy of the program in b) and modify the copy to do the calculation using an adaptive step size with the given target accuracy of $\delta = 1$ kilometer per year in the position of the comet and plot the trajectory. The result below (2) shows that the graph is identical and accurate to the plot in b) (1) as expected. However, with the half of the N points of b) for N = 250000, a step size h is now 0.00066, consequently the the calculation speeds up taking lesser time than b).

d) In the last part, I modify the program to place dots on the graph showing the position of the comet at each Runge–Kutta step around a single orbit. The result (3) shows the steps getting closer together when the comet is close to the Sun and further apart when it is far out in the solar system, as expected for a comet travelling very fast for a fly-by and for a brief period of time.

2. EXERCISE 8.14A-B: QUANTUM OSCILLATORS

Consider the one-dimensional, time-independent Schrodinger equation in a harmonic (i.e.,quadratic) potential,

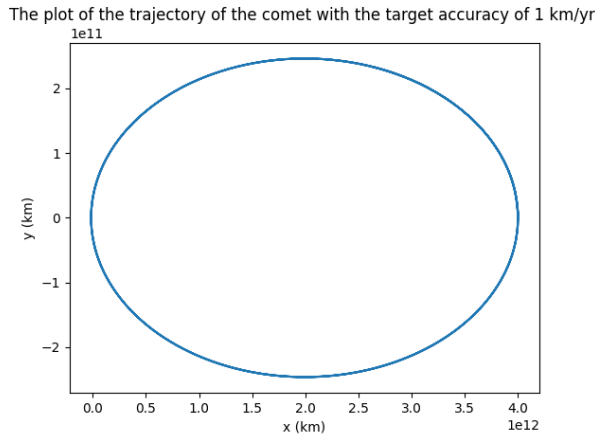$$V(x) = \frac{V_0 x^2}{a^2} \tag{3}$$

where V_0 and a are constants.

FIG. 2: The plot of the trajectory of the comet with an adaptive step size h = 0.00066, given the target accuracy of $\delta = 1$ kilometer per year
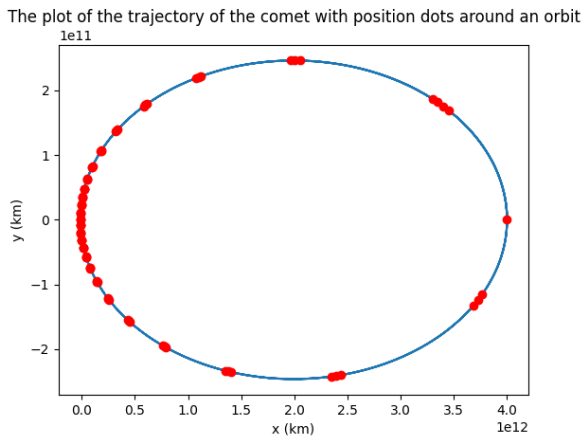

FIG. 3: The plot of the trajectory of the comet with position dots around an orbit, showing the steps getting closer together when the comet is close to the Sun and further apart when it is far out in the solar system.

a) Based on Example 8.9: Ground state energy in a square well (Newman, p.395), we can modify the program for the time-independent Schrodinger equation in a harmonic, converting it from a second-order equation to two first-order ones as in the example, so that we can find the energies of the ground state and the first two excited states for these equations when m is the electron mass, $V_0 = 50$ eV, and $a = 10^{-11}$m. For the accurate an-

swers, we need a large but finite interval, instead of x = $\pm\infty$ as in theory of the wavefunction, we use x = -10a to +10a, with the wavefunction $\psi = 0$ at both boundaries.

Since, the wavefunction is real everywhere, so we don't need to use complex variables, instead we can use evenly spaced points for the solution. I create an array of the wavefunction which is solved in a loop of the fourth-order Runge–Kutta calculation. Then, I define the main program to find the energy using the secant method, resulted in the energies of the ground state and the first two excited states of the harmonic oscillator: E_0 = 138.02397125521225 eV, E_1 = 414.0719165394641 eV, and E_2 = 690.1198621106302 eV.

