

5163, Homework Assignment 2

due on Friday, 02/04/2022, at 6pm (to be uploaded to Canvas)

This homework set consists of four problems.

Problem 1:

This problem serves as a refresher of thermodynamics: it utilizes the concepts of thermal and mechanical equilibrium as well as expressions for the temperature and the pressure in terms of the entropy.

Some substance has the entropy function

$$S = \lambda V^{1/2} (NE)^{1/4}, \quad (1)$$

where N is in moles, λ is a constant with appropriate units, and E and V denote energy and volume, respectively. A cylinder is separated by a partition into two halves, each of volume 1 m^3 . One mole of the substance with an energy of 200 J is placed in the left half, while two moles of the substance with an energy of 400 J is placed in the right half.

(a) Assuming that the partition is fixed but conducts heat, what will be the distribution of the energy between the left and right halves at equilibrium?

(b) Does your result from part (a) make sense? If so, provide an intuitive explanation of your result. If not, explain why your result does not make sense.

(c) Assuming that the partition moves freely and also conducts heat, what will be the volumes and energies of the samples in both sides at equilibrium?

(d) Does your result from part (c) make sense? If so, provide an intuitive explanation of your result. If not, explain why your result does not make sense.

Problem 2:

Suppose that the Hamiltonian \mathcal{H} contains a term that is linear in the parameter λ ,

$$\mathcal{H}(\vec{p}, \vec{q}) = \mathcal{H}_0(\vec{p}, \vec{q}) + \lambda h(\vec{p}, \vec{q}). \quad (2)$$

There are many physical situations that can be described by this type of Hamiltonian. For example, if we consider N particles in an external gravitational field, then the parameter λ can be identified as the gravitational acceleration g and the function h would take the form

$$h = m \sum_{i=1}^N z_i. \quad (3)$$

For the purpose of this problem, we will leave λ and h unspecified.

Show that the microcanonical average of the observable $h(\vec{p}, \vec{q})$ is given by

$$\langle h \rangle = -T \frac{dS}{d\lambda}. \quad (4)$$

The following will be helpful:

$$\frac{d}{d\lambda} \log f = \frac{\frac{df}{d\lambda}}{f} \quad \text{and} \quad \frac{d}{d\lambda} \theta(E - \mathcal{H}_0 - \lambda h) = -h \delta(E - \mathcal{H}_0 - \lambda h). \quad (5)$$

Problem 3:

Mathematically, there are quite a few similarity between the system considered here and the ideal gas system considered in class.

The position of a two-dimensional diatomic molecule with fixed distance between the two atoms can be described by the three coordinates (x, y, θ) , where x and y are the Cartesian coordinates of the center-of-mass of the molecule and θ gives the orientation of the molecular axis with respect to the x -axis. The conjugate momenta are denoted by (p_x, p_y, p_θ) . Physically, p_x and p_y are the linear center-of-mass momenta and p_θ is the angular momentum of the molecule about its center-of-mass. The energy ϵ of the molecule is

$$\epsilon = \frac{p_x^2 + p_y^2}{2m} + \frac{p_\theta^2}{2I}, \quad (6)$$

where I is the moment of inertia about the center-of-mass.

- (a) For a system of N non-interacting two-dimensional diatomic molecules confined to a two-dimensional area \mathcal{A} , use the microcanonical ensemble to calculate the entropy $S(N, E, \mathcal{A})$.
- (b) Using the entropy, derive the equations of state of the system, i.e., the equations that give the pressure and the energy per particle as functions of the temperature and density.
- (c) Calculate the constant volume (actually, it is better to say constant area) specific heat per particle, defined through

$$C_V = \frac{1}{N} \left(\frac{\partial E(N, T, \mathcal{A})}{\partial T} \right)_{N, \mathcal{A}}. \quad (7)$$

Note for part (b): In two dimensions, “pressure” is “force per unit length that is required to confine the particles to an area \mathcal{A} ”. It is given by a formula analogous to the three-dimensional formula, namely

$$P = T \left(\frac{\partial S}{\partial \mathcal{A}} \right)_{N, E}. \quad (8)$$

Problem 4:

For a system of N one-dimensional massless particles in a “one-dimensional box” of length L , calculate the entropy $S(N, E, L)$ of the system.

Start by thinking about the energy of a single *massless* particle.

To evaluate the required N -dimensional integral, you might consider a recursive approach. Alternatively, you might look explicitly at $N = 1, 2, \dots$ to deduce a pattern.