Lab Report 6

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Q1 a)

Lennard-Jones Potential: $V(r) \;=\; 4\epsilon[(\frac{\sigma}{r})^{12} - (\frac{\sigma}{r})^{6}]$

Take derivative of $V(r)$ to get the force: $-\frac{dV(r)}{dr} = \vec{f}(\vec{r}, t)$

Find acceleration from force: $a = \frac{\vec{f}(\vec{r},t)}{m} = \frac{d^2\vec{r}}{dt^2}$

x components of the acceleration:

$$-\frac{\partial V(x)}{\partial x} = -\frac{\partial}{\partial x}\{\, 4\epsilon[(\frac{\sigma}{\sqrt{x^2+y^2}})^{12} - (\frac{\sigma}{\sqrt{x^2+y^2}})^{6}]\} \qquad (r = \sqrt{x^2+y^2})$$

$$= \frac{48x}{(x^2+y^2)^7} - \frac{24x}{(x^2+y^2)^4} \qquad (\epsilon = 1, \text{mass} = 1, \sigma = 1)$$

y components of the acceleration:

$$-\frac{\partial V(y)}{\partial y} = -\frac{\partial}{\partial y}\{\, 4\epsilon[(\frac{\sigma}{\sqrt{x^2+y^2}})^{12} - (\frac{\sigma}{\sqrt{x^2+y^2}})^{6}]\} \qquad (r = \sqrt{x^2+y^2})$$

$$= \frac{48y}{(x^2+y^2)^7} - \frac{24y}{(x^2+y^2)^4} \qquad (\epsilon = 1, \text{mass} = 1, \sigma = 1)$$

Q1 b)

Pseudocode

```
import numpy
import matplotlib.pyplot

#Define a function that calculates x,y components of acceleration
def function(array of two vector [r_1, r_2], time):
    x = x_component of r⃗_1 - x_component of r⃗_2
    y = y_component of r⃗_1 - y_component of r⃗_2
    x-component of acceleration of r⃗_1 = 24x/(x^2+y^2)^7 - 12x/(x^2+y^2)^4
    y-component of acceleration of r⃗_1 = 24y/(x^2+y^2)^7 - 12y/(x^2+y^2)^4
    x-component of acceleration of r⃗_2 = 12x/(x^2+y^2)^4 - 24x/(x^2+y^2)^7
    y-component of acceleration of r⃗_2 = 12y/(x^2+y^2)^4 - 24y/(x^2+y^2)^7
   return [accelerations of r⃗_1 ], [accelerations of r⃗_2 ]
```

```
#Assign time step
time_step = 0.01
#Assign number of time step
number_of_time_step = 100
#Assign time
time = 0 to 1
#Assign initial velocity
initial velocity = 0

#Use Verlet method to calculate velocity and position of a
particle
```

Calculate $\vec{v}(t+\frac{h}{2}) = \vec{v}(t) + \frac{h}{2}\vec{f}(\vec{r}(t), t)$ for first step only

```
#Calculate position and velocity using for-loop
for time_step in time:
```

