PHYS H304 Homework 7

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This is the lab report write-up of the approach and methods used for the sixth problem set in PHYS H304.

1. INTRODUCTION

This is a summary of the methods and major equations used for this problem set. In this report, we explore the application of Runge-Kutta-4 algorithm to solve ordinary differential equations. The major equations used are included where appropriate and a summary of the approach used to develop the code is included as well. All equations are taken from Computational Physics by Mark Newman [1].

2. METHODS

2.1. Exercise 8.4

Due to Kepler's laws, orbits about massive objects take an elliptical form. As a result of the radial dependence of gravitational attraction, when a satellite is particularly close to its orbiting body, the speed of the satellite increases rapidly.[2] At larger distances, however, the satellite travels very slowly. An example of a physical system that operates in this way is the motion of a comet about the sun. The closest point in the orbit, with the corresponding fastest speed is known as perihelion, whereas the farthest point and slowest speed occurs at the aphelion.

For such systems, we can determine the analytical solution using various algorithms for solving ordinary differential equations, such as the Runge Kutta-4 method.This algorithm works by approximating the value of differentiable variable from the first order derivative (slope) over a range of time divided into N slices of width, or step size, "h." We make these approximations by using the first order Taylor expansions such that the set of equations shown from Eqn. 1, 2, 3, and 4. The final estimation of the variable is determined by the sum of each "k" term weighted by a factor of $\frac{1}{6}$, as shown in Eqn. 5. Note that we can set up r as a vector so that it can simultaneously solve a system of equations for the same time range. Hence, we set the first column of r to the range of angles of the pendulum as a function of time, θ and the second column as the angular velocities, ω.

$$k1 = h\mathrm{f}(\mathrm{r}, \mathrm{t}) \tag{1}$$

$$k2 = h\mathrm{f}(\mathrm{r} + 0.5\mathrm{k1}, \mathrm{t} + 0.5\mathrm{h}) \tag{2}$$

$$k3 = h\mathrm{f}(\mathrm{r} + 0.5\mathrm{k2}, \mathrm{t} + 0.5\mathrm{h}) \tag{3}$$

$$k4 = h\mathrm{f}(\mathrm{r} + \mathrm{k3}, \mathrm{t} + \mathrm{h}) \tag{4}$$

$$r(t+h) = r(t) + \frac{1}{6}(\mathrm{k1} + \mathrm{k2} + \mathrm{k3} + \mathrm{k4}) \tag{5}$$

In this method, we are using a step size of "h" that we can fix as a constant equal to $\frac{b-a}{N}$. Using a step size defined in this way and a value of N equal to 800,000, we can solve the system of differential equations corresponding to the motion of the comet about the sun. As it is traveling in a plane, its velocity has two non-zero components, which we define as v_x and v_y for its horizontal and vertical displacements of x and y. From Newton's law of gravitation, shown in Equation 6, we can define the x and y components of the radius vector "r", which we represent in Eqn. 7 8.

$$\frac{d^2 r}{dt^2} = -\frac{GMr}{r^3} \tag{6}$$

$$\frac{d^2 x}{dt^2} = -\frac{GMx}{r^3} \tag{7}$$

$$\frac{d^2 y}{dt^2} = -\frac{GMy}{r^3} \tag{8}$$

We solve the second order differential equations as a coupled system of first order ordinary differential equations. To do so, we define the velocities of the x and y components as the first order derivative of the respective displacements. Thus, we can set up the coupled system of equations as shown in Eqns. 9, 10, 11, and12.

$$\frac{dx}{dt} = v_x \tag{9}$$

$$\frac{dy}{dt} = v_y \tag{10}$$

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$$\frac{dv_x}{dt} = -\frac{GMx}{\sqrt{x^2+y^2}^2} \tag{11}$$

$$\frac{dv_y}{dt} = -\frac{GMy}{\sqrt{x^2+y^2}^2} \tag{12}$$

Then, we solve for the set of $x(t)$ and $y(t)$ that serves as the solutions to this system of equations using the given initial conditions that the comet has an initial displacement of 4.0 $x10^{12}$m along the x axis, and an initial v_y of 500m/s. We select a value for the step size by estimating the period of the comet to be roughly similar to that of Halley's comet (approximately 2.4e9 seconds) and chose a value for N that showed stability of the system such that two orbits overlayed on top of each other.

$$\rho = \frac{30h\delta}{|\epsilon_1 - \epsilon_2|} \tag{13}$$

However, since this system shows varying speeds based on the radius, we can use an adaptive step size that takes larger steps in areas where the system is slow and smaller steps where the system is traveling at fast speeds, and therefore changing very quickly. To do so, we use a zoom factor ρ defined in Eqn. 13 that we can use to increase or decrease the step size when necessary as explained in Section 8. of Newman [1].

