PHY407F: Explanatory Notes for Lab 6

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1 Question 1 - by Idil Yaktubay

(a) The interaction potential of a two-dimensional molecular dynamics system of two particles under the influence of only the Lennard-Jones potential is given by equation 1, where ϵ is the depth of the potential well, σ is the Van der Waals radius, and r is the distance between the two particles. Combining Newton's second law, the fact $\vec{F}_r = -\frac{\partial V}{\partial r}\hat{\mathbf{r}}$, and the chain rule of calculus, we can find the x and y components of the acceleration of one particle due to the presence of the other particle using equation 2, where m is the mass of the particle.

$$V(r) = 4\epsilon\left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6}\right] \tag{1}$$

$$a_x = -\frac{1}{m}\frac{\partial V}{\partial r}\frac{\partial r}{\partial x},\ a_y = -\frac{1}{m}\frac{\partial V}{\partial r}\frac{\partial V}{\partial y} \tag{2}$$

Below, we have shown the derivation of the x component of the acceleration of one particle due to the presence of the other particle. We have used the fact that the separation distance between the particles is given by $r = \sqrt{(x-x')^2 + (y-y')^2}$, where x' and y' are the coordinates of the source particle, in order to find that $\frac{\partial r}{\partial x} = \frac{x-x'}{r}$.

$$\begin{aligned}
a_x &= -\frac{1}{m}\frac{\partial V}{\partial r}\frac{\partial r}{\partial x} \\
&= -\frac{1}{m}\frac{\partial}{\partial r}\left[4\epsilon\left(\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6}\right)\right]\frac{\partial r}{\partial x} \\
&= -\frac{4\epsilon}{m}\left(-12\sigma^{12}\frac{1}{r^{13}} + 6\sigma^{6}\frac{1}{r^{7}}\right)\frac{\partial r}{\partial x} \\
&= \frac{24\epsilon\sigma^6}{m}\left(2\sigma^{6}\frac{1}{r^{13}} - \frac{1}{r^{7}}\right)\frac{\partial r}{\partial x} \\
&= \frac{24\epsilon\sigma^6}{m}\left(2\sigma^{6}\frac{1}{r^{14}} - \frac{1}{r^{8}}\right)(x-x') \\
&= \frac{24\epsilon\sigma^6}{m}\left(\frac{\sigma}{r}\right)^{6}\frac{1}{r^2}\left[2\left(\frac{\sigma}{r}\right)^{6} - 1\right](x-x')
\end{aligned}$$

The exact same steps can be followed to derive the y component of the acceleration of the same particle due to the presence of the other particle. Therefore, the expressions for the x and y components of the acceleration of one particle due to the presence of the other particle in this molecular system is given by equations 3 and 4, respectively.

$$a_x = \frac{24\epsilon\sigma^6}{m}\left(\frac{\sigma}{r}\right)^{6}\frac{1}{r^2}\left[2\left(\frac{\sigma}{r}\right)^{6} - 1\right](x-x') \tag{3}$$

$$a_y = \frac{24\epsilon\sigma^6}{m}\left(\frac{\sigma}{r}\right)^{6}\frac{1}{r^2}\left[2\left(\frac{\sigma}{r}\right)^{6} - 1\right](y-y') \tag{4}$$

(b) We have written a program to update the position of the two particles in this conservative system using the Verlet method for zero initial velocities and three sets of initial positions. We have used a time step of $dt = 0.01$ and

ran the simulation for 100 time steps (101 time points). We have used the values $\sigma = 1.0$ and $\epsilon = 1.0$ and assumed units where the masses of both particles are 1.0. Figures 1, 2 and 3 depict the trajectories of both particles for the three sets of initial conditions. Along with trajectories, we have included position versus time plots to better show features of particle behavior. Our figure captions include all the remaining relevant information about our plots.

