Entropy Revisited:

- Previously we considered each microstate of the full system to be equally likely. Thus

$$P_m = C$$

probability to be in microstate m is constant

Then $\sum_m P_m = 1$ or $C \sum_m 1 = 1$ this litterally counts the states

or

$$C\,\Omega(E) = 1 \quad \text{and} \quad \boxed{P_m = \frac{1}{\Omega(E)}}$$

Thus

$$S_{tot} = k \ln \Omega = -k \ln P_m$$

- Now we have a subsystem with probabilies $P_m \propto e^{-\mathcal{E}_m/kT}$. We would like to find the [redacted] entropy for the subsystems, with this probality distribution (see slide)

The generalzation is (as we show below)

$$\boxed{S = -\langle k \ln P_m \rangle = -k \sum_m P_m \ln P_m}$$

Let's work it out!

We will use this to find the entropy from one subsystem.

Probability and entropy for one subsystem

1	0	1	0	2	1	0	0	2	1	3	1	1	1	0	0	0	0	1	0
1	2	2	2	0	0	0	0	0	1	1	0	0	3	5	1	0	0	0	0
0	0	1	1	0	2	0	0	6	1	1	0	1	1	1	0	2	0	0	0
0	3	3	0	0	2	0	0	3	0	1	3	0	2	0	0	0	3	0	0
2	0	0	1	0	6	0	4	1	0	0	0	2	1	0	0	1	1	1	0
1	0	6	0	4	0	1	2	1	0	0	0	1	0	0	0	0	3	4	1
0	0	0	1	2	4	0	0	1	0	0	2	0	1	2	1	1	2	0	6
1	3	0	0	2	0	1	0	1	0	0	3	0	4	0	2	1	0	6	1
1	1	1	0	0	0	0	1	0	3	1	2	0	0	0	0	1	0	0	0
0	0	0	0	0	2	0	3	1	0	0	0	0	0	3	0	0	2	2	1
9	1	0	1	1	0	2	1	0	1	0	0	0	3	7	3	0	2	3	0
2	2	0	0	0	0	0	1	0	1	7	1	3	1	0	1	3	0	1	0
0	5	3	0	1	2	4	8	1	0	4	0	3	0	1	0	0	0	4	0
0	0	0	0	1	0	0	0	0	1	0	1	0	0	2	3	0	2	0	0
0	1	1	0	0	2	0	4	0	1	0	4	0	1	1	1	1	8	5	1
0	0	0	0	1	0	0	0	2	0	1	0	1	1	2	0	0	1	1	1
3	0	0	0	4	0	0	1	0	1	2	0	0	1	2	0	2	0	1	0
0	0	1	2	1	0	0	0	0	0	1	0	0	0	2	0	1	1	0	0
1	0	1	0	0	0	1	0	3	1	0	0	0	0	0	2	9	0	0	5
0	0	1	2	3	0	1	2	0	2	4	0	0	0	1	2	0	0	0	1

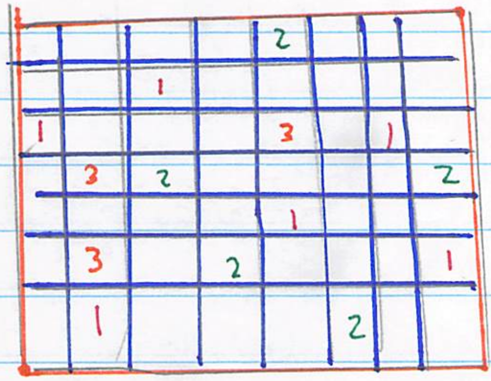
Pick a subsystem (site):
The remaining sites are the reservoir

The probability for a site
to have n quanta to be:

$$P(\epsilon_n) \propto e^{-\beta\epsilon_n} = e^{-n\,\beta\hbar\omega_0}$$

We will determine the entropy of the subsystem (one site) from this probability distribution. To find the total entropy, just multiply by the number of sites: $S_{\mathrm{tot}} = NS$

Consider a large number of subsystems   see slide



N subsystems: (blue boxes)

N_1 in state 1:

N_2 in state 2, etc

for example, probability to be in state 1 $\longrightarrow P_1 = \frac{N_1}{N} \propto e^{-\varepsilon_1/kT}$

- $S_{TOT} = k \ln (\#\text{ configurations with } N_1, N_2, \ldots \text{ fixed})$

$$= k \ln \frac{N!}{N_1!\, N_2! \cdots N_m!}$$

$$\simeq k \left(N \ln N - N - \sum_m (N_m \ln N_m - N_m) \right)$$

- So using $\sum_m N_m = N$ we have

$$S_{TOT} = k \sum_m N_m \ln N - N_m \ln N_m$$

Using $\ln N - \ln N_m = -\ln N_m/N = -\ln P_m$ we have

$$S_{TOT} = -k \sum_m N_m \ln P_m$$

- Finally the [redacted] entropy for one subsystem is

$$S = \frac{S_{TOT}}{N} = -k \sum_m \frac{N_m}{N} \ln P_m = -k \sum_m P_m \ln P_m$$