2.2. Exercise 8.14

To describe the energy levels of a system, Schrodinger's equation represents an eigenvalue equation where the energy eigenstates have eigen values that physically corresponds to the energies of each level [3]. Thus, on an atomic level, this equation shows the quantized nature of energy, as the levels only take on specific values of energy. The time dependent Schrodinger equation is shown in Eqn. 14. To transform this second order differential equation into a system of first order differential equations, we define a function ϕ as the time derivative of the wave function $\psi(t)$. We thus have a coupled system of differential equations shown in Eqn. 16 and 15.

$$\frac{d^2\psi(t)}{dt^2} = \frac{2m}{h_{bar}^2}(V(x) - E)\cdot\psi \tag{14}$$

$$\frac{d\phi(t)}{dt} = \frac{2m}{h_{bar}^2}(V(x) - E)\cdot\psi \tag{15}$$

$$\frac{d\psi(t)}{dt} = \phi \tag{16}$$

If we choose the potential energy to be a simple quadratic (shown in Eqn. **??**), which corresponds to that of the simple harmonic oscillator, we observe a potential energy well bounded by a parabolic curve. Solving this system using the fourth order Runge-Kutta method, with the initial conditions that the wavefunction is zero and its first derivative is 1, we obtain the solution of the behavior of the wavefunction as a function of time – $\psi(t)$. We then use the secant method to determine the energy eigenvalues using the boundary conditions that the wave function must equal zero at the right and left most edges.

$$V(x) = V_0\frac{x^2}{a^2} \tag{17}$$

As the secant method uses the slope to make an estimate of the eigenvalue, we must provide it with a good initial guess of the energy level we are aiming to find. Therefore, we select the guesses for the energies of the first and second excited states by making a plot of the wavefunction as a function of energies. Whenever the wavefunction is zero, the value at which this occurs is an energy eigenvalue that we can approximate as an initial guess. Due to the relative scaling of the ground state energy level and higher level energies, we plot the wavefunction against energy on a logarithmic scale.
For the second part of the problem, we follow the same process, but we use a potential of the form shown in Eqn **??**.

$$V(x) = V_0\frac{x^4}{a^4} \tag{18}$$

3. RESULTS AND CONCLUSIONS

For Exercise 8.10, we plot the trajectory of the comet as its y position for a time range that corresponds to approximate two and a quarter orbits. The step size we used to achieve this was 5192.5, and the calculation took approximately 20 seconds. The trajectory and plot of x(t) against time are shown in Figure 1. We observe that the comet does indeed follow an elliptical orbit, with the slope of x and y varying with time as the comet moves away and towards the sun. When moving away from the sun, it decelerates in the y direction. When moving towards the sun, however, the comet accelerates in the x direction.
Using the adaptive step size, I couldn't get the program to run for the target accuracy given. This was due to the adjustments required to make to putting a cap on the zoom factor ρ. When the errors are small, ρ becomes infinitely large, which we account for by manually adjusting the step size to zoom out just a little. Calibrating the exact amount it should zoom out by was done by a lot

