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.

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

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

where $n_i = 0, 1, 2, \cdots$, 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.

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

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

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

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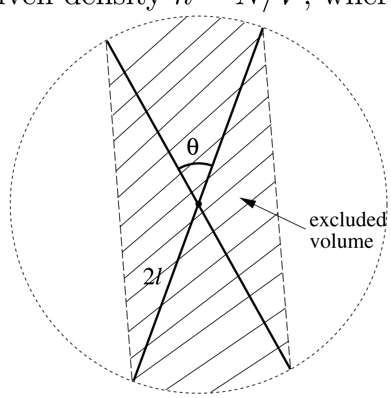
4. (Optional) *Interacting Rod-Molecules:* A collection of N asymmetric molecules in two dimensions may be modeled as a gas of rods, each of length $2l$ and lying in a plane. A rod can move by translation of its center of mass and rotation about latter, as long as it does not encounter another rod. Without 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_c on your sketch. What is the critical angle θ_c at the transition? You don't need to calculate θ_c explicitely, but give an (implicit) relation defining it. What value does θ adopt at $n < n_c$?

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Suggested Reading: Huang, Chapter 6.