Lab7 Report

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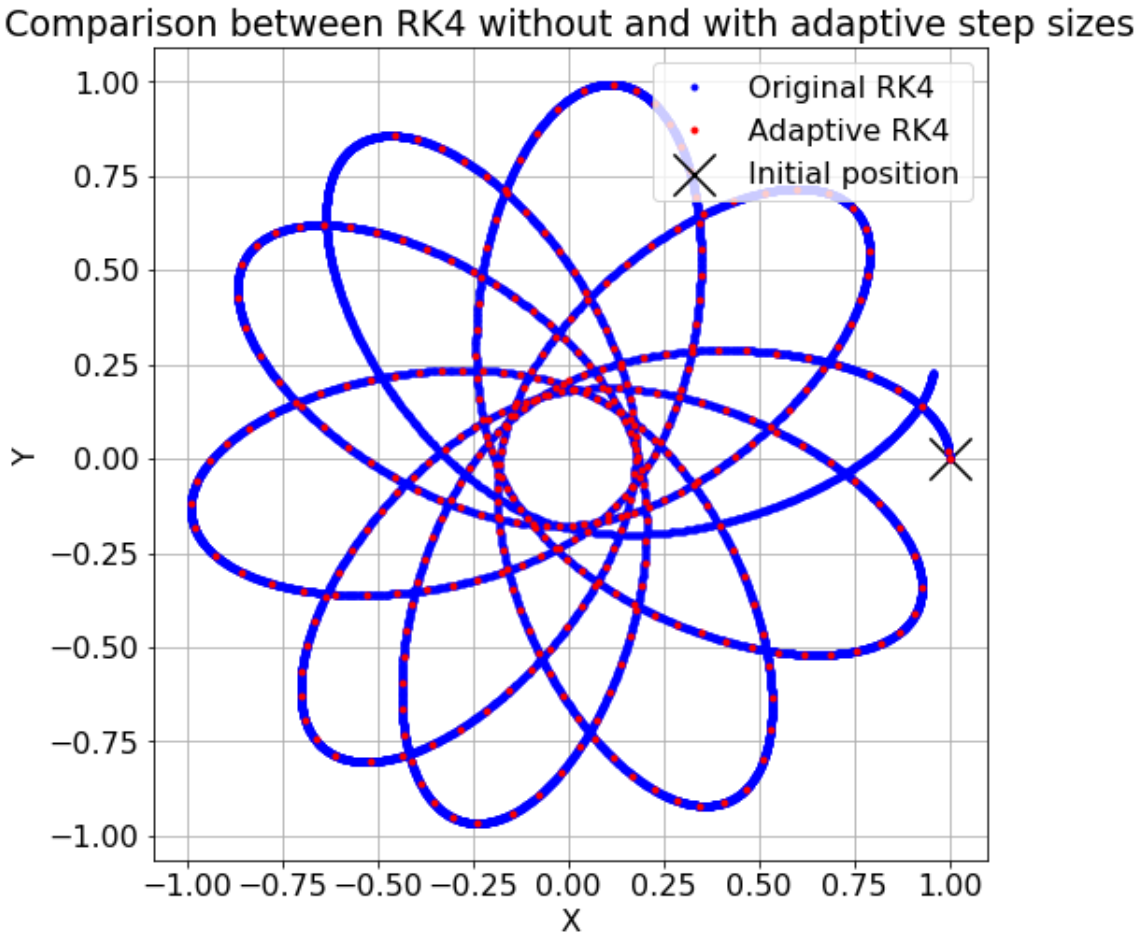
November 1, 2020

1 Question 1

1.1 Q1 (a): Plot and description



The comparison between simulated orbits of space garbage using original and

adaptive RK4 is shown above. You can see that, without steps with adaptive sizes, the RK4 algorithm will simulate densely in order to picture the shape of the orbit. Namely speaking, in order to maintain the desired accuracy, the RK4 scheme would have to data points very close to each other, without the knowledge about the non-linearity of the function. By contrast, the adaptive RK4 algorithm knows the information about the non-linearity of the function. Therefore, it increases the step sizes where the function is less non-linear and small steps are waste of computational cost. And it decreases the step sizes where there are larger variabilities and more computational effort has to be made to ensure accuracy.

