

**PHY407 Computational Physics Lab Assignment 7**  
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**Question 1: Molecular Dynamics of Argon Atoms**

For the Argon element, the forces experienced between two atoms can be modelled by the potential function:

$$V(r) = 4\epsilon \left[ \left( \frac{\sigma}{r} \right)^{12} - \left( \frac{\sigma}{r} \right)^6 \right]$$

When the atoms are relatively spread apart, there exists an attractive force created by the electric dipole moment between the atoms, which varies as  $r^{-6}$ , where  $r$  is the distance between them. When closer together though, the force becomes repulsive as the negatively charged electron clouds overlap. This force varies as  $r^{-12}$ . There is a sweet spot in between where the atoms are expected to oscillate, as these forces tend to cancel each other out. Overall then, this question means to investigate the relationships of these repulsive and attractive forces, by modelling position vs time functions of two argon atoms at various distances apart, to observe and comment on their behaviour.

**a) Nothing to Submit**

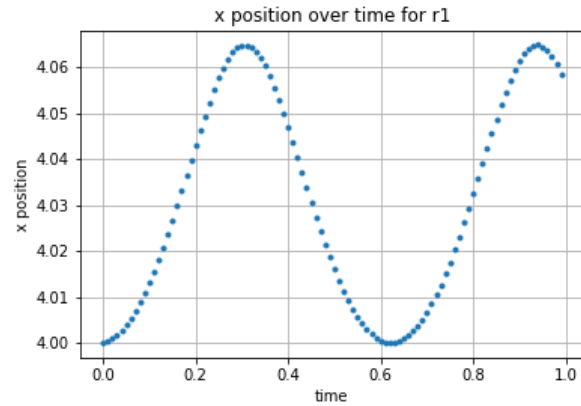
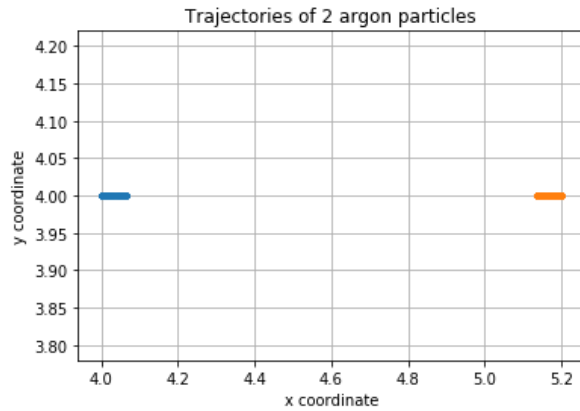
**b) (Restated Question)** For this question the goal is to apply the verlet method to update the position of two particles using a time step of  $dt = 0.01$  s for 100 steps (total of 1 second), then plot the trajectories of the particles. We did this for 3 sets of initial conditions.

**Pseudocode:**

```
# Define function to calculate distance from r1 and r2 (r)
# Define function to calculate the force by the potential in x and y
# components for both r1 and r2. Return array with 4 forces corresponding to
# the x and y for r1 and r2.
# perform verlet method in the following fashion
# initialize arrays to store the x and y positions for r1 and r2
# perform the first Euler step and obtain new velocity
# in a for loop perform the following actions
# update position from new velocity
# update distance from new position
# update force from new position and distance
# update velocity with new force
# append the new positions to the arrays and return when for loop is finished
```

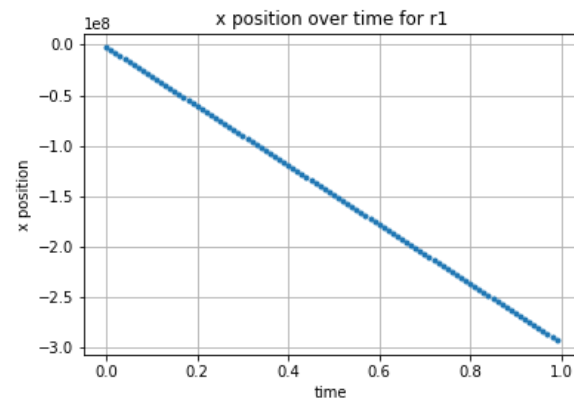
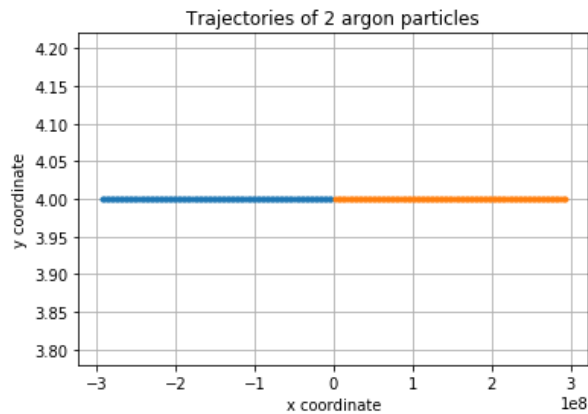
Note that since we are given dimensionless initial coordinates and unitless time steps, our graphs do not have any units.

