Problem Set 2 - Microcanonical ensembles

(Dated: PHYS403, Spring 2024)

I. Entropic "Forces"

Consider a simple toy model for a polymer made up of $N \gg 1$ segments that can each have two configurations: either long (l) or short (s) as shown in the figure, with corresponding segment lengths ℓ_l, ℓ_s respectively, with $\ell_l > \ell_s$.

Suppose we hang a mass M from the end of this polymer (ignore the mass of the polymer segments). Suppose this mass is heavy enough that we can neglect it's thermal motion, so that only its gravitational potential contributes to the energy. Also, neglect the kinetic energy of the polymer: let's just focus on its configurational entropy.

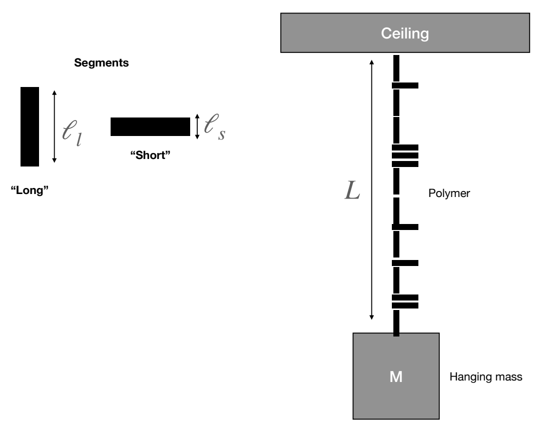

FIG. 1. (left) Polymer consisting of segments with two arrangements, (right) schematic of mass M hanging from polymer.

1. Express the length, L, of the polymer in terms of the number of long segments (N_l) and the number of short segments (N_s).

2. Write an expression for the gravitational potential energy, E, of the mass as a function of the polymer length, L (denote the acceleration due to gravity as g).

3. What is the number of micro-states, $\Omega(E)$ of the polymer with energy E?
(Hint: relate this to the two-level system, TLS, problem from class, use Stirling's approximation to extract only the leading large-N dependence, like we did for TLS's).

4. How does the length, $L(T)$, of the polymer depend on the temperature, T? Sketch a plot of $L(T)$ as a function of T labeling the position of any notable features in terms of the parameters of the problem ($\ell_{l,s}, M, g$).
Explain (physically) whether heating up the polymer cause it to expand, shrink, or stay the same length, and why.

II. Hard-sphere gas

In the ideal gas model, we neglect interactions between the particles. Here, you will explore a simple model of a gas of N particles with short-range repulsive interactions in a box of volume V. Suppose that the repulsive interactions are effectively infinitely strong but only act if the particles are closer than a fixed distance, i.e. that you can model each gas particle as a "hard sphere" of volume a. In this problem, you will analyze this model in the microcanonical ensemble at fixed total energy E.

As with the ideal gas, the the number of microstates with total energy E can be written as a product of contributions from the integral over particle positions: $\Omega_r(N, V, a)$ (which only depends on V, a, N, not E) and from the integral over particle momenta: $\Omega_p(E)$ (which only depends on the total energy not, V, a):

$$\Omega(E) = \Omega_r(N, V, a) \cdot \Omega_p(E)$$

. Note $\Omega_p(E) \sim (2mE)^{3N/2}$ is not effected by the "hard sphere" interactions, and is the same as for the ideal gas.

The integral over positions changes, however. For example, if there is one particle, its position can be anywhere inside the box, so it can explore volume V. However, the second particle can only explore volume $V - a$ because it is "blocked" from sharing the same volume as the first particle. A third particle could only explore volume $V - 2a$, et cetera. Multiplying these together we get:

$$\Omega_r(V, a) \approx \prod_{j=0}^{N-1} (V - ja)$$

.

1. Assume for the rest of this problem that the density of the gas is low: $Na \ll V$, i.e. the volume excluded by the N particles is much less than the total volume. In this case, you can approximate each term in the product as $(V - ja) = V(1 - ja/V) \approx Ve^{-ja/V}$. Using this approximation, compute $\Omega_r(N, V, a)$.

2. Compute the entropy, S, temperature, T as a function of energy, E, and volume V (the results will also depend on $N, a, ...$).

3. Compute the heat capacity, $C = \frac{dE}{dT}$ and pressure of the hard-sphere gas. as functions of T (i.e. not as functions of E, use your previous results to replace any E by the equivalent temperature $T(E)$). Comment on how the results differ from the ideal gas: can you give a qualitative explanation for these differences?.