1.2 Q1 (b): Printed output and short answer

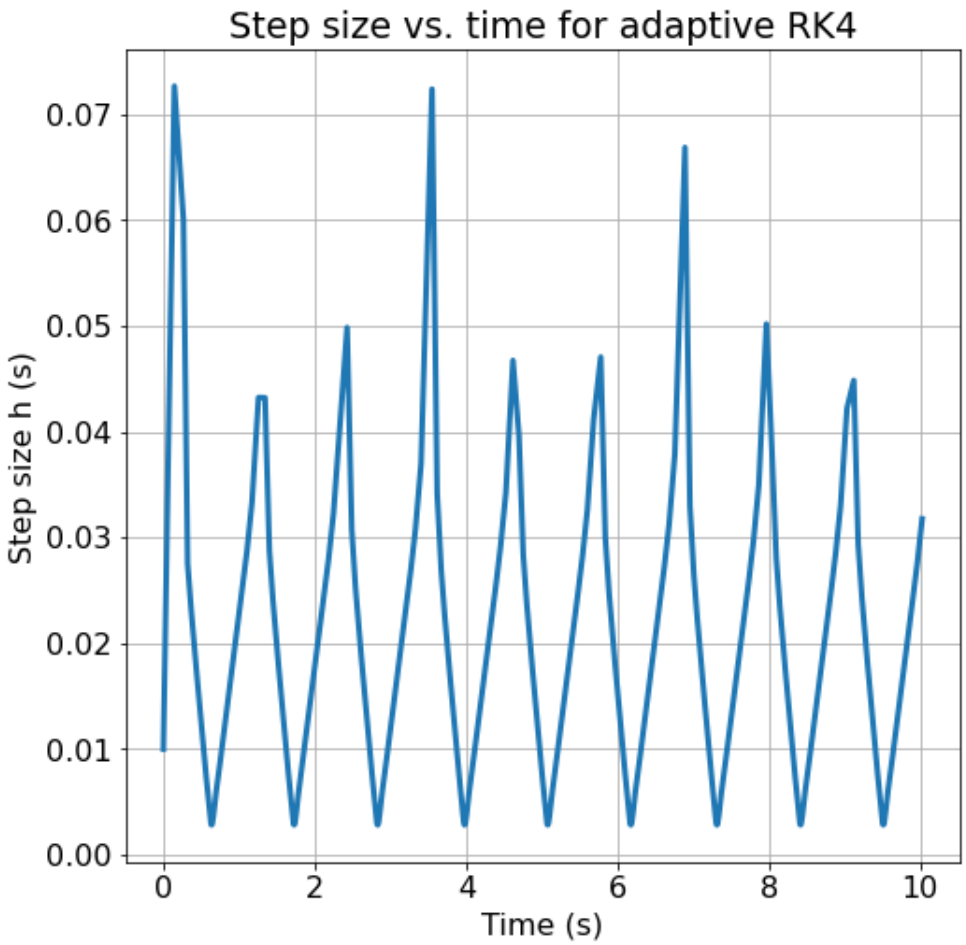
```
In [5]: runfile('C:/Users/ellen/Desktop/PHY Couses/PHY407/Lab 7/Lab07_Q1.py', wdir='C:/
Users/ellen/Desktop/PHY Couses/PHY407/Lab 7')
Reloaded modules: Lab07_Q1functions
The time taken by original RK4 is 0.395 seconds.
The time taken by adaptive RK4 is 0.079 seconds.
```

Algorithm Name	Time (second)
Original RK4	0.395
Adaptive RK4	0.079

Table 1: Timing comparison between original and adaptive RK4 schemes

The raw printed output of the timing comparison is shown above, and tabulated as well. You can see that, to an accuracy of $\delta = 1e-6$, the RK4 algorithm without adaptive step sizes took 0.395 second to finish simulating 10000 data points. By contrast, the adaptive RK4 algorithm only took 0.079 second, which was about $\frac{1}{5}$ of that by the original RK4.

