The Micro-canonical Algorithm

- The preceding discussion leads to the algorithm

- We have a system (E.g. N harmonic oscillators) with total energy E (e.g. $E = q\hbar\omega_0$), and want the temperature.

- We "just" need to count the number of ways $\Omega(E)$ for the system to share (or partition) the energy. This determines the entropy $S(E)$:

$$\boxed{S(E) = k_B \ln \Omega(E)}$$

Then

$$\boxed{\frac{\partial S(E)}{\partial E} = \frac{1}{T}}$$

This determines the relation between the temperature and energy $E(T)$.

Example of Microcanonical Algorithm

- You will do this in homework. So I will only sketch the steps here

- Take N harmonic oscillators with q units of energy $E = q\hbar\omega_0$, so the average number of vibrational quanta per oscillator is

$$\bar{n} = \frac{q}{N} = \frac{E}{N\hbar\omega_0}$$

we will consider $\bar{n} = 1$, $N = 400$

Then $\Omega(q) = \dfrac{(N+q-1)!}{q!\,(N-1)!}$ (Compute S)

$\Omega(q)$ is the number of states with q units of energy and N particles, which you will compute in homework

- Using the stirling approximation (homework!)

$$\Omega(q) = e^{N[(1+\bar{n})\ln(1+\bar{n}) - \bar{n}\ln\bar{n}]}$$

For $N = 400 = q$, $\bar{n} = 1$, $\Omega(q) = e^{555}$.

Then

- $S(E) = k\ln\Omega(E) = Nk_B\left[(1+\bar{n})\ln(1+\bar{n}) - \bar{n}\ln\bar{n}\right]$

- Then differentiating with respect to energy $\bar{n} = \dfrac{E}{N\hbar\omega_0}$

$$\frac{1}{T} = \frac{\partial S}{\partial E} = \frac{\partial S}{\partial \bar{n}} \frac{1}{N\hbar\omega_0}$$ (Find Temperature)

$$\boxed{\frac{1}{k_B T} = \frac{1}{\hbar\omega_0} \ln\left(\frac{1+\bar{n}}{\bar{n}}\right)}$$

- So, for $\bar{n} = 1$, $k_B T = \hbar\omega_0 / \ln 2 \Rightarrow \beta\hbar\omega_0 = \ln 2$

- We can also express $\bar{n}$ in terms of the temperature

$$\boxed{\bar{n} = \frac{1}{e^{\hbar\omega_0/kT} - 1}}$$ ← You will derive this this week using partition fcns!

Analysis of Thermal State

- We found the temperature of the system $k_B T = \hbar\omega_0 / \ln 2$ or $\beta\hbar\omega_0 = \ln 2$

- We can verify that this is correct numerically.

- Each site is an independent subsystem. The probability of a site having energy ε_n is

$$P(\varepsilon_n) \propto e^{-\varepsilon_n / k_B T}$$

Energy is flowing in and out of every site. The probability that a site "steals" energy ϵ_n from the bath is given by the Boltzmann factor (see slides).

- Since for a harmonic oscillator $\varepsilon_n = n\hbar\omega_0$ with $\Delta\varepsilon = \hbar\omega_0$, we expect

$$P(\varepsilon_n) \propto e^{-\beta\varepsilon_n} = e^{-n\beta\hbar\omega_0} = e^{-n\ln 2}$$

- This probability distribution is reflected in the histogram $N(n)$ which is the number of sites $N(n)$ with n vibrational quanta (see slide 2 and slide 3)

$$N(n) \propto e^{-n\ln 2}$$

- This is born out in our numerical experiment (see slide 3)

Each independent subsystem (one site in this case) has a probability distribution:

$$P_s = \frac{1}{Z} e^{-\epsilon_s/k_B T}$$

This is known as the **canonical ensemble**. The energy in each subsystem is variable, as each subsystem can "steal" energy from the others. Using the canonical ensemble we can calculate the mean properties of the subsystem and deduce the properties of the total system, i.e. the total system is just N copies of the subsystem.

The collection of subsystems (i.e. the 20x20 square of subsystems) is known as the **microcanonical ensemble**. The energy doesn't change in the total system. We can also calculate the properties of the total system by following the microcanonical approach, finding $S(E)$ and using $(\partial S/\partial E) = 1/T$. The two approaches are identical. In the next section we will derive the Boltzmann factor from the microcanonical ensemble.