$\vec{r}(t+h) = \vec{r}(t) + h\vec{v}(t+\frac{h}{2})$

$\vec{k} = h\vec{f}(\vec{r}(t+h), t+h)$

$\vec{v}(t+h) = \vec{v}(t+\frac{h}{2}) + \frac{1}{2}\vec{k}$

$\vec{v}(t+\frac{3}{2}h) = \vec{v}(t+\frac{h}{2}) + \vec{k}$

plot trajectories for $\vec{r}_1 = [4, 4], \vec{r}_2 = [5.2, 4]$

plot trajectories for $\vec{r}_1 = [4.5, 4], \vec{r}_2 = [5.2, 4]$

plot trajectories for $\vec{r}_1 = [2, 3], \vec{r}_2 = [3.5, 4.4]$

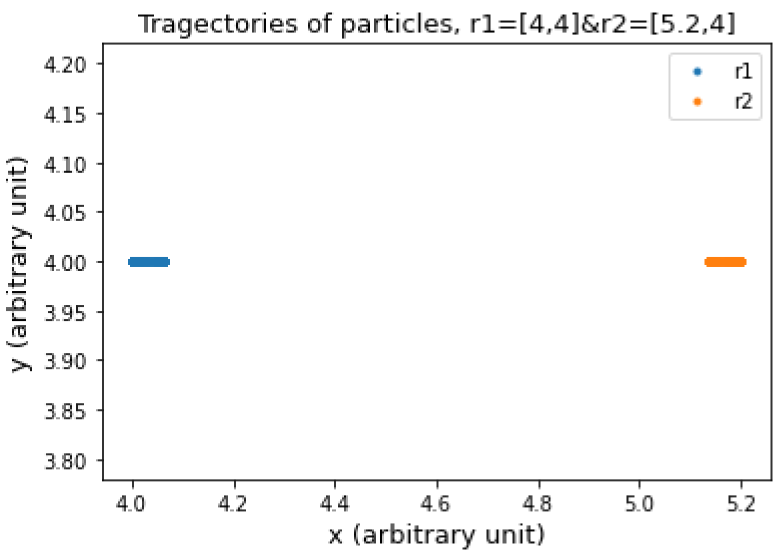

Figure 1: Trajectories of particle with initial condition $\vec{r}_1 = [4, 4], \vec{r}_2 = [5.2, 4]$

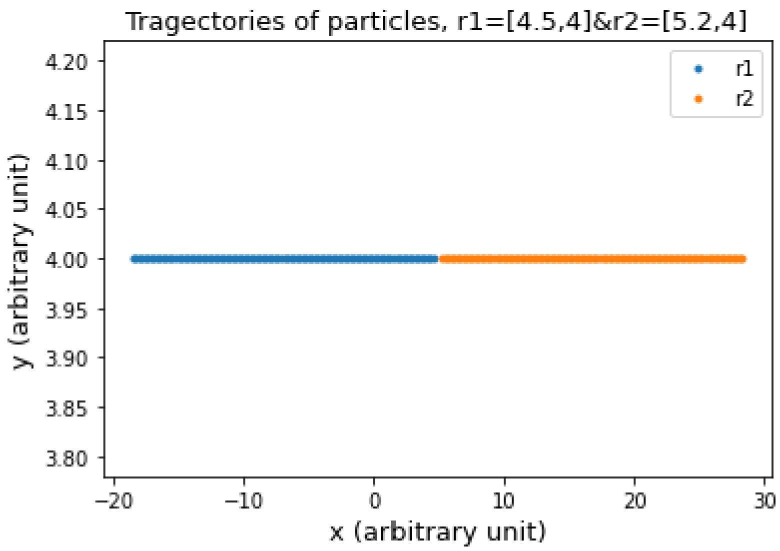

Figure 2: Trajectories of particle with initial condition $\vec{r}_1 = [4.5,\ 4]$, $\vec{r}_2 = [5.2,\ 4]$

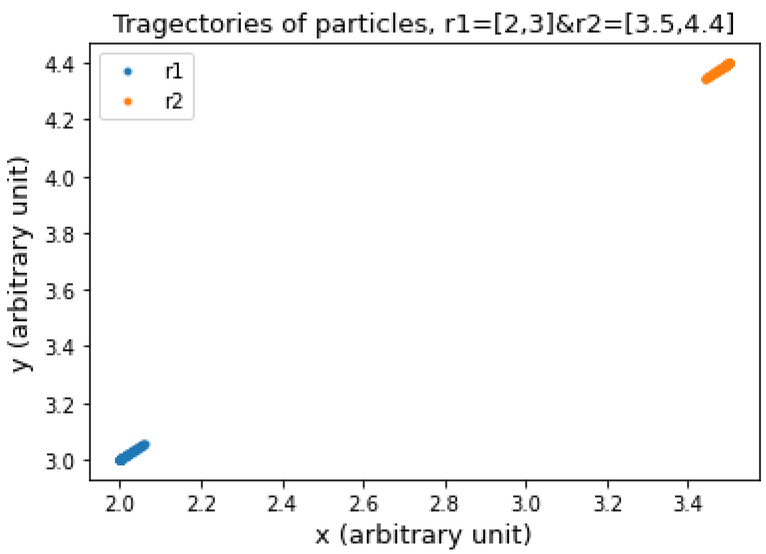

Figure 3: Trajectories of particle with initial condition $\vec{r}_1 = [2,\ 3]$, $\vec{r}_2 = [3.5,\ 4.4]$