1.3 Q1 (c): Printed output and short answer



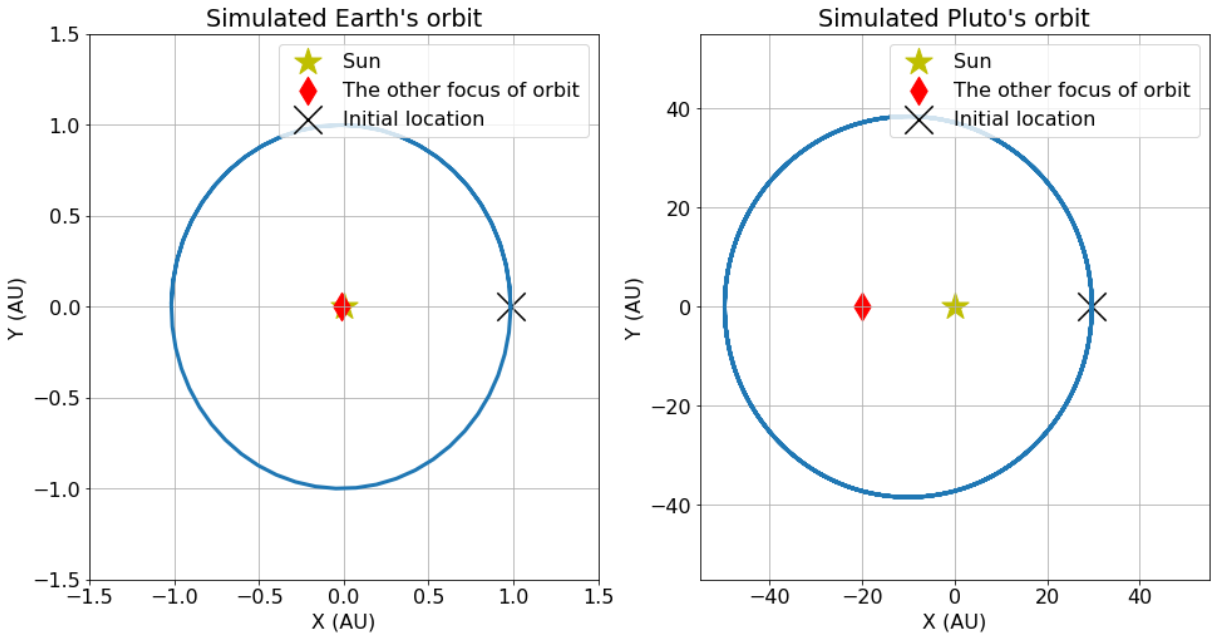
The size of time step is plotted above as a function of time. From the figure in Q1 (a), it is shown that the initial position is at the apoapsis of the orbit. As it approaches the periapsis, the orbit:

1. first becomes less non-linear as the orbit has small curvature,
2. and then more non-linear as the curvature of the orbit increases near the periapsis.

The corresponding part for this process is the first peak of the step size vs. time figure. This is just as expected, because less non-linearity requires less computational cost, which means large step sizes are desired. And vice versa for the more non-linear part of the orbit.

2 Question 2

2.1 Q2 (a) and (b): Simulated orbits of Earth and Pluto, and explanation notes



The simulated orbits of Earth and Pluto are plotted together above, in astronomical units. For computational convenience, the initial positions of both the Earth and Pluto are set to be on the positive half of the x axis, and the center of mass (one of the foci of the elliptical orbit) is set to be at the origin. Therefore, the initial velocities would be pointing in +y direction, if the observer is looking downwards above Earth's North Pole. In the figures, I plotted the initial location of Earth/Pluto, the location of the Sun, and the other foci of the orbits (calculated using the eccentricity of the orbits of Earth and Pluto from wikipedia). In the Bulirsch-Stoer scheme I coded, the positional error is calculated to be $\epsilon = \sqrt{\epsilon_x^2 + \epsilon_y^2}$ as there are two variables. For the Earth, I plotted roughly 547 days, which means 1.5 revolutions are displayed. You can see that the accuracy of the simulation has been well preserved by the Bulirsch-Stoer scheme, as there are no shifting between the 1.5 revolutions. While for the Pluto, the simulation ran for 1500 Earth years, which was roughly 6 Pluto years. It is obvious that its orbit is much more elliptical than the Earth. And the two foci of the orbit are much further away from each other. But again, the Bulirsch-Stoer scheme well preserved the accuracy of the simulation. As you can see, the orbits from 6 revolutions of the Pluto's orbit do not show any shifting between each other. Moreover, the desired positional error was set to be 1km per week, whereas the scale of the simulation is in astronomical unit.

Although the relative accuracy is on the order of $1e-8$, this high-accuracy simulation ran very fast. It could be concluded that, the Bulirsch-Stoer scheme is a highly effective method that can easily achieve high accuracy, which is very desirable in large-scale simulations, e.g. the interaction between a large number of astronomical objects in the universe.

3 Question 3

3.1 Q3b, Adjust the various parameters, discuss the impact on the energy eigen values

There are 3 adjustable parameters:

- The maximum value of r, which is r_∞. I take $r_\infty = 20a_0$, $25a_0$, and $30a_0$.
- The step size of the simulation h. I take $h = 2 \times 10^{-3}a_0$, $10^{-3}a_0$, and $5 \times 10^{-4}a_0$.
- The target energy convergence. I take target $= e/10^3$, $e/10^4$, and $e/10^5$.

So there will be total 27 possible combinations. To save space and your time, I will show only a few of them, then I will discuss the result.

