Lab 7 Report

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Q1 a

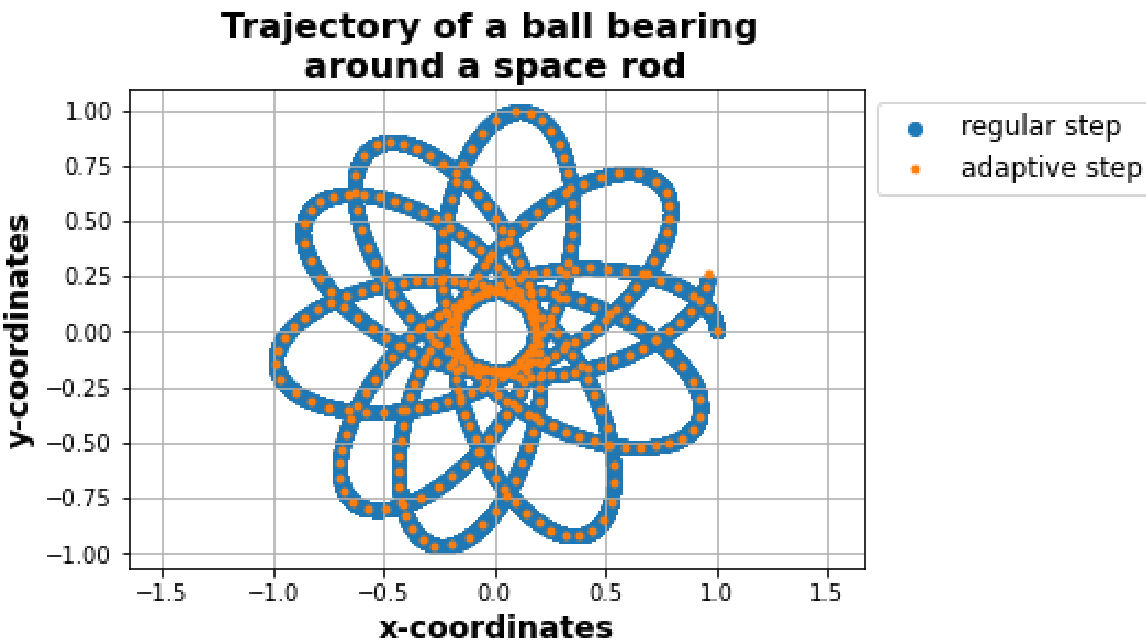

Figure 1: trajectory plot for both the adaptive and normal RK4 methods . Note that the points for the regular step method are so close together that it looks like a line.

As seen in the trajectory plot of a ball-bearing orbiting around a steel rod in Figure 1, both the regular and adaptive step methods using RK4 resulted in overlapping trajectories. The main difference between the two methods is that the adaptive step method takes more steps when the ball bearing is close to the origin (0,0) and takes fewer steps when farther away. This is a characteristic of the adaptive step method as it takes fewer steps when the ball bearing is moving slower when orbiting farther away and takes more steps when the ball bearing is moving faster when close to the sun to maintain the wanted accuracy.

Q1 b

*chose to submit short answer instead of printout, code provides time printouts when run

The time needed for the adaptive method to execute was around 0.063 seconds, while the normal method using h = 0.001 (second) size steps takes around 0.295 seconds to execute. As expected, the adaptive method takes a shorter time to complete its calculation as it saves time by altering the step size to fit the desired accuracy. Note that the timing for each method varies slightly each time the code is run.

