

$$54.5 + 54.5 + 5 = 114$$

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HW8 Write-up

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In this problem set, algorithms to calculate the cometary orbit implementing an adaptive time-step, calculate energies and plot the wavefunction for quantum oscillators were developed.

1. EXERCISE 8.10: COMETARY ORBITS

1.1. Introduction

The equation of motion of a comet is

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

where $\vec{r} = \begin{pmatrix} x \\ y \end{pmatrix}$ and $r = \sqrt{x^2 + y^2}$. Constants in the equation are the mass of the sun $M = 1.989 \times 10^{30}$ kg, and the gravitational constant $G = 6.67408 \times 10^{-11}$ m³ kg⁻¹ s⁻². Equation 1 is a second-order vector equation can be separated into 4 first-order single-variable equations,

$$\begin{aligned} \frac{dx}{dt} &= v_x & \frac{dy}{dt} &= v_y \\ \frac{dv_x}{dt} &= -GM \frac{x}{r^3} & \frac{dv_y}{dt} &= -GM \frac{y}{r^3} \end{aligned} \quad (2)$$

that can be used to track the trajectory of the comet in the solar system.

1.2. Experiment

In order to calculate the trajectory of the comet, a function implementing the fourth-order Runge-Kutta method was used to solve the equations of motion 2. This was done using a fixed time-step method and adaptive time-step method. The trajectory was calculated from an initial position $\vec{r} = \begin{pmatrix} 400 \times 10^{12} \\ 0 \end{pmatrix}$ meters with initial velocity $\vec{v} = \begin{pmatrix} 0 \\ 500 \end{pmatrix}$ meters per second.

The fixed time-step method calculated the trajectory for about 3.2 orbits. To pick a time-step, I started from an arbitrary time-step to calculate the trajectory and increased the time-step until consecutive orbital trajectories overlapped.

We made the fixed time-step simulation accurate to the eye, but with the adaptive time-step we set a specific desired level of accuracy. We set a desired accuracy δ of 1km per cometary year, or 1km per period of the comet.

To update the time-step, we calculated the comet's position after $t = t_0 + 2h$ by using Eq. 2 by updating the

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start at h = 2^0 period of stepsize, plot x vs t, to determine period, then go back to update h appropriately.
if fixed timestep use h = 1 period
else adaptive timestep use h = 1 period
use solution of 1st 4th pg to make range-kutta equations for system of 1st order equations: dx/dt = v_x, dy/dt = v_y
set r = [initial-x, initial-y, initial-vx, initial-vy]
function returns [fx, fy, vx, vy]
plot trajectory y(t) vs x(t), w/ time force
to increase h with averaging of several consecutive periods on overlapping
this decreases h
adaptive step-size:
use h = 2 * period of comet / target - you
slightly better & then necessary
bigger stepsize over -overhead of work
use while t < t_end
    range-kutta using 2h for timestep
    set pos at t1 = t0 + (k * h)/6
    range-kutta using h/6 for twice
    if |x1 - x2| > 10^-6
        calculate difference in x1 + x2 - (x1 + x2)/2
        if x1 + x2 are the same, set t10 = t1 + h/6
        otherwise calculate real h10 = 2 * pi / (x1 - x2)
        if h10 > 1, scale h down and redo calculations for that timestep
    else
        plot x(t) vs y(t) using these steps

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FIG. 1: Pseudocode for Exercise 8.10.

position once in a single large time-step versus updating the position twice in two smaller time-steps and comparing the two projected positions returned by each calculation. Then the ratio of the target accuracy to the actual accuracy was calculated according to Eq. ?? and used to scale the time-step by $\rho^{1/4}$ for the next calculation.

$$\rho = \frac{30h\delta}{|x_1 - x_2|} \quad (3)$$

If the actual accuracy matched or exceeded the target accuracy, the program saved the calculated value for \vec{r} , but if the actual accuracy did not meet the target accuracy, the time-step was decreased and the calculation was repeated until the target accuracy was reached.

Although the time-step is adaptive, the program limits the amount that the step-size can increase over a single time-step to 1.0001. This improves the accuracy of the time-step during regions of high impulse.

The accuracy of both simulations was checked by finding the maximum value and index in the list of x -values.