- $r_\infty = 20a_0$, $h = 2 \times 10^{-3}a_0$, target $= e/10^3$:

```
For n=1, l=0, with max range = 20a, stepsize = 0.002000a, target size = e/1000
The calculated energy eigen value is:
-13.50098956116753 eV
---------------------------------
For n=2, l=0, with max range = 20a, stepsize = 0.002000a, target size = e/1000
The calculated energy eigen value is:
-3.3879863689251213 eV
---------------------------------
For n=2, l=1, with max range = 20a, stepsize = 0.002000a, target size = e/1000
The calculated energy eigen value is:
-3.401393376086758 eV
---------------------------------
Check normalization
1.0
1.0000000000000002
0.9999999999999976
```

- $r_\infty = 20a_0$, $h = 10^{-3}a_0$, target $= e/10^3$:

```
For n=1, l=0, with max range = 20a, stepsize = 0.001000a, target size = e/1000
The calculated energy eigen value is:
-13.552881442389564 eV
---------------------------------
For n=2, l=0, with max range = 20a, stepsize = 0.001000a, target size = e/1000
The calculated energy eigen value is:
-3.3945105936359976 eV
---------------------------------
For n=2, l=1, with max range = 20a, stepsize = 0.001000a, target size = e/1000
The calculated energy eigen value is:
-3.4013935038719842 eV
```

```
---------------------------------
Check normalization
0.9999999999999905
1.0000000000000064
0.9999999999999921
```

- $r_\infty = 20a_0$, $h = 10^{-3}a_0$, target $= e/10^4$:

```
For n=1, l=0, with max range = 20a, stepsize = 0.001000a, target size = e/10000
The calculated energy eigen value is:
-13.552881442389564 eV
---------------------------------
For n=2, l=0, with max range = 20a, stepsize = 0.001000a, target size = e/10000
The calculated energy eigen value is:
-3.3945105936359976 eV
---------------------------------
For n=2, l=1, with max range = 20a, stepsize = 0.001000a, target size = e/10000
The calculated energy eigen value is:
-3.4013935038719842 eV
---------------------------------
Check normalization
0.9999999999999905
1.0000000000000064
0.9999999999999921
```

- $r_\infty = 25a_0$, $h = 5 \times 10^{-4}a_0$, target $= e/10^4$

```
For n=1, l=0, with max range = 25a, stepsize = 0.000500a, target size = e/10000
The calculated energy eigen value is:
-13.579326515320705 eV
---------------------------------
For n=2, l=0, with max range = 25a, stepsize = 0.000500a, target size = e/10000
The calculated energy eigen value is:
-3.3981769186608117 eV
---------------------------------
For n=2, l=1, with max range = 25a, stepsize = 0.000500a, target size = e/10000
The calculated energy eigen value is:
-3.401538111279074 eV
---------------------------------
Check normalization
1.0000000000000018
1.0000000000000215
1.0000000000000042
```

- $r_\infty = 30a_0$, $h = 5 \times 10^{-4}a_0$, target $= e/10^5$

```
For n=1, l=0, with max range = 30a, stepsize = 0.000500a, target size = e/100000
The calculated energy eigen value is:
```

```
-13.579326456642267 eV
-----------------------------------
For n=2, l=0, with max range = 30a, stepsize = 0.000500a, target size = e/100000
The calculated energy eigen value is:
-3.398183382375534 eV
-----------------------------------
For n=2, l=1, with max range = 30a, stepsize = 0.000500a, target size = e/100000
The calculated energy eigen value is:
-3.4015406531765016 eV
-----------------------------------
Check normalization
1.0000000000000124
0.999999999999994
1.00000000000001
```

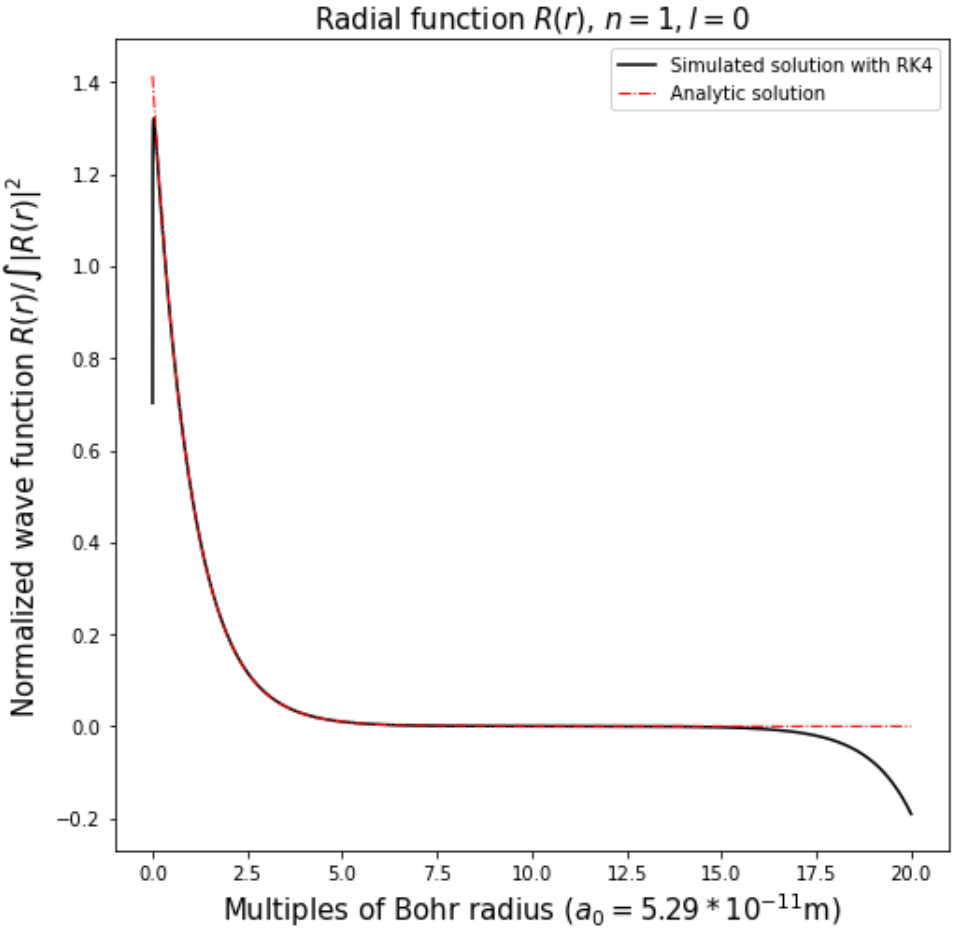
The well known energy value for hydrogen atoms is:

