PH 202 : STATISTICAL MECHANICS

ASSIGNMENT 1

Due date - 27 January 2025

1. Using the facts: i) entropy (S) is a function of microstates (Ω), i.e., $S = f(\Omega)$. ii) entropy is additive, $S = S_1 + S_2$, iii) microstates are multiplicative in nature, $\Omega = \Omega_1\Omega_2$.

   - Show that $f(\Omega) =$ "*constant*" $\times \ln\Omega$. Find out the dimension of the constant term.
   - Third law states that, $\lim_{T\to 0} S = 0$, It implies $\Omega = 1$, a unique microstate description. However, there are classical examples of both non-interacting (such as an ideal gas) and interacting (the frustrated spins in a triangular antiferromagnet) systems with a large number of (degenerate) ground states and a finite zero temperature entropy. Resolve this apparent puzzle.
   - Comment on the small T behaviour of specific heat (C). Plot for $\Delta = 0, \Delta \neq 0$. Explain. (Take $\Omega \simeq 1 + e^{-\Delta/k_BT} + correction$, $\Delta > 0$)

2. Study the statistical mechanics of an extreme relativistic gas confined in a cubical box of length L characterized by the single-particle energy states

$$\varepsilon(n_x, n_y, n_z) = \frac{hc}{2L}\left(n_x^2 + n_y^2 + n_z^2\right)^{1/2}, n_x, n_y, n_z = 1, 2, 3, ... \tag{1}$$

   Show that the ratio of C_P/C_V in this case is 4/3 instead of 5/3.

3. Variations of extensive coordinates of a thermodynamic system are related by

$$dE = TdS - PdV + \mu dN, \tag{2}$$

   where all the symbols have the usual meaning. Now, consider that extensive quantities are proportional to the size or number of particles. First, express this statement in a mathematical identity,

$$E(\lambda S, \lambda V, \lambda N) = RHS \tag{3}$$

   - What is RHS?
   - Then derive the following relation, which transfers the variations from the extrinsic to the intensive variables!

$$SdT - VdP + Nd\mu = 0 \tag{4}$$

   - **A simple application:** For a fixed amount of ideal gas going through an isothermal process, show that

$$\mu = \mu_0 - k_BT\ln\frac{V}{V_0} \tag{5}$$

     where, (P_0, V_0, μ_0) is some reference point. Did you notice that all quantities in 5 are intensive quantities, and N drops out?
   - Eq.2 is more fundamental than eq. 4, which is not valid in many astrophysical processes involving galaxies, black holes, etc. Why? More specifically, which assumptions taken above are not valid in those situations?
     Can you find out such an example where eq. 2 is valid but not eq. 4 ?

4. Two particles of mass m are attached to a massless rigid rod of length l and free to rotate in three dimensions with the center of mass fixed. It has energy E and angular momentum M.

   - What is the dimension of phase space (D)?

- Compute the volume of phase space and the number of microstates in terms of angular momentum (M).
- How does the number of microstates vary with energy (E)? Compute entropy (S) and temperature (T).
- Identify the ensemble. Does it satisfy the liouville's theorem?
- Now treat the problem quantum mechanically. The eigenvalue equation for angular momentum is $M^2 f = j(j+1)f$. Compute the microstates for a given j. Does it match your expectations?

5. Using the following relation of entropy of an ideal gas

$$S = N \ln V + \frac{3}{2} N \left[1 + \ln T\right] \tag{6}$$

- Compute the total entropy change in mixing two ideal gases A (V_1, T_1, N_1) and B(V_2, T_2, N_2). The mixing is performed in an adiabatic container so that no heat is allowed to transfer between the system and the environment.
- Would the contribution arising from this cause depend on whether the two gases were different or identical? Explain.

Numerical Assignment

This is a numerical question where you are expected to write a program in order to simulate and understand the simple processes. you will be required to submit the code, results you obtained from the code along with any discussion/answer to particular question asked. Text/question in red is something which you have to do/answer and will be considered for grading. Text marked blue is something which you can do for yourself for fun.

This question is intended to shed some light on two postulates of statistical mechanics. After carefully following through these questions you will be able understand the following:

- Why is first postulate important and its consequences.
- How it leads to concept of equilibrium and how it relates to second law of thermodynamics.

One can look for more in book - Fundamentals of Statistical Mechanics and Thermal Physics by F. reif. (chapter 2 - Statistical description of system of particles)

6. Let us consider N_s number of sections. Each section "i" consists of M_i number of compartments. All these sections are placed next to each other. We have N_b number of boxes which will be randomly placed in any compartment with equal probability.

   form of M_i for computation :

$$M_i = |i - \frac{N_s}{2}| + 5 \tag{7}$$

   This will look something like "V" shape as function of i. Take N_s=50, N_b=10000 boxes , and at each time step , assign each box to a different compartment with equal probability.

   Plot the graph with number of boxes in each section on y axis and section number on x axis. after time steps N_t = 100,1000. How does the shape look like? (you will soon realize that there is no notion of time in this exercise).

7. Now we will quantify the fluctuations. Now take first 100 iterations of your previous program and store all the iterations. Calculate the mean value (n_i) of boxes in each section. Also calculate the variance/ standard deviation (σ_i). Now define the quantity F such that

$$F = \sum_i \sigma_i \tag{8}$$

Now vary the N_b = 100-10000 with step of 500 and plot F as function of N_b and $\sqrt{N_b}$.

8. Now define another quantity

$$F_2 = \sum_i \frac{\sigma_i}{n_i} \tag{9}$$

plot its variation with N_b and $\frac{1}{\sqrt{N_b}}$. What do you understand by this exercise?. Briefly describe how you think this could be related to basic postulates? Comment on what happens if N_b is low and third law of thermodynamics.

Discussion

When a system of objects/particles if given where it system can be in many possible configurations (micro-state) , Overall distribution of objects (macro-state) changes if system was not in equilibrium to begin with. We know if system starts from some random configuration, let's say where all the particles/objects in one state, with time due to interactions, they will move to other states randomly. One can ask some questions at this point?

- How system in some initial state achieves equilibrium?
- What is so statistical about it?
- Let's say system is in equilibrium, what do this tells us about micro-states, when we know that all micro-states are equally probable.

Answer to these question lies in statistical description of the problem. Long story short, For very large number of particles, probability of system to be in one macro-state as compared to other macro-state changes. As $N \rightarrow \infty$, only one macro-state prevails which does not change with time, **state which is defined as equilibrium.**

you can see this in simulation you just did. for very small number of particles, you will see lot of fluctuations and you might not be able to make up how distribution looks. The moment you increased N_b to very large values, suddenly underlying structure of compartments emerge very clearly. even in this case, probability of finding all the boxes in one compartment is finite and every micro-state carries equal probability, but as far as macro-state is concerned, system will be in such a state where number of possible micro-states for particular macro-state is maximum. you can actually calculate this and cross check whether this is true or not for above problem.

One can now ask how system evolves to find equilibrium. This is slightly non trivial question, as it really depends on how constituents of system interacts with each other. But one can do fun simulation **(which will not be graded).** In previous example, you picked a box and randomly placed to any other compartment at each time step. In order to add notion of time (in crude way). do as follows:

- pick a box and keep it at its previous location with probability p.
- move it to other location with probability (1-p)/N_c to other compartments.

This is crude way to put in time, but here you can then define starting point, such that all the boxes are placed in compartment 1. Then if you run this simulation, you will be able to see how system actually approaches equilibrium.