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

(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

The Canonical Ensemble

- 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

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

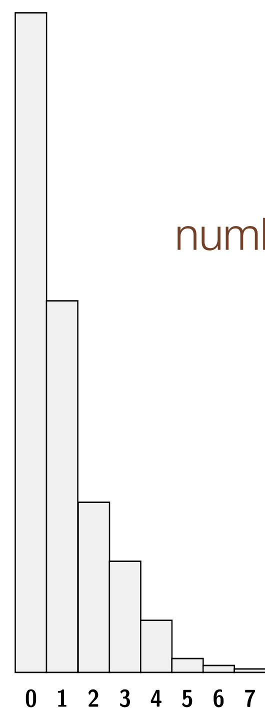
Energy is flowing in and out of every site. The probability that a site "steals" energy ϵ_n from the bath is given by the Boltzmann factor (see slides).

Analysis of the thermal state

(c)

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



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

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

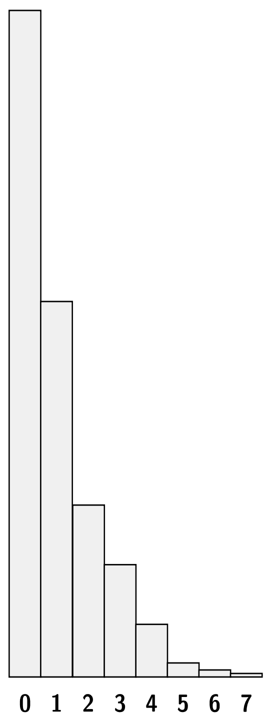
A typical histogram of the number quanta is shown above: What is $N(n)$?

What is $N(n)$?

(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

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



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

- 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

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

- This is born out in our numerical experiment

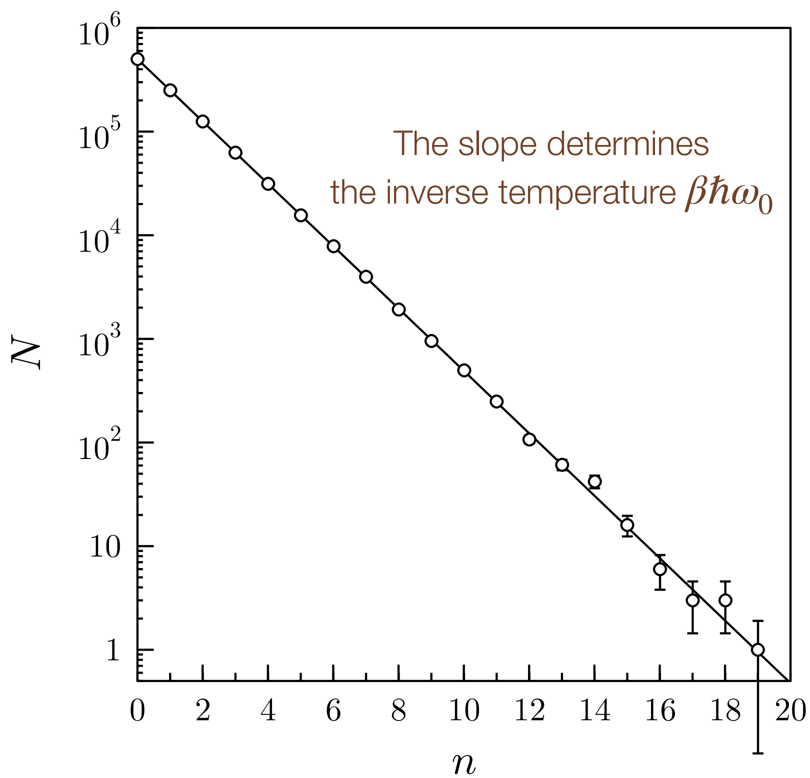
Each independent subsystem (one site in this case) has a probability distribution:

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

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.

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!

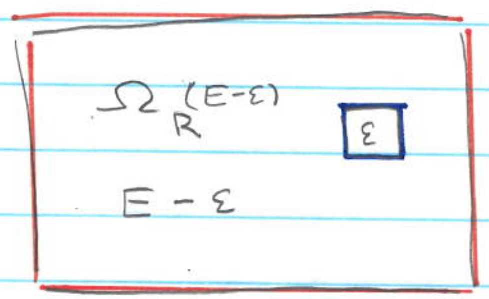
We found temperature in this problem $k_B T = \hbar\omega_0 / \ln 2$ by counting possibilities!

The Boltzmann Factor

- We can use notions of entropy to derive the Boltzmann Distribution

$$P_{\substack{\text{micro}\\ \text{state } s}} \propto e^{-\varepsilon_s/k_B T} \qquad \varepsilon_s \equiv \text{energy of microstate}$$

- Take a subsystem which is small compared to the total, interacting with a reservoir (the rest of the system):



$$\varepsilon \ll E$$

- The total system has energy E. Let us require that the subsystem be in <u>one</u> microstate with energy ε. The remaining system has energy $E-\varepsilon$. The probability of this configuation is

$$P(E-\varepsilon;\varepsilon) = \Omega_R(E-\varepsilon)\cdot 1 / \Omega(E) \leftarrow \text{constant}$$

(Before we had $\Omega_1(E_1)\,\Omega_2(E_2)$, now system 2 is in exactly one state). $\Omega_R(E-\varepsilon) = \Omega_1$ is the number of microstates associated with the reservoir, and $\Omega_2 = 1$. $\Omega(E)$ is constant since the energy is constant

- Take the log

$$\log P(\varepsilon) = \text{const} + \log \Omega_R(E-\varepsilon) + \cancel{\log 1}^{\,0}$$

- Now ε is small compared to the total system

$$\log \Omega_R(E-\varepsilon) = \log \Omega_R(E) - \left(\frac{\partial \log \Omega_R(E)}{\partial E}\right) \varepsilon$$

Or since

$$\frac{1}{k_B T} = \frac{\partial \log \Omega_R(E)}{\partial E}$$

- We have

$$\log P(\varepsilon) = \underbrace{\text{const} + \log \Omega_R(E)}_{\substack{\text{all const} \\ \text{indep of } \varepsilon}} - \frac{\varepsilon}{k_B T}$$

- So exponentiating

$$\boxed{P(\varepsilon) = (\text{Const})\, e^{-\varepsilon/k_B T}}$$

The constant can be found from normalization:

$$\sum_s P(\varepsilon_s) = 1 \quad \text{or} \quad \sum_s C e^{-\varepsilon_s/kT} = 1$$

$$C = \frac{1}{Z} \quad \text{with} \quad Z = \sum_s e^{-\varepsilon_s/kT}$$