The Microcanonical Ensemble

1. Classical Harmonic Oscillators: Consider N harmonic oscillators with coordinates and momenta $\{q_i, p_i\}$, and subject to a Hamiltonian

$$\mathcal{H}(\{q_i, p_i\}) = \sum_{i=1}^{N} \left[\frac{p_i^2}{2m} + \frac{m\omega^2 q_i^2}{2}\right].$$

(a) Calculate the entropy S, as a function of the total energy E.

(Hint: By appropriate change of scale, the surface of constant energy can be deformed into a sphere. You may then ignore the difference between the surface area and volume for $N \gg 1$. A more elegant method is to implement this deformation through a canonical transformation.)

(b) Calculate the energy E, and heat capacity C, as functions of temperature T, and N.

(c) Find the joint probability density P(p,q) for a single oscillator. Hence calculate the mean kinetic energy, and mean potential energy for each oscillator.

2. *Quantum Harmonic Oscillators:* Consider N independent quantum oscillators subject to a Hamiltonian

$$\mathcal{H}\left(\{n_i\}\right) = \sum_{i=1}^{N} \hbar \omega \left(n_i + \frac{1}{2}\right),$$

where $n_i = 0, 1, 2, \dots$, is the quantum occupation number for the *i*th oscillator.

(a) Calculate the entropy S, as a function of the total energy E.

(Hint: $\Omega(E)$ can be regarded as the number of ways of rearranging $M = \sum_{i} n_i$ balls, and N-1 partitions along a line.)

(b) Calculate the energy E, and heat capacity C, as functions of temperature T, and N.

(c) Find the probability p(n) that a particular oscillator is in its n^{th} quantum level.

(d) Comment on the difference between heat capacities for classical and quantum oscillators.

3. Hard Sphere Gas: Consider a gas of N hard spheres in a box. A single sphere occupies volume ω , while its center of mass can explore a volume V (if the box is otherwise empty).

There are no other interactions between the spheres, except for the constraints of hard-core exclusion.

(a) Calculate the entropy S, as a function of the total energy E.

(Hint:
$$(V - a\omega)(V - (N - a)\omega) \approx (V - N\omega/2)^2$$
.)

(b) Calculate the equation of state of this gas.

(c) Show that the isothermal compressibility, $\kappa_T = -V^{-1} \left. \frac{\partial V}{\partial P} \right|_T$, is always positive.

4. (Optional) Interacting Rod-Molecules: A collection of N asymmetric molecules in two dimensions may be modeled as a gas of rods, each of length 2l and lying in a plane. A rod can move by translation of its center of mass and rotation about latter, as long as it does not encounter another rod. Without treating the hard-core interaction exactly, we can incorporate it approximately by assuming that the rotational motion of each rod is restricted (by the other rods) to an angle θ , which in turn introduces an excluded volume $\Omega(\theta)$ (associated with each rod). The value of θ is then calculated self consistently by maximizing the entropy at a given density n = N/V, where V is the total accessible area.



(a) Write down the entropy of such a collection of rods in terms of N, n, Ω , and $A(\theta)$, the entropy associated to the rotational freedom of a *single* rod. (You may ignore the momentum contributions throughout, and consider the large N limit.)

(b) Extremizing the entropy as a function of θ , relate the density to Ω , A, and their derivatives Ω' , A'; express your result in the form $n = f(\Omega, A, \Omega', A')$.

(c) Express the excluded volume Ω in terms of θ and sketch f as a function of $\theta \in [0, \pi]$, assuming $A \propto \theta$.

(d) Describe the equilibrium state at high densities. Can you identify a phase transition as the density is decreased? Draw the corresponding critical density $n_{\rm c}$ on your sketch. What is the critical angle $\theta_{\rm c}$ at the transition? You don't need to calculate $\theta_{\rm c}$ explicitly, but give an (implicit) relation defining it. What value does θ adopt at $n < n_{\rm c}$?

Suggested Reading: Huang, Chapter 6.