For the first set of conditions:  $\mathbf{r1} = [4,4]$ ,  $\mathbf{r2} = [5.2,4]$  we obtain:



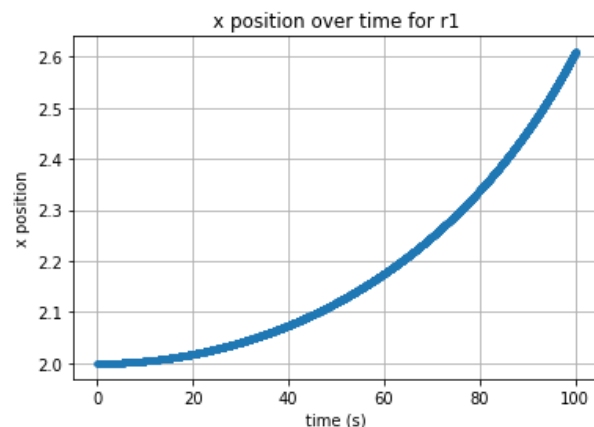
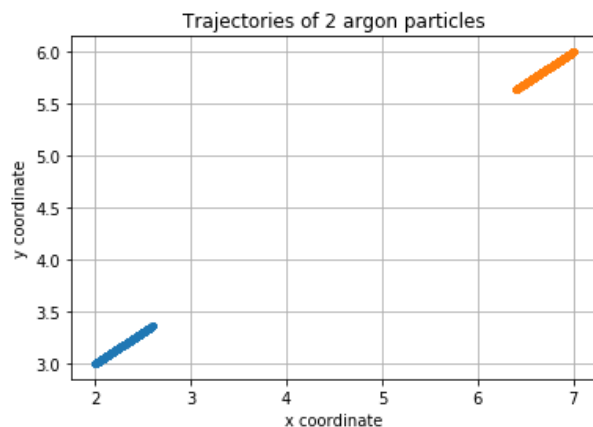
While its tricky to see in the first plot, the second plot illustrates the oscillatory nature of the particles quite well.

For the second set of conditions:  $\mathbf{r1} = [4.9, 4]$ ,  $\mathbf{r2} = [5.1, 4]$  we obtain:



Here, it's again clear from the second plot that the particles are close enough together to repel entirely, the particle starts at a zero position, and moves away (in the negative direction) from the other argon atom. Also take note of the scale of x axis which is  $1e8$  meaning they got repelled very far away, which is reflected when we look at x position over time.

For the final set of conditions:  $\mathbf{r1} = [2, 3]$ ,  $\mathbf{r2} = [7, 6]$  we obtain:



For this final set of conditions, it's clear that the first particle is far enough away from the second that it accelerates towards it, as shown by the exponential nature of the position time graph from the second plot.

- c) The first set of conditions is the only one which exhibits oscillatory motion from both particles. The second set was too close, the third, too far.

This is likely because the potential function:

$$V(r) = 4\epsilon \left[ \left( \frac{\sigma}{r} \right)^{12} - \left( \frac{\sigma}{r} \right)^6 \right]$$

would need to go to zero in order for the repellent portion of the function to cancel with the attractive. Given the values we have for sigma, that would happen close to when  $r \sim 1$  as  $1^{12} = 1^6$ . In our first case, this was almost precisely true, with  $r = 1.2$ . But in the second case, when  $r = 0.2$ , the repelling component  $r^{-12}$  dominated and create a repulsive potential, while the opposite happened in the last case, as the  $r$  value went up to around 5.83 causing the  $r^{-6}$  to now dominate, creating an attractive potential.

## Question 2: Time Independent Schrodinger Equation.

The time independent Schrödinger equation gives solutions which represent the possible energy values at different states in a quantum system. For this question, the systems in question will be a harmonic oscillator (a quadratic potential) and an anharmonic oscillator (a potential that varies as  $x^4$ ).

The goal will be to produce programs which output the corresponding energy values for the ground and first two excited states of the systems, as well as plot the wave functions vs position.

- a) **(Restate Question):** The goal for this question is to convert the Schrodinger equation from a second-order differential into two first order differentials. Next, given a set of conditions describing a particular quantum harmonic oscillator, we are asked to find the energy levels of the first three states (ground and first two excited).