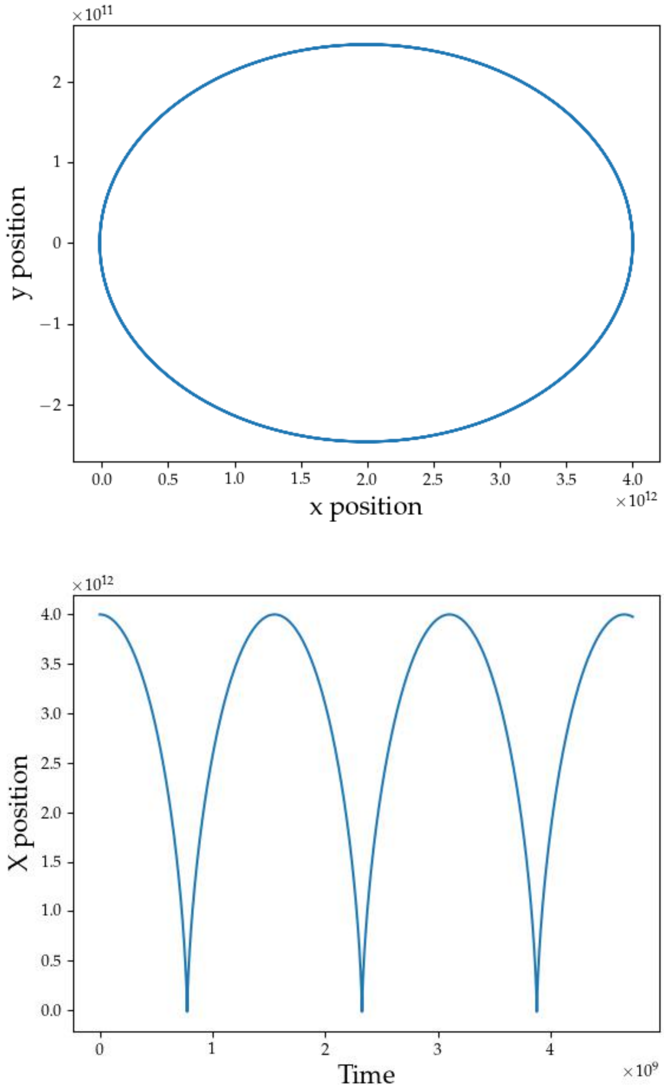

FIG. 1: A plot of the trajectory of the comet, showing an elliptical orbit. It also shows periodicity of the orbit, as after two periods of the orbit, the two cycles are overlayed on top of each other as one orbital path. Both axes are given in meters. The second plot shows the behavior of x as a function of time, which shows multiple periods of the comet's orbit.

of trial and error, and I could not determine the exact amount as the threshold for the given target accuracy was very sensitive to small adjustments.

For a lower threshold, with a target accuracy of roughly 100 times that of the given accuracy of 1km/yr 0.0000317m/s, we obtain the plot shown in Figure 2. We expect to see that the dots on the leftmost side would be more spaced out around the x axis and the dots to get more and more closely spaced as we approach the x axis on the right most side (the perihelion). At this scale, it is not noticeable in the figure how spaced out the dots are. However, we do see that we only needed 333,755

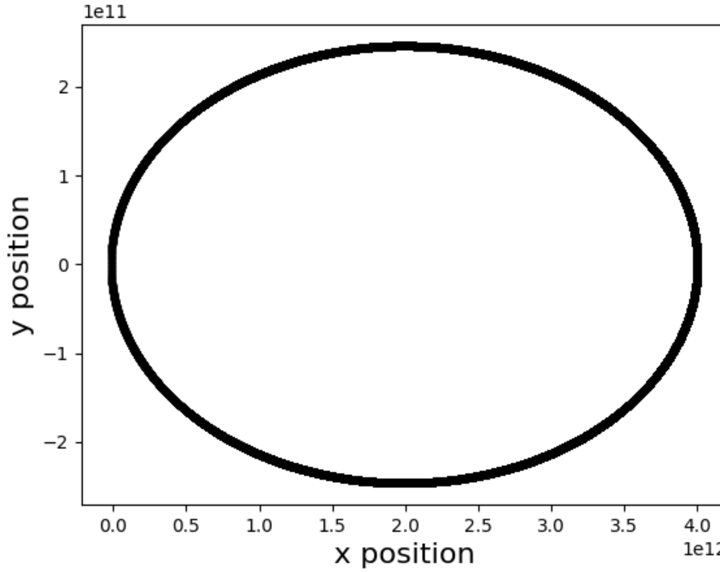

FIG. 2: A plot of the trajectory of the comet, showing an elliptical orbit, using an adaptive step size. We note that we need about 500,000 less steps to plot the trajectory in this way than when using a fixed step size.

steps as opposed to the full 800,000. This shows that the step size is indeed adapting based on the value of ρ. The program does not run much faster than the first - this may be due to the number of small adjustments that are being made, although we would expect that the adaptive method should run faster as it requires less steps.

