Homework 3: Ensemble Theory

BY YUEJIAN MO 11510511

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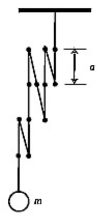
1. A chain made of N segments of length **a** hangs from the ceiling. A mass **m** is attached to other end under gravity. Each segment can be in either of two states, up and down, as illustrated.



   a. The ceiling is chosen as the reference point of the poetical energy, if the mass is L away from the ceiling, what is the entropy of this system?

   Assume that a link can be up or down independently. The partition function is the product of the partition functions of individual links. We think that the energy is $-mga$ when a segment is donw while energy is mga when segement is up. We ignore the fact that the energy of nth link depends on its height, and restriction that the link can not higher than ceiling. So the Hamiltonian is

$$\mathcal{H} = \sum_i^N (-mga)n_i, \text{where}\, n_i = \pm 1$$

   Then the partition function is

$$\begin{aligned} Z = \sum_{n_i=\pm 1, i=1,2\ldots,N} e^{-\beta H} &= \sum_{n_i=\pm 1, i=1,2\ldots,N} e^{-\beta \sum_i^N (-mga)n_i} \\ &= \sum_{n_i=\pm 1, i=1,2\ldots,N} e^{-\beta mga(n_1+n_2+\ldots+n_N)} \\ &= \left(e^{-\beta mga} + e^{\beta mga}\right)^N \end{aligned}$$

   We obatain free energy and entropy from partition function

$$\begin{aligned} F(T,N) &= -k_B T \,\mathrm{In}\, Z \\ &= -N k_B T \,\mathrm{In}(e^{-\beta mga} + e^{\beta mga}) \\ S &= -\frac{\partial F}{\partial T} = N k_B \mathrm{In}(e^{-\beta mga} + e^{\beta mga}) \\ &= N k_B \mathrm{In}(2\cosh \beta mga) \end{aligned}$$

b. If the temperature of the system is T, what is the length of L as a function of T?

$$
\begin{aligned}
E &= -\frac{\partial \mathrm{In}\, Z}{\partial \beta} = -N\frac{\partial \mathrm{In}(e^{-\beta mga} + e^{\beta mga})}{\partial \beta} \\
&= -N\frac{mga(-e^{-\beta mga} + e^{\beta mga})}{e^{-\beta mga} + e^{\beta mga}} \\
&= -mgaN\tanh(\mathrm{mg}\, a)
\end{aligned}
$$

$$
F = E - TS
$$

$$
\Longrightarrow
$$

$$
\begin{aligned}
T &= \frac{E-F}{S} = \frac{-mgaN\tanh(\mathrm{mg}\, a) + Nk_BT\,\mathrm{In}(e^{-\beta mga} + e^{\beta mga})}{Nk_B\mathrm{In}(2\mathrm{cosh}\beta mga)} \\
&=
\end{aligned}
$$

c. What is the free energy of the system at T?

$$
\begin{aligned}
F(T,N) &= -k_BT\,\mathrm{In}\, Z \\
&= -Nk_BT\,\mathrm{In}(e^{-\beta mga} + e^{\beta mga})
\end{aligned}
$$

2. *Relativistic particles: N indistinguishable* relativistic particles move in *one dimension* subject to a Hamiltonian

$$
\mathcal{H}(\{p_i, q_i\}) = \sum_{i=1}^{N} [c|p_i| + U(q_i)],
$$

with $U(q_i) = 0$ for $0 \leqslant q_i \leqslant L$, and $U(q_i) = \infty$ otherwise. Consider a *microcanonical* ensemble of total energy E.

a. Compute the contribution of the coordinates q_i to the available volume in phase space $\Omega(E, L, N)$.

Each of N coordinates explore a length L, for an overall contribution $L^N / N!$. Division by $N!$ ensure no over-counting of phase space for indistinguished particles.

b. Compute the contribution of the momenta p_i to $\Omega(E,\ L,\ N)$.(*Hint.* The volume of the hyperyramid defined by $\sum_{i=1}^{d} x_i \leqslant R$, and $x_i \geqslant 0$, in d dimensions is $R^d / d!$.)