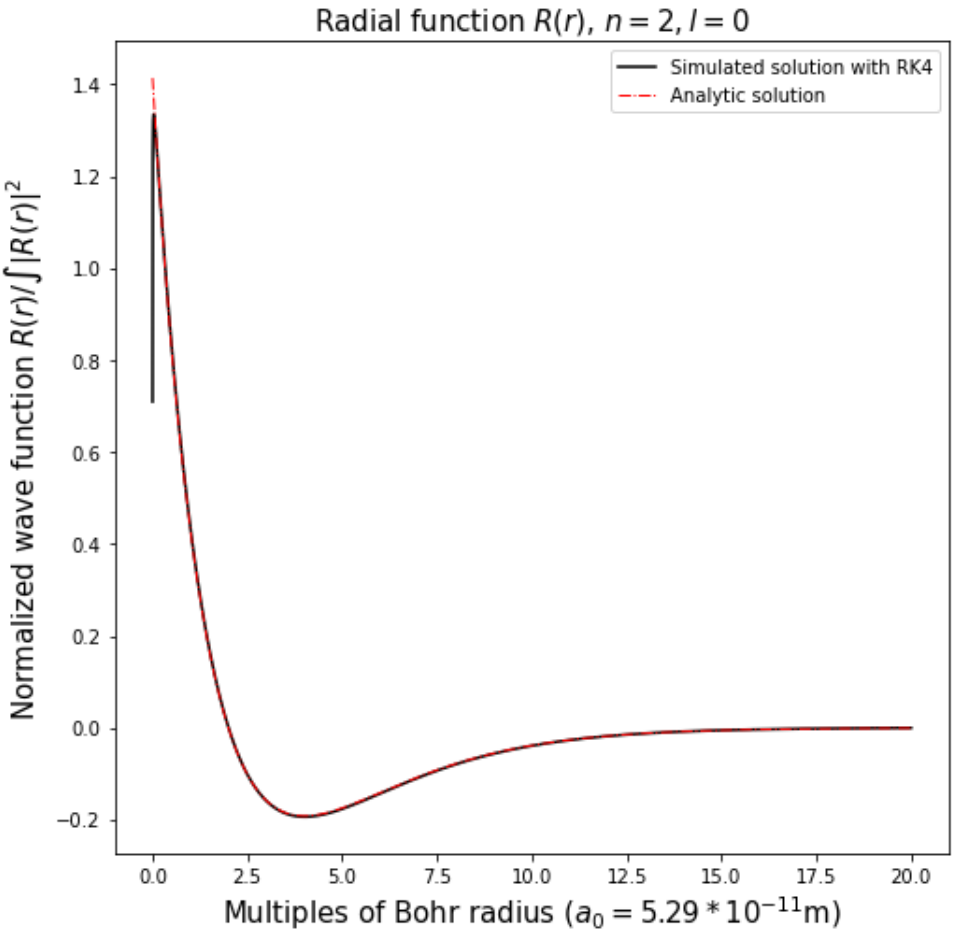
$$E_n = -\frac{E_0}{n^2} \quad \text{where } E_0 \approx 13.6\text{eV},\ n \text{ is the energy level.}$$