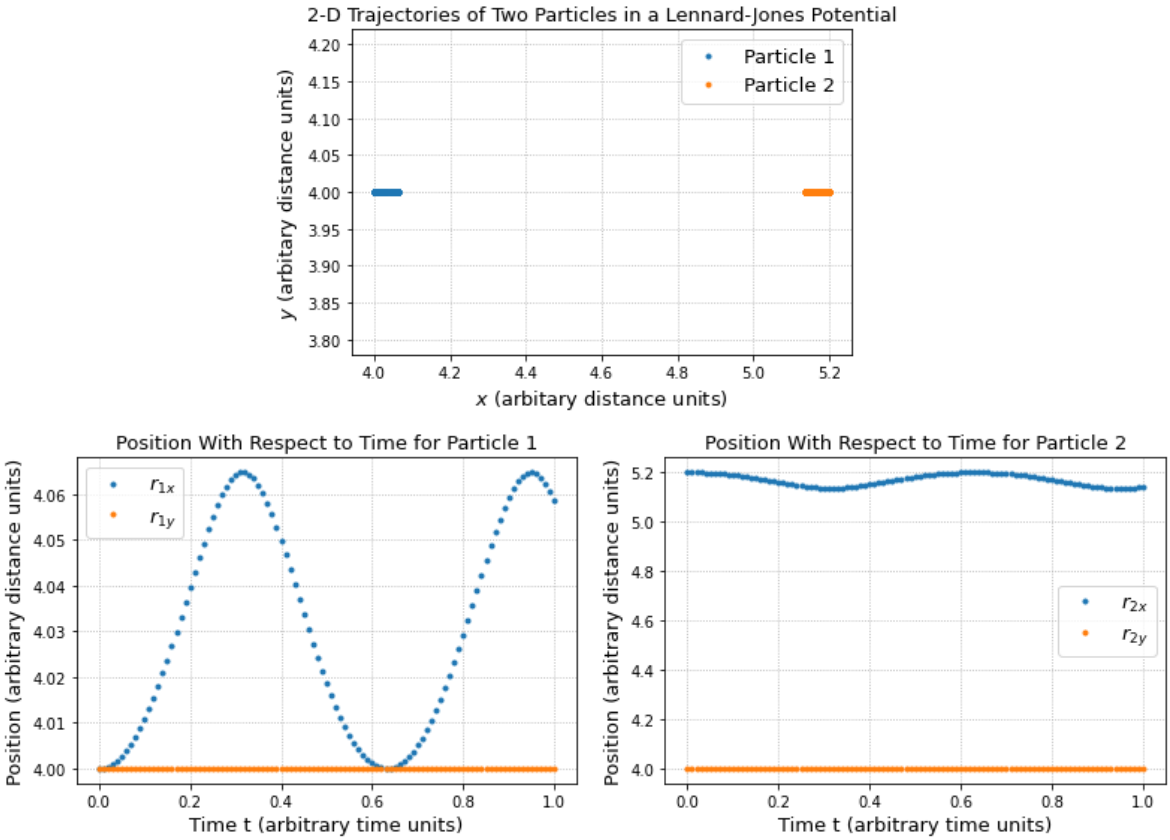
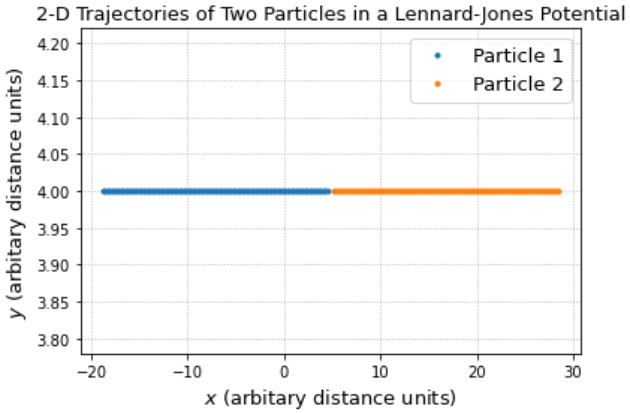
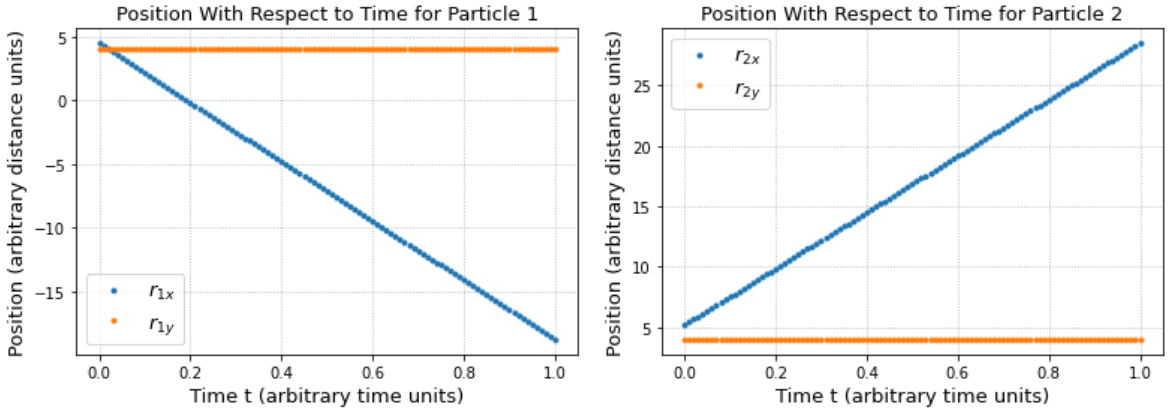


Figure 1: Trajectories and positions with respect to time of two particles under the influence of only the Lennard-Jones potential for the first set of initial conditions. Here, the initial conditions are given by zero initial velocities and initial positions $\vec{r}_1 = [4, 4], \vec{r}_2 = [5.2, 4]$. The trajectories are depicted by the top plot, whereas the position with respect to time of particles 1 and 2 are depicted by the bottom left and bottom right plots, respectively. As the bottom two plots suggest, both particles engage in oscillatory motion along the x direction.