Q1 c)

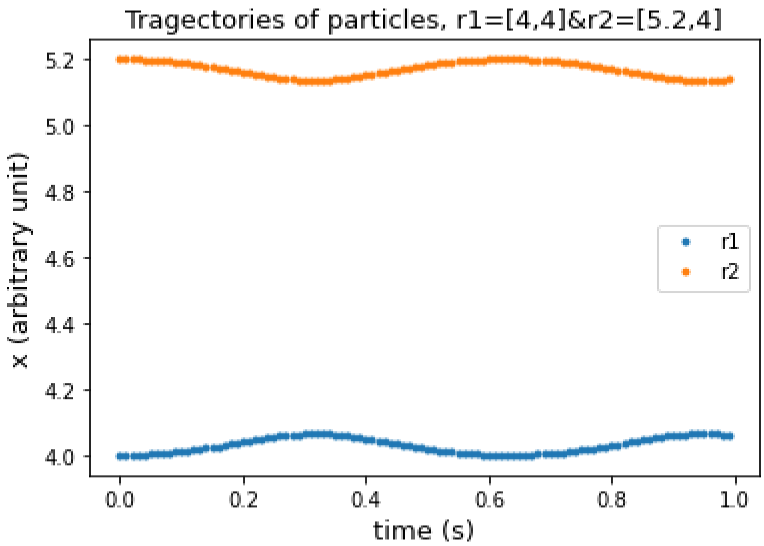

Figure 4: Oscillatory motion of a particle with initial position $\vec{r}_1 = [4, 4]$, $\vec{r}_2 = [5.2, 4]$

The case with initial position $\vec{r}_1 = [4, 4]$, $\vec{r}_2 = [5.2, 4]$ leads to oscillatory motion for both of the particles. They show oscillatory motion because given Lennard-Jones potential equation with $\epsilon = 1$ which is the depth of the potential well, particles with given initial position $\vec{r}_1$ and $\vec{r}_2$ and initial velocity of 0 do not have enough kinetic energy to escape the potential well (i.e. they are “trapped” inside the potential well). If we plot t vs x, we can indeed see that they show oscillatory motion.

Q2 a)

Pseudocode

```
import numpy
import matplotlib.pyplot

#Define a Verlet method. Note that f⃗ is the same as acceleration.
def verlet(matrix of r, time-step, time):
    position_value = [] #Make an empty array to store x and y
    velocity_value = [] #Make an empty array to store v_x and v_y
    On the first step, calculate v⃗(t + h/2) = v⃗(t) + (h/2)f⃗(r⃗(t), t).
    Then repeatedly apply the equations using a for loop:

    for t in number_of_time_steps:
        r⃗(t + h) = r⃗(t) + hv⃗(t + h/2) #position of the particle
        k⃗ = hf⃗(r⃗(t + h), t + h) #time step times acceleration
        v⃗(t + h) = v⃗(t + h/2) + (1/2)k⃗ #velocity of the particle
        v⃗(t + (3/2)h) = v⃗(t + h/2) + k⃗ #next step of velocity
        append x and y to position_value
        append v_x and v_y to velocity_value
    return position_value, velocity_value


#Define a function that calculates x,y components of acceleration
def acceleration(2d array r that contains x and y position):
   acceleration_value = [] #Make an empty array to store a_x and a_y
    #i is the particle we want to calculate a_x and a_y for
    #j is the other particles that affects particle i
    while i < number of particles:
        while j < number of particles:
            if i = j:
                don't do anything because it's a same particle
            else:
               x = x_i − x_j #x distance between particles i and j
               y = y_i − y_j #y distance between particles i and j
               #sum up all accelerations on particles i
               a_x += 48x/(√(x²+y²))⁷ − 24x/(√(x²+y²))⁴ #x acceleration of particle i
               a_y += 48y/(√(x²+y²))⁷ − 24y/(√(x²+y²))⁴ #y acceleration of particle i
          j+=1
      i+=1
      append a_x and a_y to acceleration_value
    return acceleration_value
```

```
#Use the code snippet provided from Lab instruction to find the
initial position of particles. Below x_initial and y_initial are
the values we obtain after using the code snippet.
x_initial = [0.5 1.5 2.5 3.5 0.5 1.5 2.5 3.5 0.5 1.5 2.5 3.5 0.5
1.5 2.5 3.5]
y_initial = 0.5 0.5 0.5 0.5 1.5 1.5 1.5 1.5 2.5 2.5 2.5 2.5 3.5
3.5 3.5 3.5]

h = 0.01 #Time step
N = 1000 #Number of time step
T = 0 to N*dt with time step h

Use the verlet function we defined to calculate the positions and
velocities of 16 particles.

plot trajectories for 16 particles.
```