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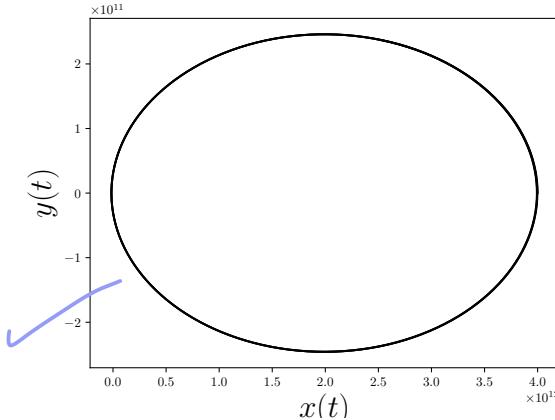


FIG. 2: Trajectory of a comet for approximately 3.2 orbits starting from $(400 \times 10^{12}, 0)$ km

This tests if there is any non-physical drifting in the period. If no drifting is occurring, the expected maximum value would be equal to the initial set value. For the adaptive program, the maximum value for one period should be around $x_{t=0} + \delta$.

1.3. Results

The simulation using a fixed time-step produced an elliptical trajectory shown in Fig 2. The time-step used to produce the orbit was 5.78 hours. Because the trajectory for over 3 consecutive orbits overlapped evenly as expected, it can be considered that this time-step produces a sufficiently stable and accurate orbit. The maximum value for x was 4.0×10^{12} and the index was 0. That the maximum value for x was the initial set value indicates no drifting occurred over the course of 3 orbits.

The calculation took 5 seconds, which is reasonable for this application but if this program was extended to a larger, more complex system it could rapidly result in an unreasonably lengthy wait time. Therefore, an adaptive time-step was implemented in order to improve the speed of the simulation.

The simulation using the adaptive step-size ran for about 30 seconds. As seen in Fig 3, the adaptive step size produced larger spacing between position points on the trajectory when the comet was nearest to the sun. This is because of the high speed and increasing acceleration of the comet as it passes the sun results in bigger jumps over a smaller time-step. When the comet is farther away from the sun, the time-step is larger but the comet does not move as quickly so the points stay really close-together on the trajectory.

The accuracy of the simulation with a fixed step-size program was less than the desired Over a single period of the comet projected by the simulation using an adaptive time-step, the maximum x -value was returned to be

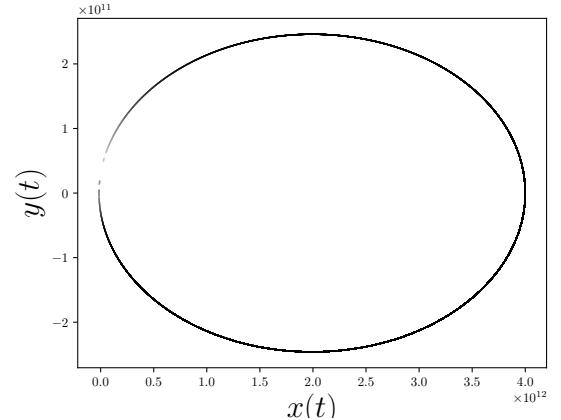


FIG. 3: Trajectory of a comet showing the implementation of an adaptive time-step for a single orbit starting from $(400 \times 10^{12}, 0)$

4000000064669.8335. This has 6.5-times the desired error input into the program. More drift in the system occurred than intended.

1.4. Conclusions

The accuracy of the simulation with a fixed step-size program was better than the simulation with the adaptive step-size, and the speed of the fixed step-size was faster. The adaptive time-step is smallest when the comet is nearest to the sun and the spacing of position calculations on the trajectory is largest when the comet is passing the sun.