The code provided illustrates the methods used, but it is similar to that used in example 8.9 in the Computational physics by Mark Newman text (page 395). The energy values we obtained are the following:

**E\_0 = 138.02881165268067 eV**

**E\_1 = 414.08643773118314 eV**

**E\_2 = 690.1440640968267 eV**

These values make sense given the hint provided for the range of the ground state energy

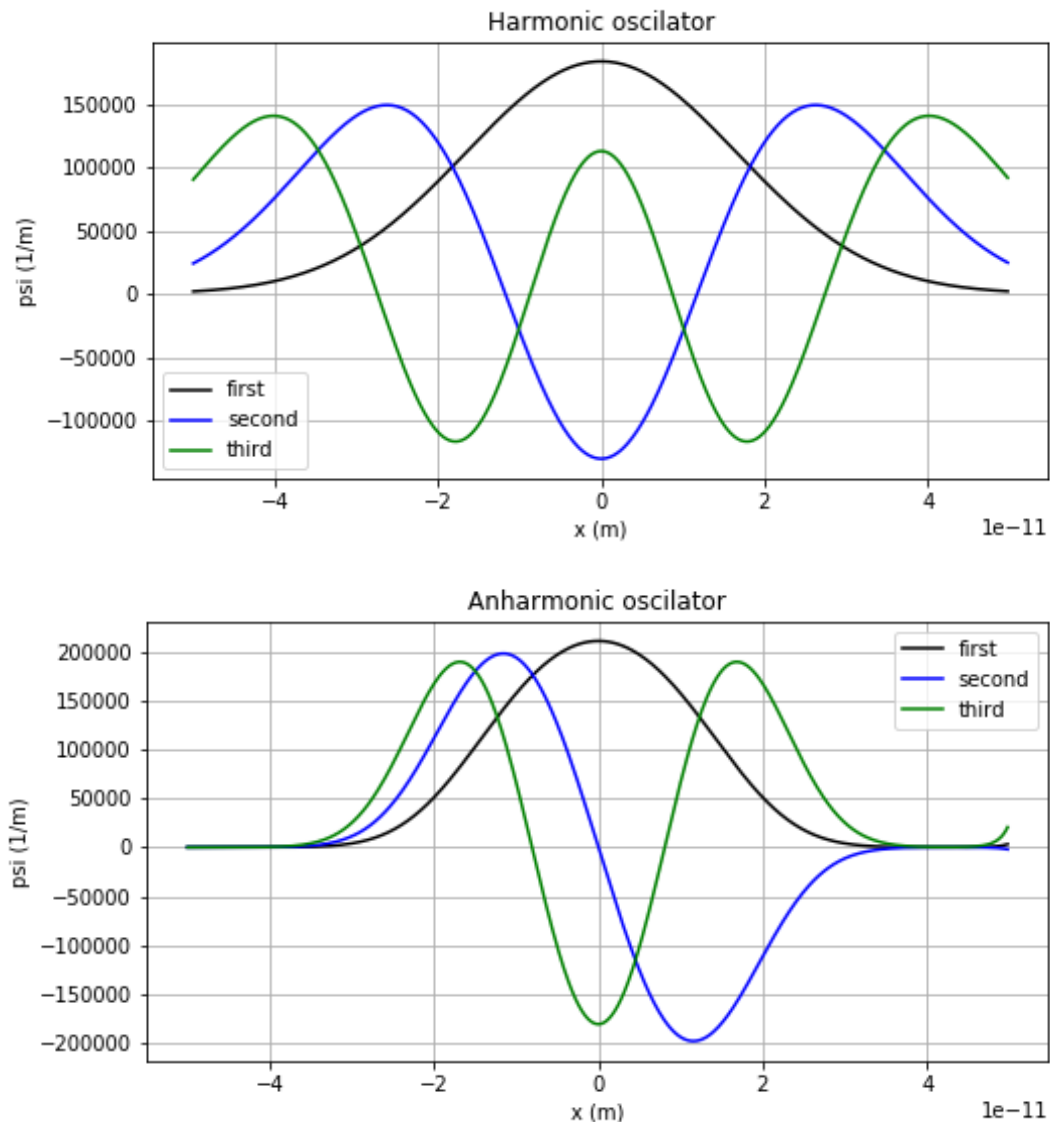
b) **(Restated Question)** For this question, we wanted to run the same test, except this time using a potential function representing an anharmonic oscillator. Here, the only differences we made to the code were the potential function as well as the ranges we guessed for the energies in our secant root function. The resulting energies were the following:

$E_0 = 205.31650347109755 \text{ eV}$

$E_1 = 735.7256474286083 \text{ eV}$

$E_2 = 1443.636921666496 \text{ eV}$

c) **(Restated Question)** This final part asks us to modify our program to incorporate normalized wave functions of our anharmonic oscillator for the 3 states, and to plot them on the same axis over the range  $-5a$  to  $5a$ . We ended up using Simpson's rule to calculate our integral for this part. The desired plots are the following:



One thing to notice in the anharmonic plot is the small spike at the far right end of the plot (most noticable in the plot for psi2). Printing the array of values for these functions gives an increase in value up to the magnitude of  $10^{48}$ . This massive increase is likely due to the potential wall at the end not being a true block (can only program it so accurately), so the normalization caused division close to zero in this region (where there should be infinite potential, and therefore no continued x values) rather than just ending the wave function, resulting in these extremely large numbers near the bounds.

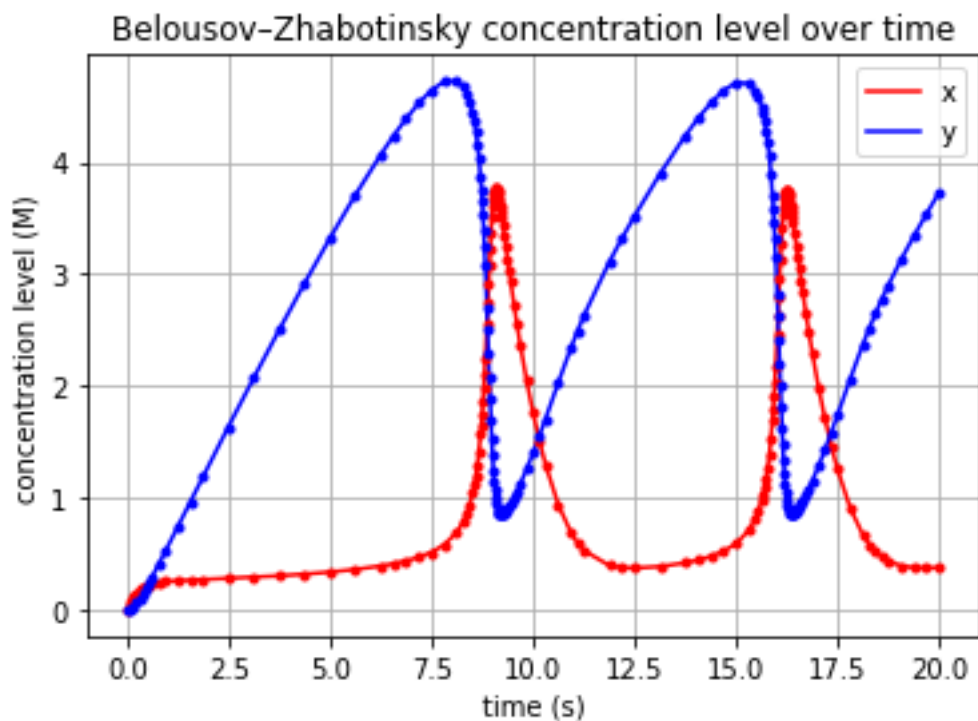
### Question 3: Oscillating Chemical Reactions:

The Belousov-Zhabotinsky reaction represents what happens when a particular chemical mixture reacts with heat. When heated, the mixture tends to oscillate between 2 extremes concentrations. These oscillations are represented mathematically by the following two first order differential equations:

$$\begin{aligned}\frac{dx}{dt} &= 1 - (b+1)x + ax^2y, \\ \frac{dy}{dt} &= bx - ax^2y.\end{aligned}$$

The purpose of this question is to investigate these relationships with a plot of the x and y values vs time to better understand how the concentration oscillates when exposed to heat over time.

- a) **Only code to submit here refer to the python file**
- b) **Nothing to submit here**
- c) **(Restated Question)** The goal here is to plot the solutions for the Belousov-Zhabotinsky reaction using the adaptive Bulirsch-Stoer method in both x and y per unit time. The time allowed was between 0-20 seconds. The following is the plot resulting from the code:



From the graph, we can see that the concentration of  $x$  and  $y$  are in an opposition trend. When  $y$  is increasing,  $x$  is decreasing or remaining almost constant. Then when  $y$  drops suddenly,  $x$  would peak. This is a direct reflection of the experiment where the concentration of the mixture oscillates between two extremes, which would correspond to the sudden change of color.

It is also worth noting that the points near the sudden drops and peaks are much close together which is what we would expect from what the question suggests.