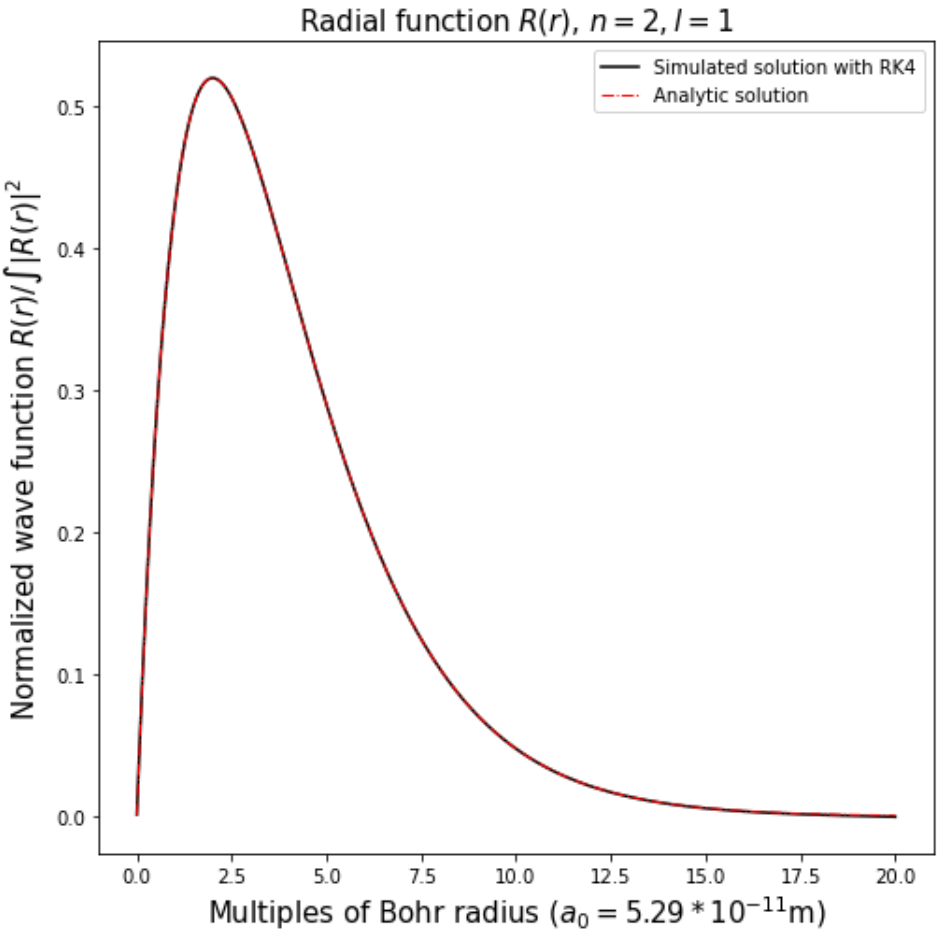
So, for $n = 1$, $E_1 = -13.6$eV, and for $n = 2$, $E_2 = -3.4$eV. All the simulation results give pretty good approximation.
From the data, we can tell that the step size h has the greatest impact on the calculated energy value. The maximum range r_∞ and the target size, however, have very little impact, almost negligible.
This makes quite sense. The step size h is the most important parameter of the simulation accuracy. The maximum range r_∞ and the target size become less important when they hit certain accuracy extent.

3.2 Q3d, Plots of normalized $R(r)$, comparison with analytic solution

So I plot the simulated $R(r)$ with the analytical solutions for $n = 0, l = 0$, $n = 2, l = 0$, and $n = 2, l = 1$.
These plots are under the parameters: $r_\infty = 20a_0$, $h = 10^{-3}a_0$, target $= e/10^4$, which are the optimal parameters according to my experience in this lab.




Radial function $R(r)$, $n = 2, l = 0$
Simulated solution with RK4
Analytic solution
Normalized wave function $R(r)/\int |R(r)|^2$
1.4
1.2
1.0
0.8
0.6
0.4
0.2
0.0
−0.2
0.0
2.5
5.0
7.5
10.0
12.5
15.0
17.5
20.0
Multiples of Bohr radius ($a_0 = 5.29 * 10^{-11}$m)