2. EXERCISE 8.14: QUANTUM OSCILLATORS

2.1. Introduction

The system used in this experiment is an electron in a quantum oscillator. The wavefunction for the electron is found using the time-independent Schrödinger equation:

$$\frac{d^2}{dx^2}\psi(x) = \frac{2m}{\hbar^2} (V(x) - E) \psi(x) \quad (4)$$

where m is the mass of an electron, and $V(x)$ is the potential of the well bounding the electron in the oscillator. In this experiment, we explore two types of quantum oscillators: the harmonic and anharmonic oscillators. A harmonic oscillator has a potential of

$$V(x) = V_0 \frac{x^2}{a^2}, \quad (5)$$

and an anharmonic oscillator has a potential

$$V(x) = V_0 \frac{x^4}{a^4} \quad (6)$$

Energy level (eV)	Harmonic	Anharmonic	Anharmonic
	$-10a \leq x \leq +10a$	$-10a \leq x \leq +10a$	$-5a \leq x \leq +5a$
Ground state	138.0229806174276	205.30592105321895	205.30592083367358
First excited state	414.0689444719685	735.6877266764313	735.6877266507154
Second excited state	690.1149086041061	1443.5625135562536	1443.5625134468467

TABLE I: Calculated energy values for the ground state and first two excited states of quantum oscillators in quadratic and quartic potential wells.

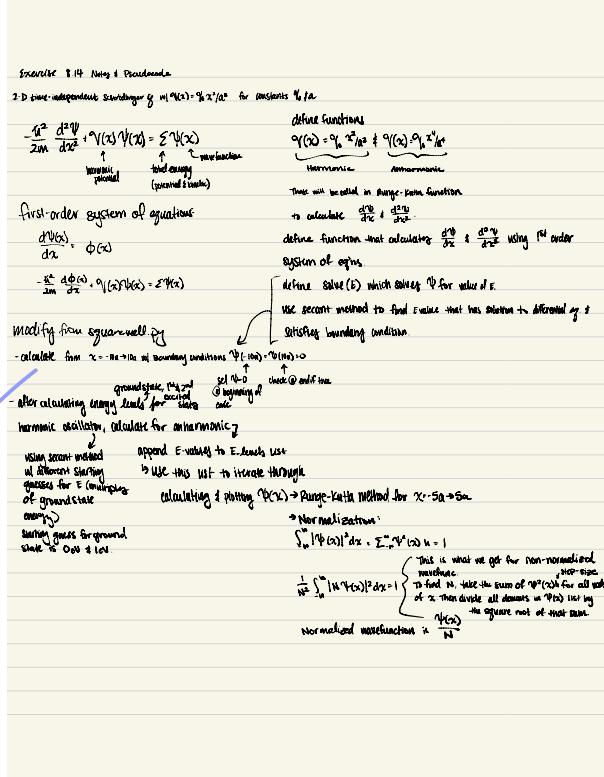


FIG. 4: Exercise 8.14 pseudocode and notes.

for constants V_0 and a . These two potential wells bound the electron inside the oscillator. Within the quantum oscillator, the electron has finite energy that is determined by the quantum energy level. It is not possible for the electron to have an energy value intermediate to these energy levels. The ground state is the lowest energy the electron can have, and the energy for each excited state above the ground state for the harmonic oscillator is equally spaced.[1]

2.2. Experiment

In this experiment, I developed an algorithm described in Fig.4 that solved for the energy levels for the ground state and first two excited states of a quadratic potential well and a quartic potential well for $V_0 = 50\text{eV}$ and $a = 10^{(-11)}\text{m}$. Since the Schrödinger equation, Eq.4, is

a second-order differential equation, when building an algorithm to it we break up the second-order equation into two first-order differential equations:

$$\begin{aligned} \frac{d}{dx}\psi(x) &= \phi(x) \\ \frac{d}{dx}\phi(x) &= \frac{2m}{\hbar^2} (V(x) - E) \psi(x) \end{aligned} \quad (7)$$

In this way, we keep track of both the change in ψ and ϕ to accurately calculate and update the next value of the wavefunction with respect to x .

To solve for the wavefunction, the fourth-order Runge-Kutta method is used over a domain $-10a \leq x \leq +10a$. Because the domain of the wavefunction is infinite, this effectively puts the particle in a box from $-10a \leq x \leq +10a$. However, because of the quadratic or quartic dependence on x of the potential well, as $|x|$ increases, the value of the potential grows exponentially. Since the particle only has a finite energy per excited state, it is confined within a finite range of the potential well, and outside of this range the wavefunction is zero. This property allows us to impose the boundary of the box for high potentials without significantly altering the solutions of the wavefunction or energy values for the oscillators.

