Lab 6 PHY407

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Question 1a

Answer

To find the x and y components of acceleration we must first write Newtons equation of motion in terms of the Lennard-Jones Potential, V(r) where V(r) is the interactive potential and is taken to be the derivative of the net force since we assume a closed system.

$$a = \frac{F}{m}$$

So

$$a = \frac{1}{m}\frac{d}{dr}[-V(r)]$$

To simplify this further we need to write out the equation of V(r) which is:

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

Hence the derivative of V(r) w.r.t r is:

$$\frac{d}{dr}[-V(r)] = 48\epsilon(\frac{\sigma^{12}}{r^{13}}) - 24\epsilon(\frac{\sigma^{6}}{r^{7}})$$

In the question, we are given that the masses of the molecules are m = 1.0, $\sigma = 1$ and $\epsilon = 1$. So the net acceleration of one of the particles, caused by the other particle is given by:

$$a = 48(\frac{1}{r^{13}}) - 24(\frac{1}{r^{7}})$$

To find the acceleration in the x and y direction we can use Pythagoras' Theorem. Taking the distance between the two particles to be r, where r is:

$$r = \sqrt{(dx^2 + dy^2)}$$

Where dx and dy are the distances between the particles in the x and y directions, given as follows:

$$dx = (r_{1_x} - r_{2_x})$$

$$dy = (r_{1_y} - r_{2_y})$$

Therefore the acceleration in the x direction (a_x) and the y direction (a_y) can be calculated with the equations:

$$a_x = [48(\frac{1}{r^{13}}) - 24(\frac{1}{r^{7}})]\frac{dx}{r}$$

$$a_y = [48(\frac{1}{r^{13}}) - 24(\frac{1}{r^{7}})]\frac{dy}{r}$$

Question 1b

Pseudocode

```
# Define a function for the potential, V(r)
# Define a function for the acceleration in the x and y directions as shown in part a
# Create a list(list) for the 3 sets of initial conditions
# Create a time array, step h = 0.01, length 100
# For each of the initial conditions, complete the Verlet algorithm,
appending each x1,y1,x2,y2,vx1,vy1,vx2,vy2 points per iteration
# Plot the results
```

Plots

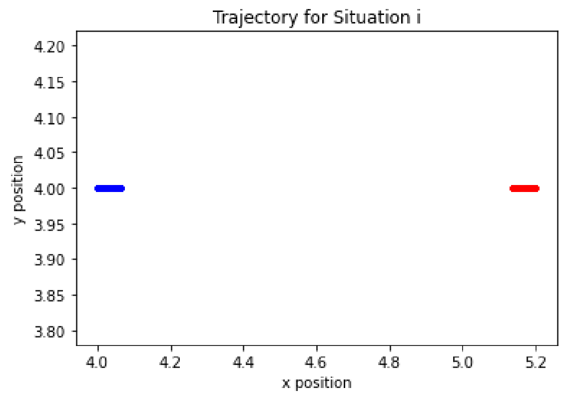

Figure 1:

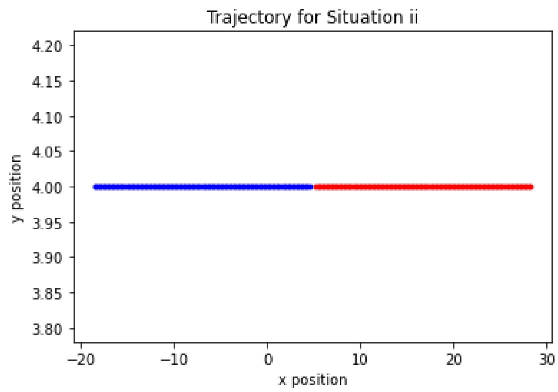

Figure 2:

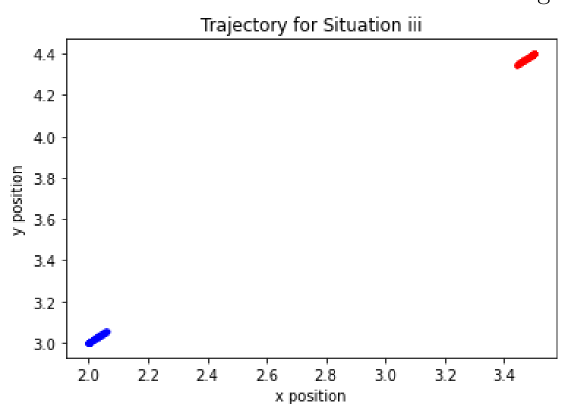

Figure 3:

Question 1c

Plot and Answer

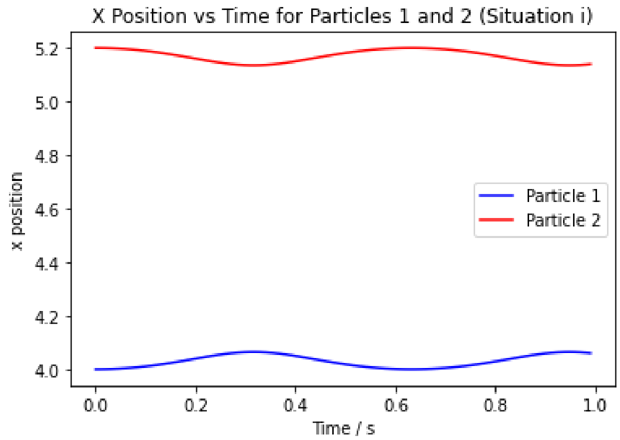

Figure 4:

It is situation (i) as seen above that causes the particles to show oscillatory motion. This is because we have set up the simulation so the particles have no initial kinetic energy. Therefore, as the potential in the system changes, in order to conserve energy, the particles must gain some kinetic energy, therefore, start to oscillate.