Q1 c

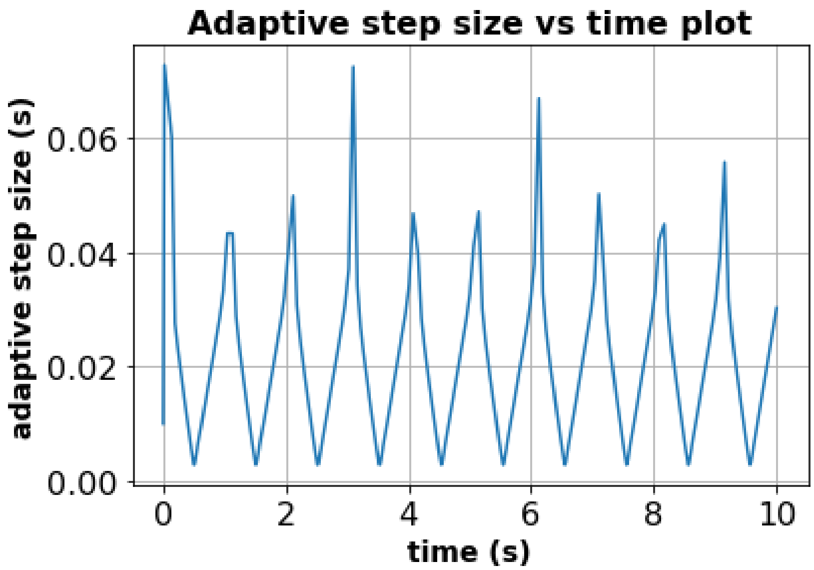

Figure 2: Adaptive step size vs time plot showing the changing step sizes generated by the adaptive method

Observing Figure 2, the step size can be seen changing through the 10 seconds. As mentioned before, the adaptive step method will take smaller steps when the ball bearing is near the origin (space rod) where it is moving faster. On the other hand, the adaptive method takes smaller steps when the ball bearing is farther from the origin (rod) where it moves slower. As a result, Figure 2 depicts a oscillatory pattern where the adaptive steps changes size depending on where the ball bearing is located in its orbital path.

Question 2b

For this question, the goal is to see how the calculated energy values change when we change the target energy convergence, the stepsize h, and r_∞. Firstly, we test 3 different target energy convergence values. Those are

- $\frac{\mathbf{e}}{10^3}$
- $\frac{\mathbf{e}}{10^4}$
- $\frac{\mathbf{e}}{10^5}$

where e is the charge of an electron; $\mathbf{e} = 1.6022 * 10^{-19}$C The initial values of h and r_∞ used here are $h = 0.002a$ where a is the Bohr radius $\approx 5 * 10^{-11}$m and $r_\infty = 20a$ For the purpose of comparing our calculated values vs the true values, we note down the ground state energy

$$E_1 = 13.6\mathbf{eV}$$

and the first excited state

$$E_2 = -3.4\mathbf{eV}$$

h=0.002a, $r_\infty = 20a$	**Target = e/1000**	**Target = e/10000**	**Target = e/100000**
n=1,l=0	E = -13.500384118560786 eV	E= -13.5003871026901 eV	E= -13.5003871026901 eV
n=2, l=0	E = -3.3878408777380575 eV	E = -3.3878408777380575 eV	E = -3.3878408475151334 eV
n=2, l=1	E = -3.401250045627208 eV	E = -3.401250045627208 eV	E = -3.401249804554267 eV

We can see that when we changed the target energy convergence to $e/10^4$, it always gave a value that was closer to the true value than the other two target boundaries. Therefore, for the next parts of this question, we will use this target energy convergence ($e/10^4$).

The table below shows the different energy values we get when we make h smaller.

Target = e/10000, r_∞ = 20a	**h = 0.001a**	**h = 0.0002a**
n=1, l=0	E = -13.552289727347661 eV	E =-13.594795553726513 eV
n=2, l=0	E = -3.394366246172148 eV	E = -3.399695094874986 eV
n=2, l=1	E = -3.401249942244761 eV	E = -3.401249828568291 eV

Notice that using h=0.0002a gave us the most accurate ground state energy eigenvalue energy (13.59. . .).

Finally, we change the values of r_∞ and make it larger to see if the solution we get is an improvement from how close it was when we changed h. To save time, we will take $h = 0.001a$ because it is more accurate then $h = 0.002a$ and doesn't take as much time to run as $h = 0.0002a$. We already found the ground state and first excited state energy for $r_\infty = 20a$, now we set it to $30a$ and $40a$.

