Subsystem of a Closed System

($\sim$ Canonical Ensemble)

As just discussed microcanonical ensemble describes a closed (i.e. an isolated) system. It is interesting to consider subsystem of such a closed system. Recall our discussion of 2^{nd} law above where we argued that the entropy associated with the density matrix of a subsystem typically increases with time. A natural question is: what is the probability distribution for the subsystem after the entropy has become maximal and the subsytem has reached a steady state?

As a specific example, consider free, non-relativistic gas we studied earlier. Let us ask: if a subsystem consists of a single particle out of N particles, what is the p.d.f. of its momentum?

$$\text{Probability } P(\vec{P}_1) = \underbrace{\int d^d q_1 \prod_{i=2}^{N} d^d q_i \, d^d p_i}_{\text{Trace over everything except } \vec{P}_1} \underbrace{P(\{p\},\{q\})}_{\text{p.d.f. of all particles}}$$

$$= \frac{\displaystyle\int_{\substack{q_i \in \text{box} \\ \sum_i \frac{p_i^2}{2m} = E}} d^d q_1 \prod_{i=2}^{N} \int d^d q_i \, d^d p_i}{\displaystyle\int_{\substack{q_i \in \text{box},\ \sum_i \frac{p_i^2}{2m} = E}} \prod_{i=1}^{N} d^d p_i \, d^d q_i}$$

Note that one can do trace over $\vec{q}_1$ without tracing over $\vec{p}_1$ only classically since quantum mechanically $[q, p] = i$. In QM, one can only do partial trace over particle # 1's whole Hilbert space

$$= \frac{V \, \Omega\left(E - \frac{p_1^2}{2m}, V, N-1\right)}{\Omega(E, V, N)}$$

Recall from previous calculation, $(L^d = V)$

$$\Omega = \frac{1}{N!} \frac{L^{dN}}{\lambda^{dN}}.$$

where $\lambda = \frac{h}{\sqrt{2m(E/N)}}$

$$\Rightarrow P(\vec{p}_1) = \frac{N}{V} \frac{\left[\sqrt{\frac{2m\left[E - \frac{p_1^2}{2m}\right]}{N-1}}\right]^{d(N-1)}}{\left[\sqrt{\frac{2mE}{N}}\right]^{dN}}$$

$(N \gg 1)$

$$\propto \left[1 - \frac{p_1^2}{2mE}\right]^{\frac{dN}{2}}$$ upto normalization for $N \gg 1$

$\left[\underset{N\to\infty}{\mathrm{Lt}} \left(1+\frac{x}{N}\right)^N = e^x\right]$

$$= a\, e^{-\frac{dN}{2}\frac{p_1^2}{2mE}}$$ where a is the normalization

Using the condition $\int d^d\vec{p}_1 P(\vec{p}_1) = 1$, one can fix the normalization 'a'. For example, when $d=3$,

$$P(\vec{p}_1) = \left[\frac{3N}{4\pi m E}\right]^{3/2} e^{-\frac{3N}{2}\frac{p_1^2}{2mE}}$$

This is the Maxwell-Boltzmann's distribution,

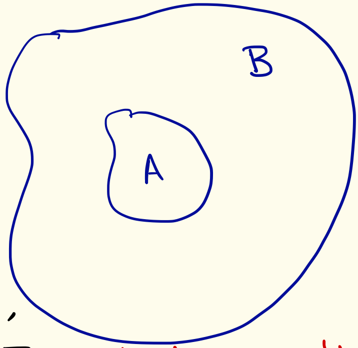
i.e. $P(\vec{p}_1) \propto e^{-\frac{p_1^2}{2mT}}$ with temperature

$$T = \frac{2E}{3N}$$

Indeed using $\beta = \frac{1}{T} = \frac{\partial S}{\partial E}$, one finds $T = \frac{2E}{3N}$ via expression for S derived earlier.

The main message of this calculation is that a subsystem of a closed system looks as if it is coupled to a heat bath at $(\text{temperature})^{-1} = \frac{\partial S}{\partial E}$. Let's derive this more generally.

Canonical Ensemble (Classical)



Consider a subsystem A of a total closed system $A \cup B$. We ask, if the total system is described an energy-entroy curre $S(E)$, and is at a given energy E, What is the probability of finding a specific configuration 'C_A' in region A that happens to have an energy $E_A(C_A)$? Assuming ergodicity, all configurations in $A \cup B$ with energy E are equally likely $\Rightarrow$ probability of finding configuration C_A in A $\propto$

$$\frac{\text{No. of configurations where the configuration in region } A = C_A \text{ and the configuration in region B arbitrary}}{\text{Total no. of configurations in } A \cup B}$$

$$= \frac{\Omega_B(E - E_A(C_A))}{\Omega(E)} = \frac{e^{S_B(E - E_A(C_A))}}{e^{S(E)}}$$

Assuming volume of region A $V_A \ll V_{A \cup B}$

$\Rightarrow$ $E_A(C_A) \ll E$. This allows one to taylor expand the numerator in above ratio:

$$P(C_A) \propto \frac{e^{\left[S_B(E) - \frac{\partial S_B}{\partial E}\Big|_{E_B=E} E_A(C_A)\right]}}{e^{S(E)}}$$

$$\propto e^{-\beta E_A(C_A)}$$

Thus, the normalized probability is given by

$$P(C_A) = \frac{e^{-\beta E_A(C_A)}}{\sum_{C_A} e^{-\beta E_A(C_A)}} \stackrel{?}{=} \frac{1}{e^{S_A(E_A)}}$$

where the sum in the denominator is over all configurations in region A – there is no restriction on the energy now, it can fluctuate a bit (we will quantify that below). What is fixed now is the temperature, which is β^{-1}.

From now on, we will drop the subscript A in C_A and E_A because we will focus solely on observables in region A.

We will rewrite the above equation as. :

$$P(C) = \frac{e^{-\beta H(C)}}{\sum_{C} e^{-\beta H(C)}}$$

Where H is the classical Hamiltonian and 'C' is a specific configuration.

The expectation value of any observable O is given by :

$$\langle O \rangle = \sum_{C} P(C)\, O(C)$$

$$= \frac{\sum_{C} O(C)\, e^{-\beta H(C)}}{\sum_{C} e^{-\beta H(C)}}$$

The denominator, $\sum_{C} e^{-\beta H(C)}$, is called 'Partition Function' and is a useful quantity for calculating any expectation value, as we will soon see.