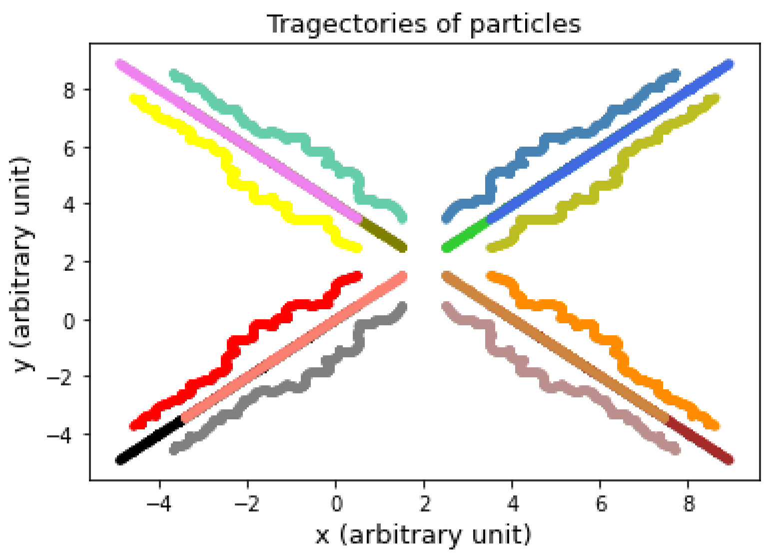

Figure 5: Trajectory motions of 16 particles

Q2 b)

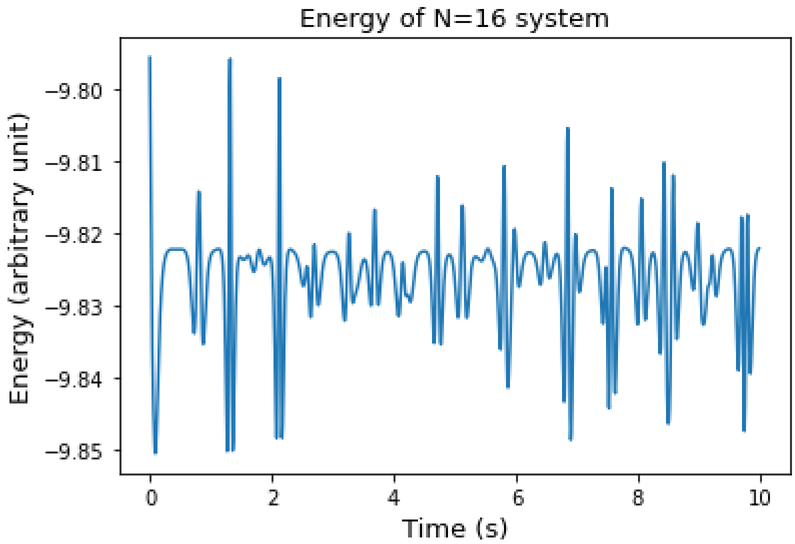

Figure 6: Total energy, calculated using $\frac{1}{2}m\vec{v}^2 + V(r)$

Figure 6 shows the plot for total energy, which is the sum of kinetic energy and potential energy. Maximum relative error for Figure 6 is within ~0.6% using a formula $\frac{max-min}{min} \times 100\%$, which is within the 1% of accepted bound.