Below is a table outlining the calculated energy eigenvalues we found from increasing the value of r_∞.

Target = e/10000, h=0.001a	**r_∞ = 30a**	**r_∞ = 40a**
n=1, l=0	E = -13.552289510606393 eV	E = -13.552289731125164 eV
n=2, l=0	E = -3.394723730618744 eV	E = -3.3947238340228796 eV
n=2, l=1	E = -3.4013961274404076 eV	E = -3.4013960127239087 eV

We now can compare these values to the known energies for the hydrogen atom. Clearly we can see that the lower the target energy convergence value the closer the energy is to the known hydrogen energy at ground state and first excited state. Furthermore, using a smaller h and a larger r also improves the accuracy of our calculation. We found that the energy was closest to the ground state energy when we used the smallest target energy convergence, h=0.0002a and r = 40a. So using these 3 constants, we get $E_1 = -13.594795601821422 eV$. However, when h=0.001a, the energy eigenvalue -13.5522. . . was still pretty close to the true value -13.6. In addition, changing the value of h affects our calculation more than changing r or the target convergence. We came to this conclusion by comparing the values in the tables. The values in the table where we varied h changed the most, as well as the eigenvalues were closest to what the analytical eigenvalue is supposed to be, relative to when we changed r and our convergence boundary.

Question 2c

These graphs were found using the constants h=0.001a, $r_\infty = 20a$, and $e/10^4$ for the target energy convergence.

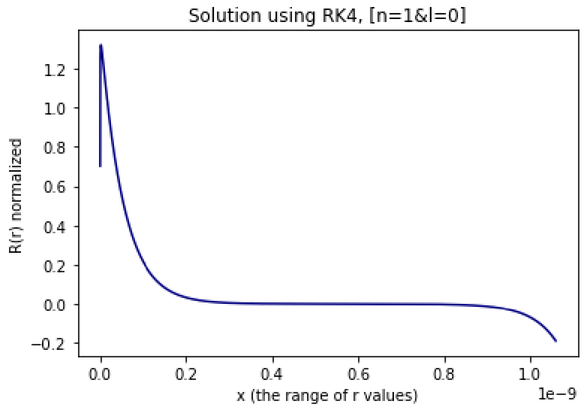

Figure 3: n=1, l=0

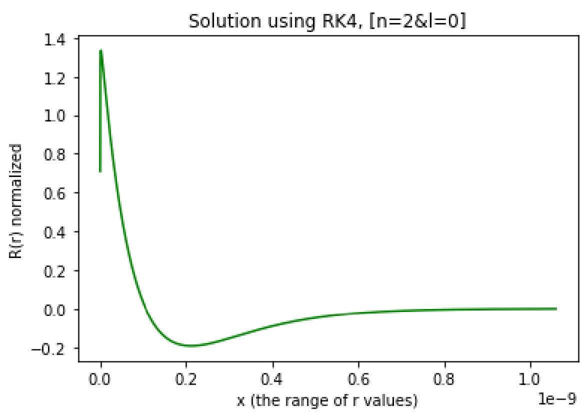

Figure 4: n=2, l=0

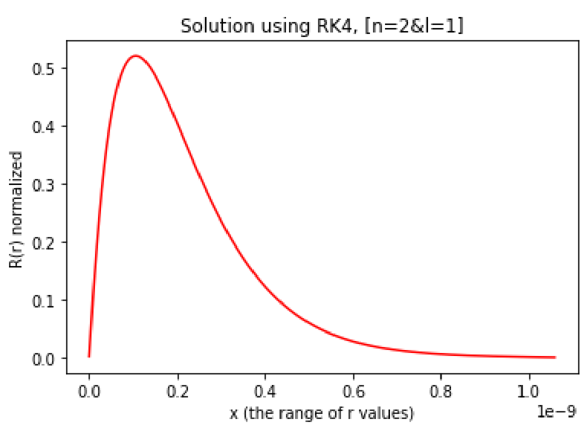

Figure 5: n=2, l=1