The quantum harmonic oscillator is known to have energy states that are equally spaced, and the ground state has energy in the range 100 to 200 eV. The properties are according to the answers as the ground state is calculated at 138.02397125521225 eV, and the energy jump in a step of roughly 276, hence our calculation was reasonably precise.

b) In this part, I modify the program to calculate the same three energies for the anharmonic oscillator with

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

,with the same parameter values in the same programming approach. The energies of the ground state and the first two excited states of the anharmonic oscillator: E_0 = 205.30690346934273 eV, E_1 = 735.691247040212 eV, and E_2 = 1443.5694214051405 eV. The answers do not share the same the properties as the quantum harmonic oscillator which is expected.

3.   FEEDBACK

I spent about 16 hours (could be around 10-12 hours without the health challenges during the semester) on this homework including meeting with classmates and attending office hours outside of classes. I think this problem set leans toward the more challenging side just a little bit in terms of programming as I spent most of my time for this homework planing and working on the codes. Nonetheless, the problems are appropriate and very fun to tackle. I found an adaptive size method to be very helpful as a computational skill.

Computational Physics/Astrophysics, Winter 2023: Grading Rubrics [1]

Haverford College, Prof. Daniel Grin

For coding assignments, roughly 25 points will be available per problem.

1. Does the program complete without crashing in a reasonable time frame? If yes, up to +3 points.

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

3. Does the code follow the problem specifications (i.e numerical method; output requested etc.) Up to +2 points

4. Is the answer correct? Up to +4 points

5. Is the code readable? Up to +2 points

    .   5.1. Are variables named reasonably?

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

    .   5.3. Are units explained (if necessary)?

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

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

6. Is the code well documented? +3points

    . 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?

7. LaTeX writeup (up to 10 points)
    . Are key figures and numbers from the problem given? (3 points)
    . Is a brief explanation of physical context given? (2 points)
    . If relevant, are helpful analytic scalings or known solutions given? (1 point)
    . Are 3-4 key equations listed (preferably the ones solved in the programming assignment) and algorithms named? (2 points)
    . Are collaborators clearly acknowledged? (1 point)
    . Are any outside references appropriately cited? (1 point)

Note, even if (1), (2), (3), or (4) are not correct, one can still obtain many points via (5), (6), and (7).

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304   HW7

8.10

$$\frac{d^2x}{dt^2} = -GM\frac{x}{r^3} \quad , \quad \frac{d^2y}{dt^2} = -GM\frac{y}{r^3} \quad \text{when } r = \sqrt{x^2+y^2}$$

→ Constant ─────────────→ $x = 4$ b km
$y = 0$

a), b) → def d(c,t)   → rk4 $V_x = 0$
$V_y = 500 \text{ ms}^{-1}$

x $r = 0$
y $r = 1$
Vx $r = 2$
Vy $r = 3$

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

→ return the system
↳ as array

$N = $ large!
$h = \dfrac{t_f - t_a}{N}$ → small!   8.4 p. 355 ☆

$\hookrightarrow$ Rk4

→ Plot y vs x Look Newman 8   ☆
adaptive step size

c) → $h =$ adapt time → bigger! → faster!
⇒ Plot $\delta = 1$ km/yr

d) ☆ → Plot with dots

8.14 $V(x) = V_0 x^2 / a^2$, V_0 and a are constants.

a) $\implies$ Look at Example 8.9   ••••

$\underset{\text{P.393}}{\text{Example.8}}$

→ $V_0 = 50$ eV

$a = 10^{-11}$ m

$x = -10a$ to $+10a$

$U = 0$

→ def $V(x)$ for TISEQ

→ Punt E_0, E_1, E_2

ψ_0 ψ_1 ψ_2 secant method.

b)   for $V(x) = V_0 x^4 / a^4$