The N momenta satify the constraint $\sum_{i=1}^{N} |p_i| = \frac{E}{c}$. For a particular choice of the signs of $\{p_i\}$, this constrain describes the surface of a hyper pramid in N dimensions. If we ignore the difference between the surface area and volume in the large N limit, we can calculate the volume in momentum space from the experssion given in the hits as

$$
\Omega_p = 2^N \cdot \frac{1}{N!} \cdot \left(\frac{E}{c}\right)^N.
$$

The factor of 2^N takes into account the two possible signs for each p_i. The surface area of pyramid is given by $\sqrt{d}R^{d-1}/(d-1)!$; the additional factor of $\sqrt{d}$ with respect to $d\,\text{volume}/dR$ is the ratio of the normal to the base to the side of the pyramid. Thus, the volume of a shell of energy uncertainty Δ_E, is

$$\Omega_p' = 2^N \cdot \frac{\sqrt{N}}{(N-1)!} \cdot \left(\frac{E}{c}\right)^{N-1} \cdot \frac{\Delta_E}{c}$$

We can use the two experssion interchangeably, as their difference is subleading in N

c. Compute the entropy $S(E,L,N)$.

Taking into account quantum modifications due to indistinguishability, and phase space measure, we have

$$\Omega(E,L,N) = \frac{1}{h^N} \cdot \frac{L^N}{N!} \cdot 2^N \cdot \frac{\sqrt{N}}{(N-1)!} \cdot \left(\frac{E}{c}\right)^{N-1} \cdot \frac{\Delta_E}{c}$$

Ignoring subleading terms in the large N limit, the entropy is given by

$$S(E,L,N) = Nk_B \text{In}\left(\frac{2e^2}{hc} \cdot \frac{L}{N} \cdot \frac{E}{N}\right)$$

d. Calculate the one-dimensional pressure P

From $dE = T\,\text{dS} - PdV + \mu dN$, the pressure is given by

$$P = T\frac{\partial S}{\partial L}|_{E,N} = \frac{Nk_BT}{L}$$

e. Obtain the heat capacities C_L and C_P.

Temperature and energy are related by

$$\frac{1}{T} = \frac{\partial S}{\partial E}|_{L,N} = \frac{Nk_B}{E}, \Longrightarrow E = Nk_BT, \Longrightarrow C_L = \frac{\partial E}{\partial T}|_{L,N} = Nk_B$$

Including the work done against external pressure, and using the equation of state,

$$C_P = \frac{\partial E}{\partial T}|_{P,N} + P\frac{\partial L}{\partial T}|_{P,N} = 2Nk_B$$

f. What is the probablity $p(p_1)$ of finding a particle with momentum p_1

Having fixed p_1 for the first particle, the remaining $N-1$ particles are left to share an energy of $(E - c|p_1)$. Since we are not interested in the coordinates, we can get the probability from the ratio of phase space for the momenta, that is

$$
\begin{aligned}
p(p_1) \; &= \frac{\Omega_p(E - c|p_1|, N-1)}{\Omega_p(E, N)} \\
&= \left[\frac{2^{N-1}}{(N-1)!} \cdot \left(\frac{E - c|p_1|}{c} \right)^{N-1} \right] \times \left[\frac{N!}{2^N} \cdot \left(\frac{c}{E} \right)^N \right] \\
&\approx \frac{cN}{2E} \cdot \left(1 - \frac{c|p_1|}{E} \right)^N \approx \frac{cN}{2E} \cdot \exp\left(- \frac{c|p_1|}{E} \right)
\end{aligned}
$$

Substituting $E = Nk_BT$, we obtain the (properly normalized) Boltzmann weight

$$
p(p_1) = \frac{c}{2k_BT} \cdot \exp\left(- \frac{c|p_1|}{k_BT} \right)
$$

(refer from Mehran Karder book)