Entropy of subsystem

1	0	1	0	2	1	0	0	2	1	3	1	1	1	0	0	0	0	1	0
1	2	2	2	0	0	0	0	0	1	1	0	0	3	5	1	0	0	0	0
0	0	1	1	0	2	0	0	6	1	1	0	1	1	1	0	2	0	0	0
0	3	3	0	0	2	0	0	3	0	1	3	0	2	0	0	0	3	0	0
2	0	0	1	0	6	0	4	1	0	0	0	2	1	0	0	1	1	1	0
1	0	6	0	4	0	1	2	1	0	0	0	1	0	0	0	0	3	4	1
0	0	0	1	2	4	0	0	1	0	0	2	0	1	2	1	1	2	0	6
1	3	0	0	2	0	1	0	1	0	0	3	0	4	0	2	1	0	6	1
1	1	1	0	0	0	0	1	0	3	1	2	0	0	0	0	1	0	0	0
0	0	0	0	0	2	0	3	1	0	0	0	0	0	3	0	0	2	2	1
9	1	0	1	1	0	2	1	0	1	0	0	0	3	7	3	0	2	3	0
2	2	0	0	0	0	0	1	0	1	7	1	3	1	0	1	3	0	1	0
0	5	3	0	1	2	4	8	1	0	4	0	3	0	1	0	0	0	4	0
0	0	0	0	1	0	0	0	0	1	0	1	0	0	2	3	0	2	0	0
0	1	1	0	0	2	0	4	0	1	0	4	0	1	1	1	1	8	5	1
0	0	0	0	1	0	0	0	2	0	1	0	1	1	2	0	0	1	1	1
3	0	0	0	4	0	0	1	0	1	2	0	0	1	2	0	2	0	1	0
0	0	1	2	1	0	0	0	0	0	1	0	0	0	2	0	1	1	0	0
1	0	1	0	0	0	1	0	3	1	0	0	0	0	0	2	9	0	0	5
0	0	1	2	3	0	1	2	0	2	4	0	0	0	1	2	0	0	0	1

There are N sites in total

N_0 are in state 0,
N_1 are in state 1,
N_2 are in state 2,
N_3 are in state 3…

$P_r = N_r / N$ is the probability of a subsystem to be in the r-th state

So we have an important result:

$$\boxed{S = -k \sum_m P_m \log P_m}$$

this expression for S is valid for any probality distribution, P_m

<u>Notes</u>

(1) If $P_m = \frac{1}{\Omega}$ is the microcanonical (or equally likely distribution)

Then

$$S = -k \sum_m \frac{1}{\Omega} \log \frac{1}{\Omega} = +k \log \Omega \underbrace{\sum_m \frac{1}{\Omega}}_{}$$

Sum over states divided by # of states

$$S = +k \log \Omega$$ ⟵ This is what we had before:

(2) If $P_m = \frac{1}{Z} e^{-\beta E_m}$, this is the canonical ensemble

Then

$$S = -k \sum_m \frac{1}{Z} e^{-\beta E_m} \log \left(\frac{1}{Z} e^{-\beta E_m} \right)$$

$$= -k \frac{1}{Z} \sum_m (-\beta E_m) e^{-\beta E_m} + k \log Z \overbrace{\frac{1}{Z} \sum_m e^{-\beta E_m}}^{1}$$

$$\boxed{S = k\beta \bar{E} + k \log Z}$$

So

$$\boxed{S = \frac{\bar{E}}{T} + k \log Z}$$

this is how the entropy can be computed from the partition function Z

$$\bar{E} = \frac{-1}{Z}\frac{\partial Z}{\partial \beta}$$

We also note that if I have two *independent* subsystems A and B, the entropy of the combined systems is the the entropy A plus the entropy of B

$$S_{AB} = S_A + S_B$$

. You will prove this in homework directly from the formula $S = -\sum_m P_m \ln P_m$.

- Finally lets calculate the entroply of the Einstein Model

with $E = 400\hbar\omega$

$N = 400$

$$\boxed{S_{\text{one site}} = \frac{\bar{E}}{T} + k \ln Z}$$

this is general.

$$\frac{S_{\text{one site}}}{k} = \frac{\bar{E}}{kT} + \ln Z$$

- Putting in $\bar{E} = \hbar\omega/(e^{\hbar\omega/kT} - 1)$ $\quad Z = \dfrac{1}{1 - e^{-\hbar\omega/kT}}$

we have

$$\boxed{\frac{S_{\text{one}}}{k} = \frac{\beta\hbar\omega_0}{e^{\beta\hbar\omega_0} - 1} - \ln(1 - e^{-\hbar\omega_0\beta})}$$

entropy of SHO at temperature T

Using $\hbar\omega_0/\ln 2 = k_B T$ and multiplying by $N = 400$

we have, $\beta\hbar\omega_0 = \ln 2$

$$\frac{S}{k} = N\frac{S_{\text{one site}}}{k} = N\, 2\ln 2 \simeq 554.$$

this is in agreement with the direct counting result we quoted earlier.