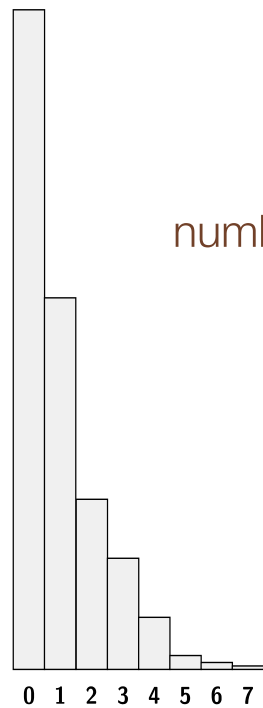
Analysis of the thermal state

(c)

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

Only one site with 7 quanta. Energy is constantly flowing in and out of each site

Histogram of energies in units of $\Delta\epsilon = \hbar\omega_0$



Histogram of N(n) , i.e. the number of sites, N(n), with n quanta of energy, $\epsilon_n \equiv n\hbar\omega_0$

A typical histogram of the number quanta is shown above: What is $N(n)$?

What is $N(n)$?

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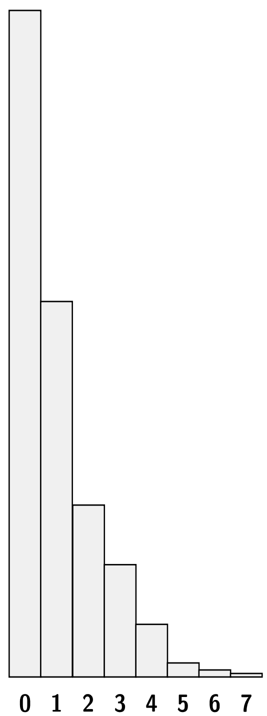
Histogram of energies
in units of $\Delta\epsilon = \hbar\omega_0$

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



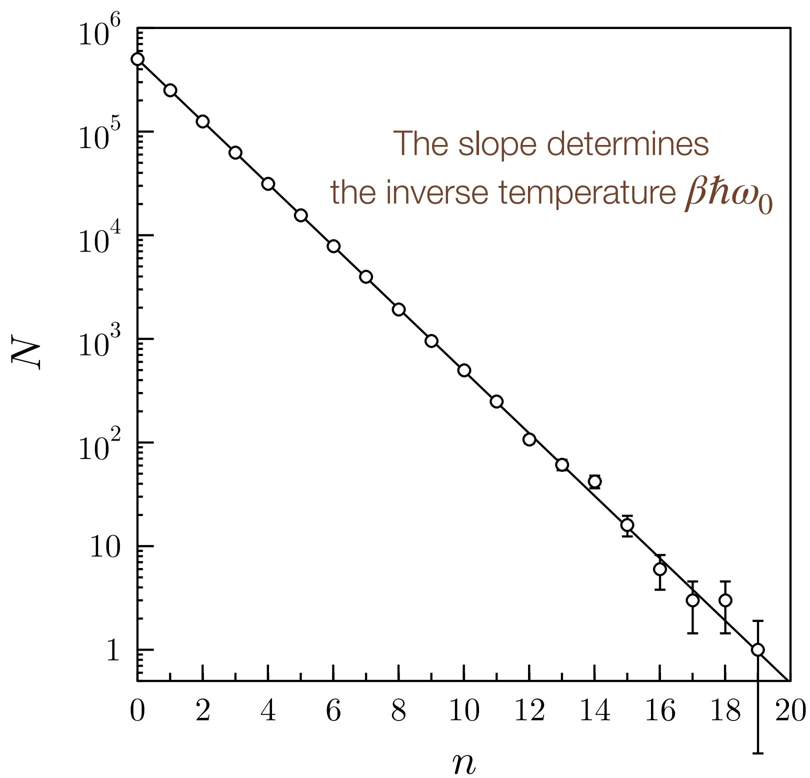
Pick a site:
The remaining sites are the reservoir

Expect the probability for a site to have n quanta to be:

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

The histogram N(n) is the number of sites with n quanta, and should be P_n up to normalization

Numerical verification: number of sites, $N(n)$, with n quanta on 1000x1000 grid



What you are seeing (on a log scale) is

$$N(n) = N_0\, e^{-Cn}$$

The log of $N(n)$ is the line you see

$$\ln N(n) = \ln N_0 - Cn$$

The slope should be $C = \beta\hbar\omega_0 = \ln 2$
set by the temperature. It is!

We found temperature in this problem $k_B T = \hbar\omega_0 / \ln 2$ by counting possibilities!