Lab Report 7

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Q1 a)

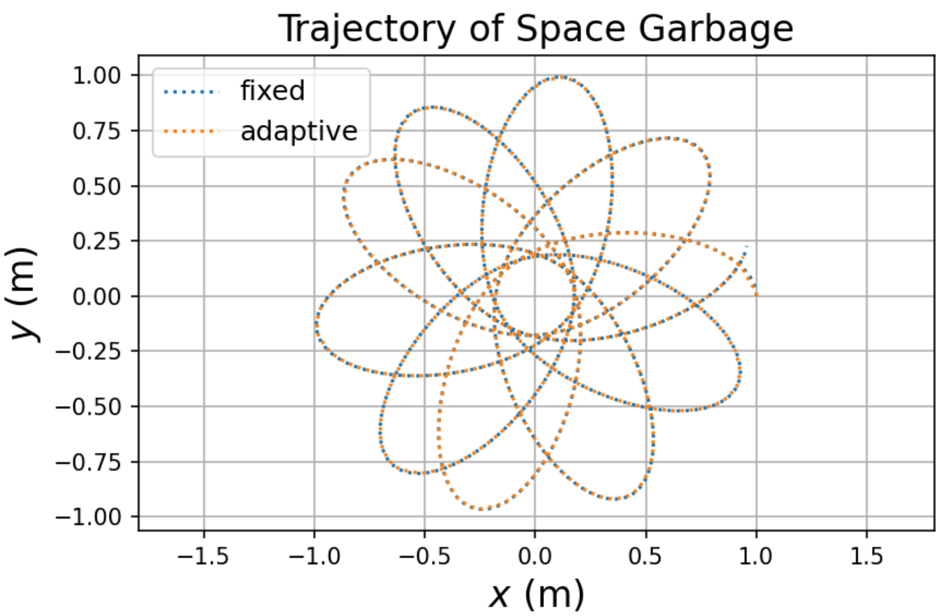

Figure 1: The trajectory of Space Garbage with fixed and adaptive time steps

Figure 1 shows the trajectories of a space garbage obtained by using both fixed step size and adaptive step size, where fixed step size is $h = 0.001$ and adaptive step size approached with the initial $h = 0.01$. The overall motion of the trajectories are the same for both fixed and adaptive step sizes, but individual points of position (x,y) are different. This happens because the adaptive step size varies as the position of the space garbage changes, so it does not perfectly align with the fixed time step of $h = 0.001$.

Q1 b)

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Time it takes for fixed step size 0.39710116386413574 seconds

Time it takes for adaptive step size 0.08101844787597656 seconds
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Figure 2: Time it takes for fixed timestep and adaptive timesteps

$(h = 0.001,\ N = 10000,\ \delta = 10^{-6})$

The adaptive time step method takes less amount of time compared to fixed time step method, as the adaptive step size method changes its size of time step depending on how fast the solution varies. Therefore, the adaptive time step method takes less number of calculations.

Q1 c)

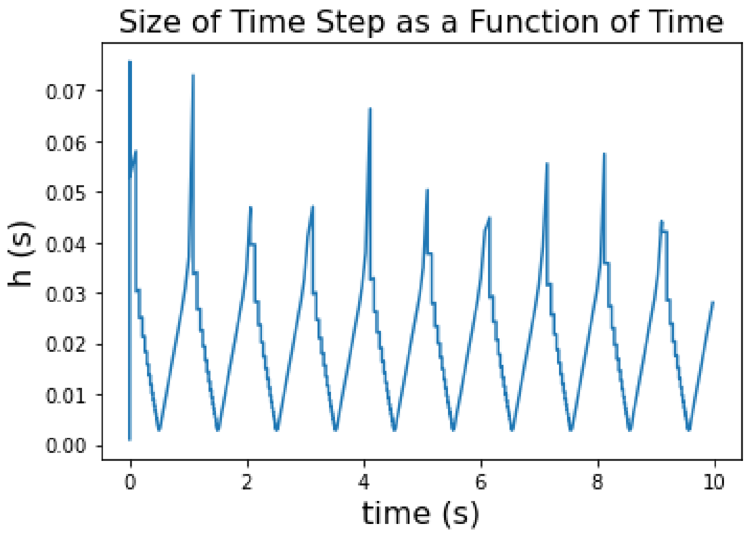

Figure 3: Size of a time step as a function of time

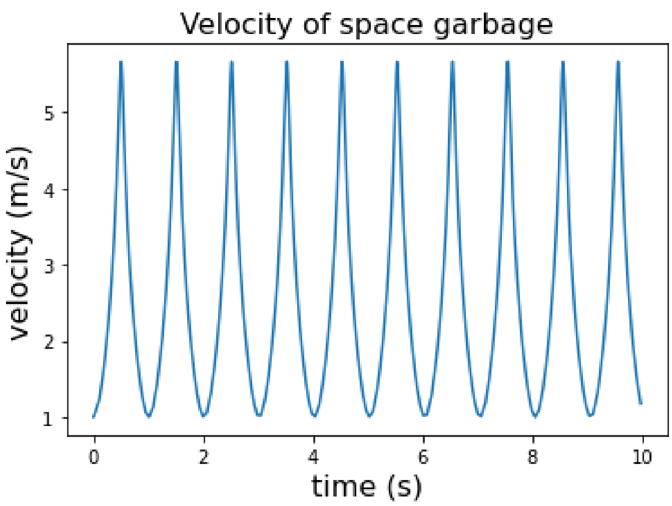

Figure 4: Velocity of space garbage

Notice that on figure 3, the size of a time step changes periodically. At high velocity, program takes smaller adaptive step size h, and at low velocity, program takes bigger adaptive step size h. Figure 4 shows the velocity of space garbage, which indeed shows the trend that as velocity gets higher time step gets smaller, and when velocity gets smaller time step gets bigger.