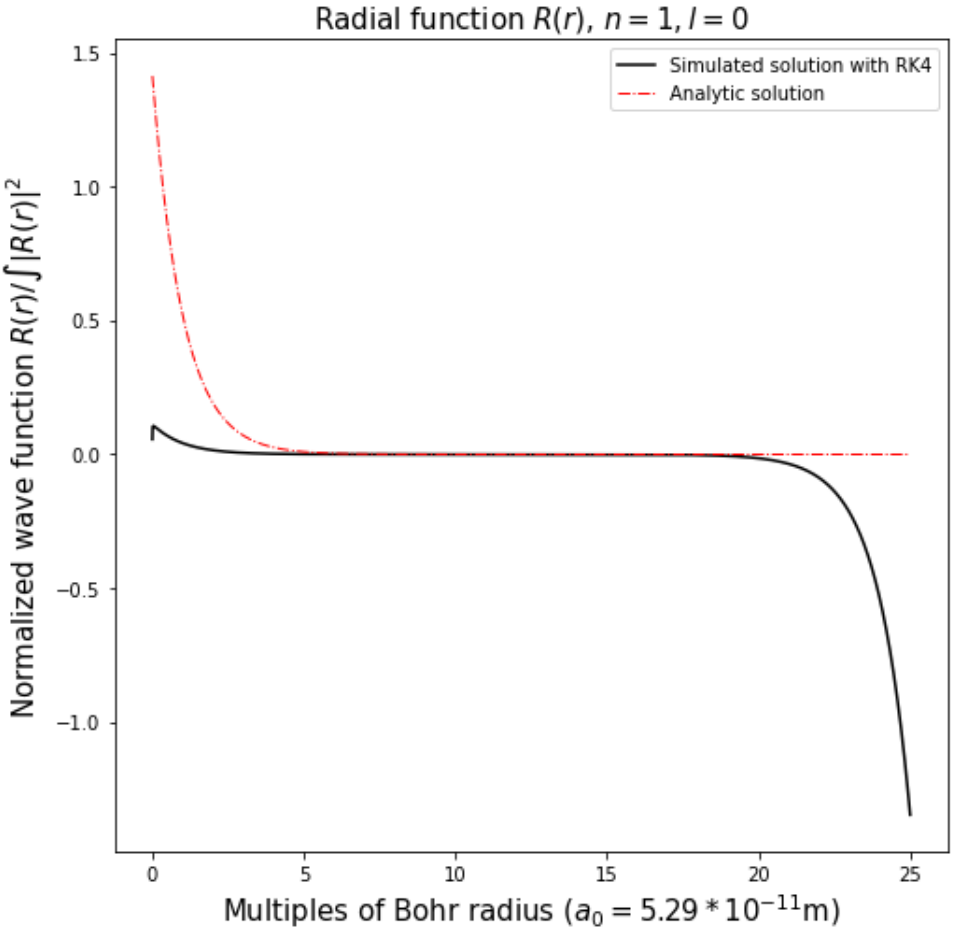
From the plots above, we can tell that for $n = 2, l = 0$ and $n = 2, l = 1$, the simulated result agrees with the analytic solution very well. Except there is a dip close to the origin in the $n = 2, l = 0$ plot, since we set the initial value for $R(h) = 0$.

The $n = 0, l = 0$ plot, however, tells a different story. The simulated solution agrees with the analytic solution at the beginning, expect for the initial dip. Then, it drops down fiercely towards the end.

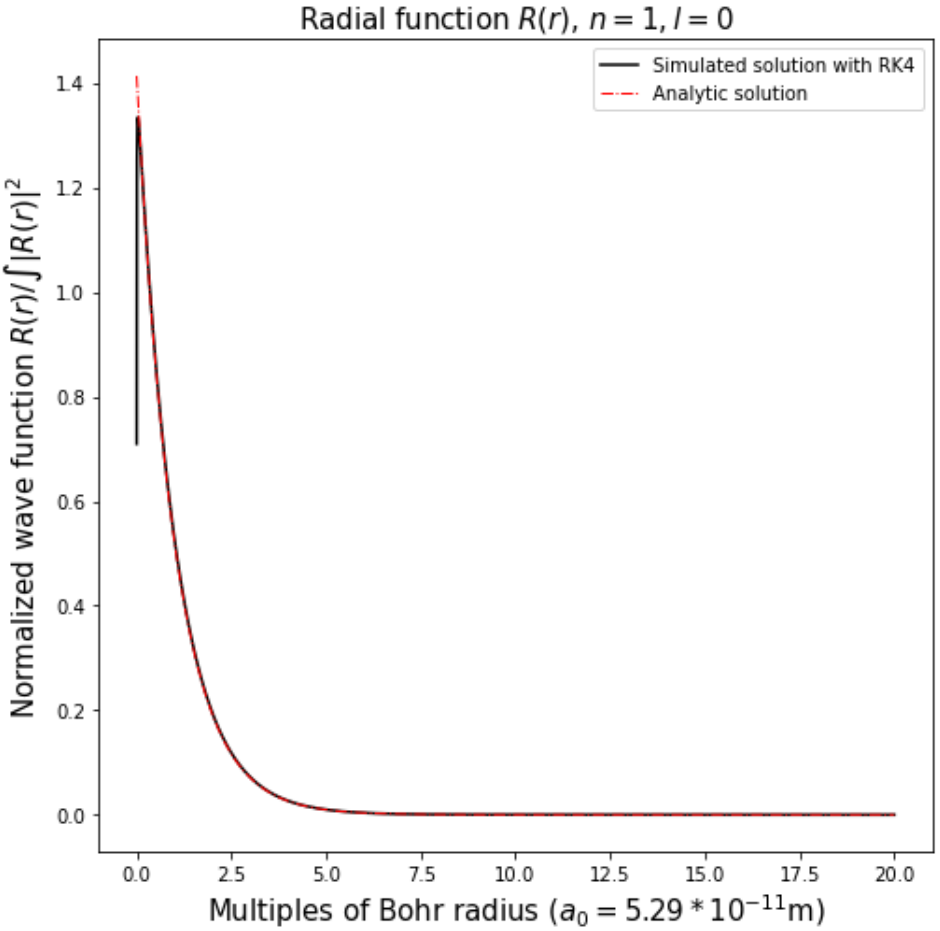
This wired trend does not effect the energy value as it was said in the lab hand-out. Also, it does not effect the normalization, I check the probability integral $\int |R(r)|^2$ at the end of the program and it is 1.