For Exercise 8.14a, we determined the energy level estimates using the figure shown in Figure 3. Using these guesses, we found that the energy level for the first and second excited states are approximately 966eV and 1518 eV respectively. The ground state energy has a value of 138eV. We note that the energy levels are equally spaced, where the first excited state is a multiple of two times the ground state, the third state is a multiple of three times the ground state and so on. Hence, we can conclude that the energy levels have the form shown in Eqn. 19, where E_1 represents the ground state. This is consistent with the energy level spacing for a quantum harmonic oscillator as discussed in Smith [4].

$$E_n = (2n + 1) \cdot E_1 \tag{19}$$

From the anharmonic potential, we determine that the energy levels of the first and second excited states are approximately 1443eV and 2254 eV respectively using guesses determined from the zeros determined in Figure 4. The ground state energy level is approximately 205eV. We note that the energy levels for this system are not evenly spaced; they become increasingly widely spaced for higher n.

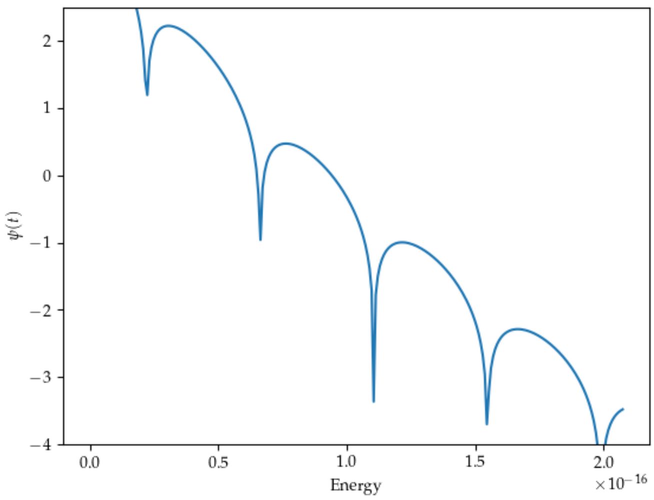

FIG. 3: A plot of the value of the wavefunction evaluated at different energies. At the boundary conditions for finding the eigenvalues, we require that the wave function is zero. Hence, at points where the wavefunction is zero on this plot (points where the function dips sharply, as this is a logarithmic scale), the energy corresponds to the energy associated with a particular energy level for the harmonic oscillator with a potential proportional to x^2

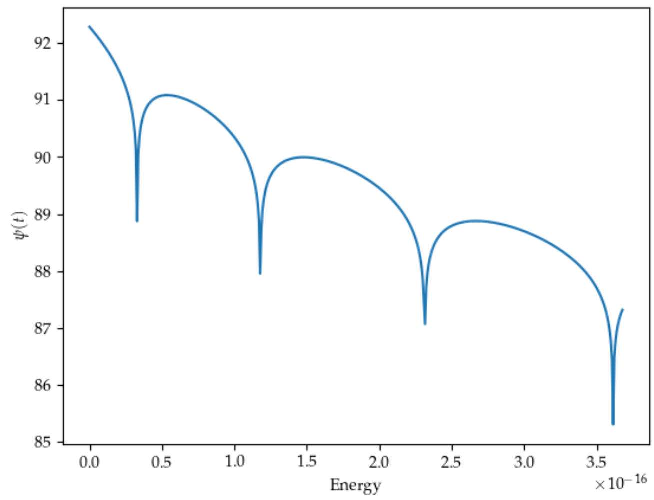

FIG. 4: A plot of the value of the wavefunction evaluated at different energies. At the boundary conditions for finding the eigenvalues, we require that the wave function is zero. Hence, at points where the wavefunction is zero on this plot (points where the function dips sharply, as this is a logarithmic scale), the energy corresponds to the energy associated with a particular energy level for the anharmonic oscillator with a potential proportional to x^4

4. SURVEY QUESTION

The most interesting problem was 8.14. The homework took me about 24 hours to complete. I learnt how to apply the coding we have been learning to practical concepts in Physics, particularly in solving ODEs. I think the problem set length was fine, but the difficulty was harder to manage than other weeks. 8.10 in particular was difficult in terms of step size.

[1] M. Newman, *Computational Physics* ([Createspace], 2012), URL http://www-personal.umich.edu/~mejn/cp/index.html.

[2] B. Ryden and B. M. Peterson, *Foundations of Astrophysics* (Cambridge University Press, 2020).

[3] J. S. Townsend, *Quantum Physics: A Fundamental Approach to Modern Physics* ([University Science Books], 2010).

[4] W. F. Smith, *Waves and Oscillations: A Prelude to Quantum Mechanics* ([Oxford University Press], 2010).