Q2 b)

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E = -13.499996656010751eV
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Figure 5: Numerical calculation of $n = 1$ and $l = 0$ (ground state)

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E = -3.38780555418903eV
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Figure 6: Numerical calculation of $n = 2$ and $l = 0$ (first excited state)

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E = -3.4012769902292989eV
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Figure 7: Numerical calculation of $n = 2$ and $l = 1$ (first excited state)

Figure 5, 6 and 7 are the numerical calculations of the energy level of a hydrogen atom. On our program we used timestep $h = 0.002a$, right-hand boundary (which analytically should be positive infinity) $r_{inf} = 20a$, and target energy convergence $\frac{e}{1000}$ where a is a bohr radius and e is an electron charge. From Bohr model, it is well known that at ground state, hydrogen atom has the electron energy of $-13.6eV$, and at first excited state it has $-3.4eV$. Figure 5, 6 and 7 shows similar numerical calculations to such known values. Changing the time step h tends to increase the accuracy of calculation, but it also significantly affects the calculation time it takes. Changing the right-hand boundary r_{inf} too low or too high tends to drop the accuracy of calculation. Changing target energy convergence affects the significant digit of calculation.

Q2 c)

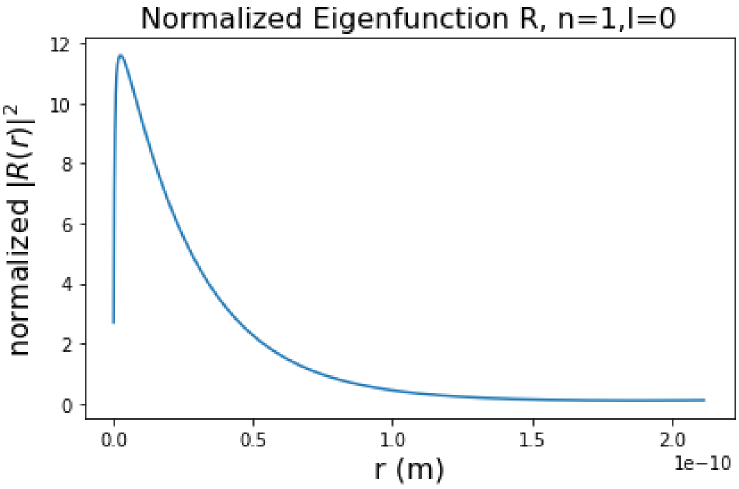

Figure 8: Normalized $|R(r)|^2$ with $n = 1$, $l = 0$

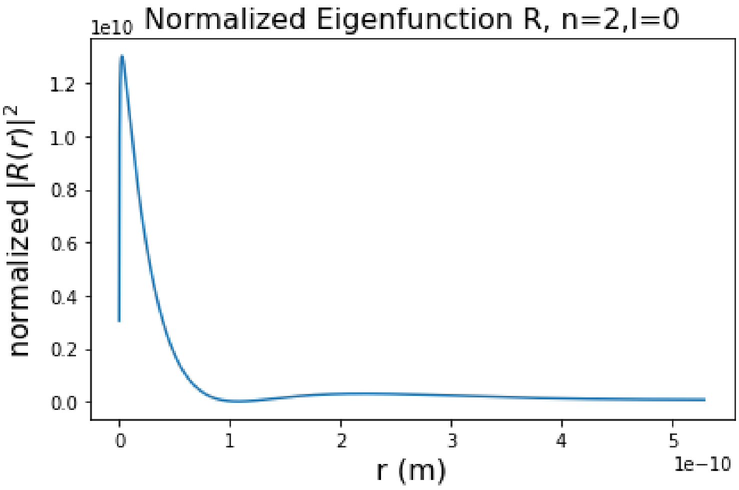

Figure 9: Normalized $|R(r)|^2$ with $n = 1$, $l = 0$

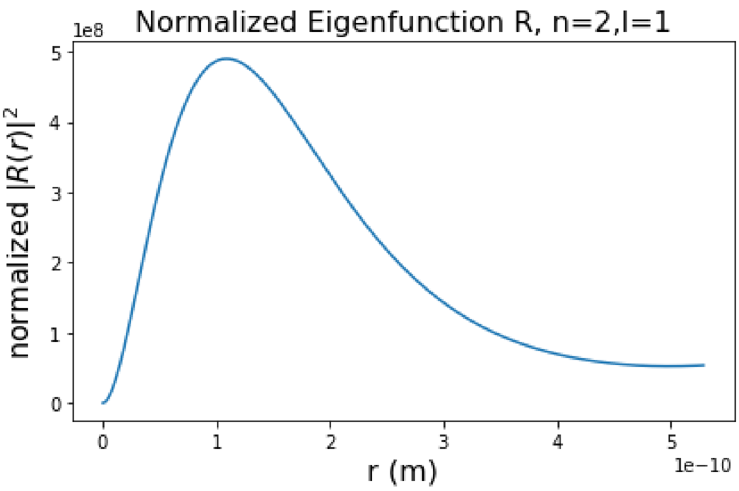

Figure 10: Normalized $|R(r)|^2$ with $n = 2$, $l = 1$