Things are way more interesting with the $n = 0, l = 0$ plot. It changes greatly when I toggle the parameters:

- $r_\infty = 25a_0$, $h = 10^{-3}a_0$, target $= e/10^4$

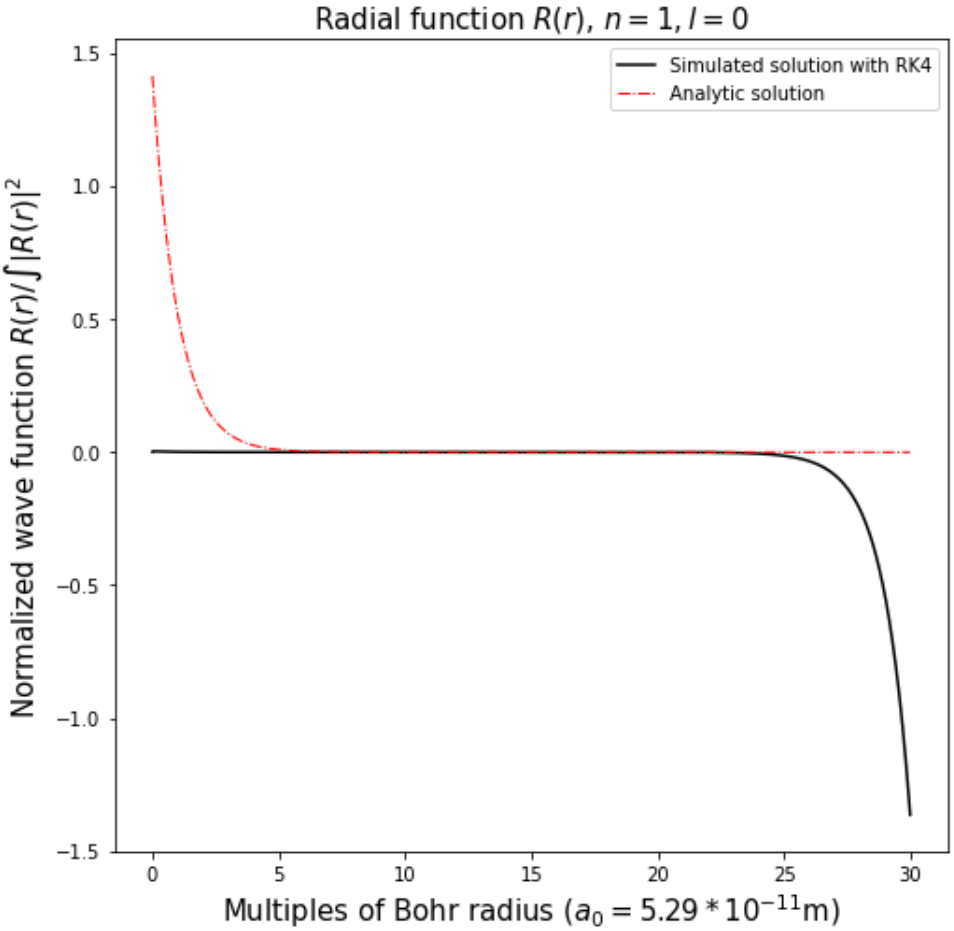


- $r_\infty = 20a_0$, $h = 10^{-3}a_0$, target $= e/10^5$



This time, the simulation fits perfectly with the analytic result.

- $r_\infty = 30a_0$, $h = 5 \times 10^{-4} a_0$, target $= e/10^5$



This time, with max accuracy parameters, the plot turns out to be the worst.

Although the plots for $n = 0, l = 0$ changes a lot, the energy value and the normalization are always correct.
Meanwhile, the other two plots are not affected by changing parameters, and agree with the analytic solution well.
We can conclude that the $n = 0, l = 0$ plot is way more sensitive to the energy value than the other two. There also must be some interesting science behind this which I don't know so far.