Problem 1. Classical harmonic oscillator. Consider two atoms in 1D with positions $R_1$ and $R_2$ and mass $M_1$ and $M_2$ interacting via a quadratic potential energy: $\frac{1}{2} K (R_1 - R_2)^2$. This could represent a di-atomic molecule interacting with quadratic bond-stretch potential.

Question 1.1: Which expression below represents the Hamiltonian of the system?

$$\begin{align*}
\text{a)} & \quad \frac{1}{2} K (R_1 - R_2)^2 \\
\text{b)} & \quad \frac{1}{2} M_1 \dot{R}_1^2 + \frac{1}{2} M_2 \dot{R}_2^2 + \frac{1}{2} K (R_1 - R_2)^2 \\
\text{c)} & \quad M_1 \dot{R}_1 \\
\text{d)} & \quad \frac{P_1^2}{2 M_1} + \frac{P_2^2}{2 M_2} + \frac{1}{2} K (R_1 - R_2)^2 \quad \text{with} \quad P_i = M_i \dot{R}_i
\end{align*}$$

Question 1.2: Four equations of motion are derived from this Hamiltonian, one for each of the variables. The ones corresponding to particle 1 are:

$$\begin{align*}
\text{a)} & \quad \dot{R}_1 = \frac{P_1}{M_1}; \quad \dot{P}_1 = -K R_1 \\
\text{b)} & \quad \dot{R}_1 = \frac{P_1}{M_1}; \quad \dot{P}_1 = -K (R_1 - R_2) \\
\text{c)} & \quad \dot{R}_1 = \frac{P_1}{M_1}; \quad \dot{P}_1 = K (R_1 - R_2)
\end{align*}$$
This system can be solved analytically and to do so we will perform a change of variable into normal modes. We will see that this coupled system can be described as two uncoupled harmonic oscillators. To do so, we will perform the following change of variables: \( R_{CM} = \frac{M_1 R_1 + M_2 R_2}{M_1 + M_2} \) and \( R = R_2 - R_1 \). In terms of the new variables representing the center of mass of the molecule and the bond distance the original variables can be written as: \( R_1 = R_{CM} - \frac{M_2}{M_1 + M_2} R \) and \( R_2 = R_{CM} + \frac{M_1}{M_1 + M_2} R \).

**Question 1.3.** The Hamiltonian in terms of the new variables and their time-derivatives is:

a) \[ \frac{1}{2} \left( M_1 M_2 \right) \dot{R}_{CM}^2 + \frac{1}{2} \frac{M_1 M_2}{M_1 + M_2} \dot{R}^2 + \frac{1}{2} K R^2 \]

b) \[ \frac{1}{2} \left( M_1 + M_2 \right) \dot{R}_{CM}^2 + \frac{1}{2} \frac{M_1 M_2}{M_1 + M_2} \dot{R}^2 + \frac{1}{2} K R^2 \]

c) \[ \frac{1}{2} \left( M_1 - M_2 \right) \dot{R}_{CM}^2 + \frac{1}{2} \frac{M_1 M_2}{M_1 + M_2} \dot{R}^2 + \frac{1}{2} K R^2 \]

This expression is not strictly speaking a Hamiltonian since the kinetic energy is not written in terms of momenta but velocities. The actual Hamiltonian in terms of the momenta associated with the center of mass (\( P_{CM} \)) and bond distance (\( P \)) is:

\[ \frac{P_{CM}^2}{2(M_1 + M_2)} + \frac{1}{2} \frac{P^2}{\mu} + \frac{1}{2} K R^2 \]
Question 1.4. The reduced mass ($\mu$) is:

   a) $\mu = \frac{M_1 M_2}{M_1 + M_2}$

   b) $\mu = \frac{M_1 + M_2}{M_1 M_2}$

Question 1.5 Obtain the two equations of motion for the center of mass position and momenta. Which of the following statements is true:

   a) The position of the center of mass of the molecule will remain constant
   b) The momentum of the center of mass is constant
   c) The center of mass will experience a constant acceleration

Problem 2. The harmonic oscillator. Consider a 1D harmonic oscillator with Hamiltonian: $\frac{1}{2} \frac{P^2}{\mu} + \frac{1}{2} K R^2$. Show that $R(t) = A \sin(\omega t)$ is a solution to the equations of motion and obtain an expression for the characteristic frequency $\omega$.

Question 2.1. The frequency is:

   a) $\omega = \sqrt{\frac{K}{\mu}}$

   b) $\omega = \frac{K}{\mu}$
**Question 2.2.** Compute expressions for total and kinetic energies as a function of time. The total energy as a function of time is (select the best answer):

a) \( \frac{1}{2} KA^2 \)

b) \( \frac{1}{2} KA^2 \sin^2(\omega t) + \frac{1}{2} \mu A^2 \omega^2 \cos^2(\omega t) \)

c) \( \frac{1}{2} KA^2 \sin^2(\omega t) \)

d) a) and b)

**Question 2.3.** Compute the average kinetic and potential energies in one oscillation period and identify which of the following statements is correct:

a) The average kinetic energy is twice as large as the average potential energy.

b) The average kinetic and potential energies are equal in value.

c) The average potential energy is larger than the kinetic energy.