

# CHM 325 Assignment 4

October 25, 2022

Due on 2<sup>nd</sup> November, 2022.

1. The Lagrangian for a classical many-particle system is given as  $L(\{q_i, \dot{q}_i, t\}) = \sum_{i=1}^N \frac{1}{2} m \dot{q}_i^2 - V(\{q_i\}, t)$ , where  $q_i, \dot{q}_i$  are the generalized coordinates and velocities of the particles, respectively. The Lagrange equations of motion for the particles are given as

$$\frac{d}{dt} \frac{\partial}{\partial \dot{q}_i} L(\{q_i, \dot{q}_i, t\}) - \frac{\partial}{\partial q_i} L(\{q_i, \dot{q}_i, t\}) = 0$$

- (a) Defining the canonical momentum as  $p_i = \frac{\partial}{\partial \dot{q}_i} L(\{q_i, \dot{q}_i\})$ , obtain an expression for the Legendre transform of  $L$  over the velocities,  $-H(\{q_i, p_i, t\})$ . ( $H$  is called the Hamiltonian).
- (b) Using the above definitions, obtain the Hamilton's equations of motion for the system:

$$\dot{q}_i = \frac{p_i}{m_i}$$
$$\dot{p}_i = -\frac{\partial}{\partial q_i} V(\{q_i\}, t)$$

- (c) If the potential energy has no explicit time dependence, then show that  $\frac{dH}{dt} = 0$ , i.e. the total energy is conserved during motion.
2. A classical two particle system, confined to move along the  $x$ -axis, has an interaction potential energy given by  $V(x_1, x_2) = V(|x_2 - x_1|)$ .

- (a) From the Lagrangian (see above), derive the Hamiltonian for the system.
- (b) Define the new coordinates,  $X = \frac{m_1 x_1 + m_2 x_2}{m_1 + m_2}$  and  $x = x_2 - x_1$  (centre of mass and relative coordinates, respectively). Rewrite the Hamiltonian in terms of these new coordinates and derive the corresponding equations of motion.
3. If the two particle system described above were treated by quantum instead of classical mechanics, then the kinetic energy operator of the system would be given by  $\hat{T} = -\frac{\hbar^2}{2m} \left[ \frac{\partial^2}{\partial x_1^2} + \frac{\partial^2}{\partial x_2^2} \right]$ , where we have assumed  $m = m_1 = m_2$ . Derive an expression for the kinetic energy operator in terms centre of mass and relative coordinates.
4. The Laplacian in cartesian coordinates is given as  $\nabla^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}$ . Convert this spherical polar coordinates.
5. (a) Show that  $f_{xy} = f_{yx}$  for (a)  $f(x, y) = x^2 e^{-y^2}$ , and (b)  $e^{-y} \cos xy$ .  
 (b) Check if  $f_{xy}$ ,  $f_{yx}$  exist and are equal, explaining your results, for the function

$$f(x, y) = \begin{cases} \frac{xy}{x^2+y^2} & (x, y) \neq (0, 0) \\ 0 & (x, y) = (0, 0) \end{cases}$$

6. Given the heat capacity at constant volume is defined by  $C_V = \left( \frac{\partial U}{\partial T} \right)_V$ , and the expression  $\left( \frac{\partial U}{\partial V} \right)_T = T \left( \frac{\partial P}{\partial T} \right)_V - P$ , derive the equation  $\left( \frac{\partial C_V}{\partial V} \right)_T = T \left( \frac{\partial^2 P}{\partial T^2} \right)_V$ .
7. Find the rectangle of maximum area that can be inscribed in the ellipse described by  $\frac{x^2}{a^2} + \frac{y^2}{b^2} = 1$ .
8. If  $\sigma(x, y)$  is the mass density (mass per unit area) in a 2-dimensional sheet, the total mass of the sheet is given by  $M = \int \int_R \sigma(x, y) dx dy$ . Calculate the total mass of a circular sheet of radius  $a$  if  $\sigma(x, y) = x^2 y^2$ .
9. Evaluate the following integrals by reversing the order of integration:  
 (a)  $\int_0^1 dy \int_0^{\cos^{-1} y} dx \sec x$ , (b)  $\int_0^1 dy \int_y^1 dx \frac{ye^x}{x}$ .

10. Show that  $\int_0^{\pi/2} dx \int_x^{\pi/2} \frac{\sin u}{u} du = 1$ .