(First part of Figure 2)



(Figure 2 continued)

Figure 2: Trajectories and positions with respect to time of two particles under the influence of only the Lennard-Jones potential for the second set of initial conditions. Here, the initial conditions are given by zero initial velocities and the initial positions $\vec{r}_1 = [4.5, 4], \vec{r}_2 = [5.2, 4]$. The trajectories are depicted by the top plot, whereas the position with respect to time of particles 1 and 2 are depicted by the bottom left and bottom right plots, respectively. As the bottom two plots suggest, both particles move away from each other along the x direction.

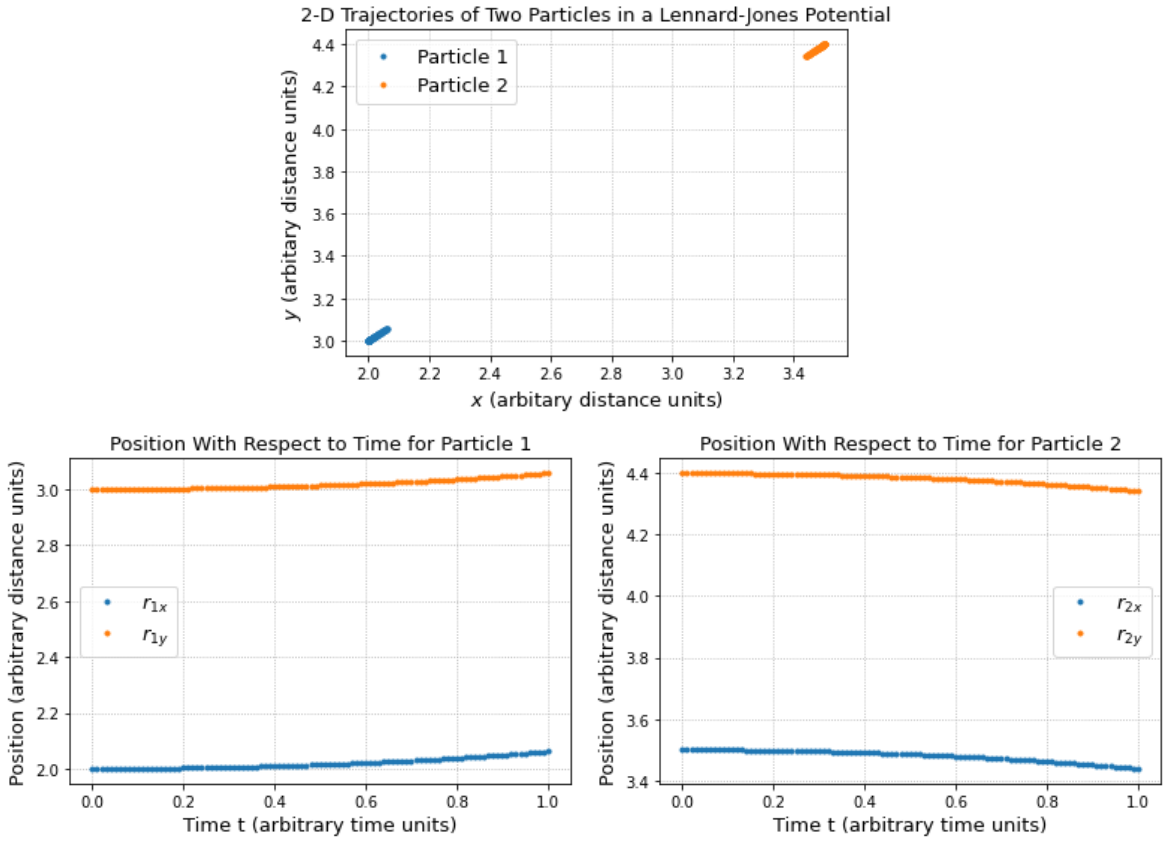


Figure 3: Trajectories and positions with respect to time of two particles under the influence of only the Lennard-Jones potential for the third set of initial conditions. Here, the initial conditions are given by zero initial velocities and $\vec{r}_1 = [2, 3], \vec{r}_2 = [3.5, 4.4]$. The trajectories are depicted by the top plot, whereas the position with respect to time of particles 1 and 2 are depicted by the bottom left and bottom right plots, respectively. As the bottom two plots suggest, both particles move towards each other along the x and y directions.