The energy for each energy level is calculated using the secant method starting with a multiple of the ground state energy to find the eigenvalue of the schrodinger equation. Using the calculated energy levels of the anharmonic oscillator, I solved for the wavefunction for each of the first three energy levels as functions of x over the domain $-5a \leq x \leq +5a$, shown in Fig.5.

A normalized wavefunction satisfies the requirement $\int_{-\infty}^{\infty} |\psi(x)|^2 dx = 1$. However, the Runge-Kutta method produces a wavefunction that was not normalized. To normalize the wavefunction, all values of $\psi(x)$ are squared and summed to find the normalization constant N^2 in Eq. 8. Then, each value of $\psi(x)$ was divided by N to produce the normalized wavefunction.

$$N^2 = \int_{-\infty}^{\infty} |N\psi(x)|^2 dx \quad (8)$$

Because we assume the wavefunction is zero outside of the domain $-5a \leq x \leq +5a$, we can assume that $\int_{-\infty}^{\infty} |\psi(x)|^2 dx = \int_{-5a}^{5a} |\psi(x)|^2 dx$.

2.3. Results

When the energies were calculated using the smaller domain, they were nearly identical to the energies calculated from the larger range as shown in Table I, so we know it is a good approximation. For better accuracy, I used the energies calculated over the larger range to calculate the wavefunction as a function of position in the oscillator.

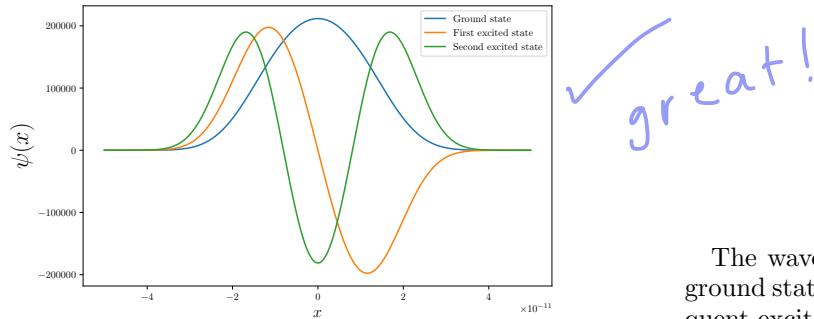


FIG. 5: The normalized wavefunction $\psi(x)$ for the ground state, first two excited states.

The wavefunction is symmetrical around $x = 0$. The ground state takes the form of a gaussian, and each subsequent excited state has an additional node. The altitude of the wavefunction decreases slightly for increasing excitation. The probability that the electron will be found at $|x| \geq 4$ is effectively zero.

- [1] M. Newman, *Computational Physics* (2013), revised and expanded ed., ISBN 978-1-4801-4551-1.

Appendix A: Statement of Collaborators

I collaborated with Rachel and Tessa on this assignment.

was longer than I'd prefer but it was doable. The most interesting question was the cometary orbits problem. It was somewhat surprising to me that the adaptive step-size caused bigger jumps in sampling the position on the trajectory. Something I learned was that I feel like I understand better what the secant method can be used for and how to implement it.

Appendix B: Survey Question

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The report for this assignment took 7 hours and coding took 6 hours. I thought the length of this assignment

8.10

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Computational Physics/Astrophysics, Winter 2024:

Grading Rubrics¹

Haverford College, Prof. Daniel Grin

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

4

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

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)

3.5

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

error with adaptive step size, we expect smaller steps on left side of graph -0.5

3

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)?
- . 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)

- . 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) *adaptive step size difficult to see in Fig 3*
- 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

54.5/56

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- 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).
- 2.5 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)? *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)

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- . 6.2. Are the functions described and ambiguous variables defined?
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- ✓* . 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)
- 3* . Do figures have a sufficient number of points to infer the claimed/desired trends? (+ 3 points)
- 1* . Is a brief explanation of physical context given? (+2 points) *expand on the difference between harmonic and anharmonic solutions*
- 1* . If relevant, are helpful analytic scalings or known solutions given? (+1 point)
- 3* . Is the algorithm used explicitly stated and justified? (+3 points) *-anharmonic solutions -1*
- 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)