Question 2a

Pseudocode

- define fucntion that calculates the force on each particle i as a sum of the interaction forces between particle 'i' and all other particles
  - create arrays fx and fy for the initial positions for particles in x and y direction
  - make 2 for loops to loop over all the particles and add an if statement so the particle doesnt interact with itself (i != j)
  - calculate distance between particles i and j in x and y direction (dx and dy, respectively)
  - multiply force formula we derived in question 1 by the distances found above
  - sum over these values in the arrays fx and fy and let the function return fx,fy
- create 2 empty arrays for the trajectories of the 16 particles in each direction (x_points ,y_points)
- use a for loop to add an array to x_points and y_points each iteration so that every one of the 16 particles gets its own array
  - append the initial positions to x_points and y_points arrays

Note: Now we start the Verlet method

- set the time step h=0.01 and create array for time from 0-10s
- create 4 zeros arrays with size N=16 for when we calculate $v(t+h)$ (one in x and one in y direction) and $v(t+\frac{1}{2}h)$ (vx_half and vy_half)
- calculate k by plugging in the initial x and y values in the function we defined above
- create arrays for x and y and set them to the initial positions
- calculate $v(x+\frac{1}{2}h)$

- loop over the time points in the array time and then loop over every particle in each time step
  - calculate x and y by multiplying h by $v(x + \frac{1}{2}h)$ (we get $r(t + h)$
  - append these new points to the initial points x and y
  - find new kx and ky by plugging in these new points into the force function and multiplying by h
  - loop up to N and calculate $v(t + h)$ and $v(t + \frac{3}{2}h)$
- loop over every particle and plot its trajectory (so all 16 are on one graph)

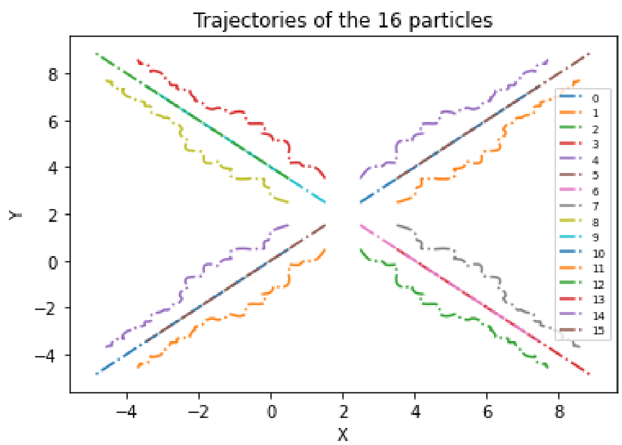

Figure 5: Each line represents the particles trajectory from t=0 to t=10s. Note that here, particle 1 is represented as particle 0 (blue), particle 2 is particle 1 (orange), and so on.

Question 2b

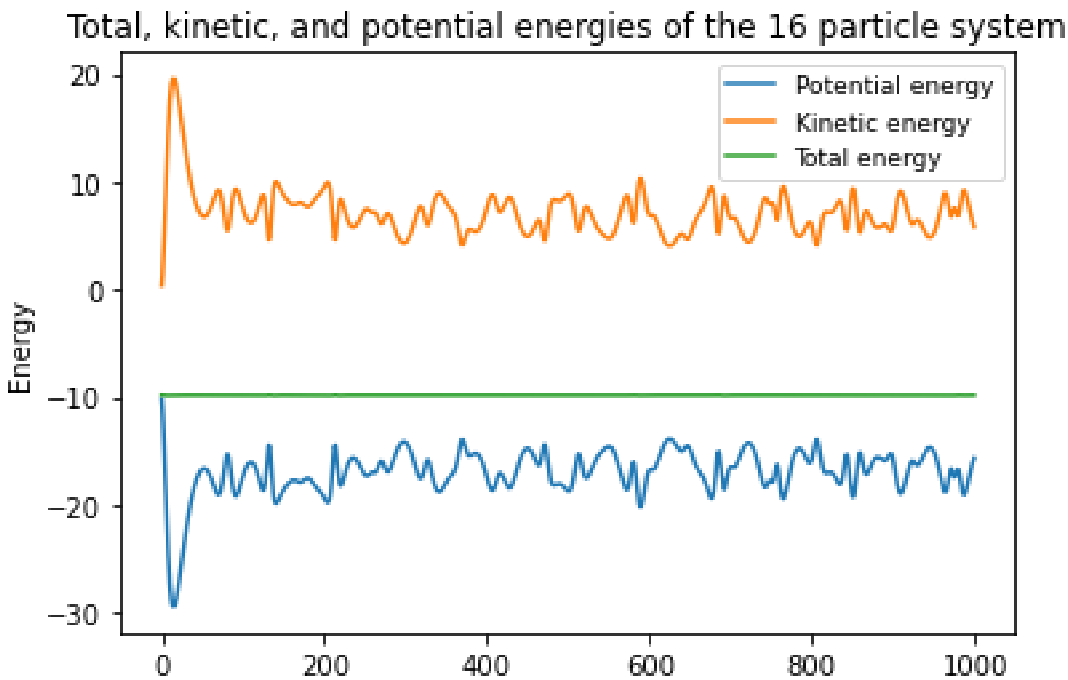

Figure 6: This plot shows the total energy of the 16 particle system is conserved as the total energy is a straight horizontal line at -10. We can clearly tell that the potential energy is the negative of the kinetic energy ($U = -K$)