(c) As we have seen, the set of initial conditions corresponding to the plots from Figure 1 leads to oscillatory motion for both particles along the x direction. This is because this set of initial conditions correspond to an initial separation distance of 1.2 distance units, which sits inside the Lennard-Jones potential well. Therefore, the two particles constantly move in a way to reach an equilibrium (the bottom of the well). In other words, the particles are

trapped inside this potential well in a way that conserves the total energy of the system with oscillating kinetic and potential energies (simple harmonic motion). We have found that this conserved total energy corresponds to about -0.89 energy units. However, in the second case, the particles start off too close together for this to happen, and instead, they move away from each other due to the strong repulsive force between them. Whereas in the third case, although the particles will *eventually* have oscillatory motion by falling into the well, our time domain simply isn't long enough to show this.

2 Question 2 - By Idil Yaktubay and Souren Salehi

(a) We have updated our code from question 1 to plot the trajectories of 16 identical particles with zero initial velocities and initial positions given by Figure 4. Our updated code calculates the net acceleration of each particle at each point in time as a result of its interaction with the remaining particles particles. We have ran our code for 1000 time steps (1001 time points) with $dt = 0.01$. Once again, we have used the Verlet method to update the particle positions. Figure 4 depicts the trajectories of these 16 particles within the time period we have defined.

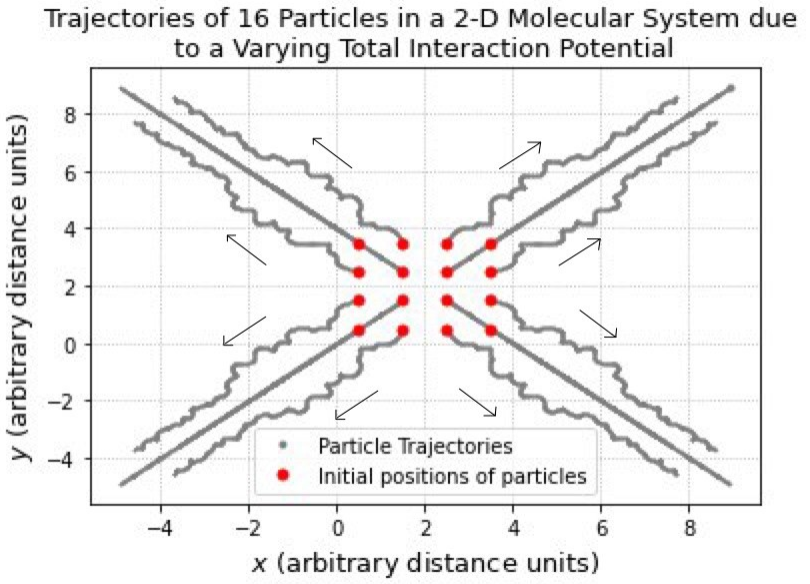


Figure 4: Trajectories of 16 particles under the influence of only the Lennard-Jones interaction potentials. The red dots represent the initial position of the particles, whereas the grey sets of dots that trail each red dot represent the trajectories of the corresponding particles. The black arrows show the direction of particle movement. As expected, the trajectories are symmetric, meaning that the energy is conserved.

(b) Lastly, we have computed the total energy of this 16-particle system at each point in time. We have found the initial total energy of this system to be about -9.8 energy units. Due to the limited accuracy of our program, the total energy deviates from this value by a maximum deviation of about 0.6% within the time period we have defined. Figure 5 shows the conservation of total energy with these minor deviations.

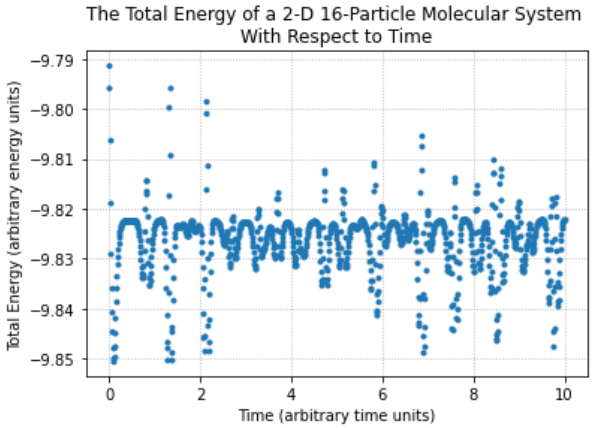


Figure 5: The total energy of the 2-D 16-particle Lennard-Jones system with respect to time. The maximum energy value is ≈ -9.79 energy units (the initial value of total energy), whereas the minimum energy value is ≈ -9.85 energy units. Therefore, the maximum deviation from the initial energy is $\approx 0.6\%$, indicating energy conservation.