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

(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

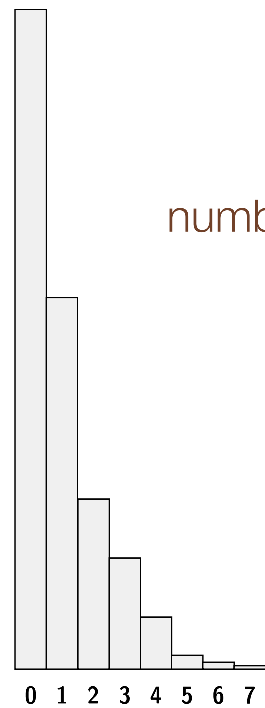
$$P(\varepsilon_n) \propto e^{-\varepsilon_n/k_B T}$$

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

Energy is flowing in and out of this site



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

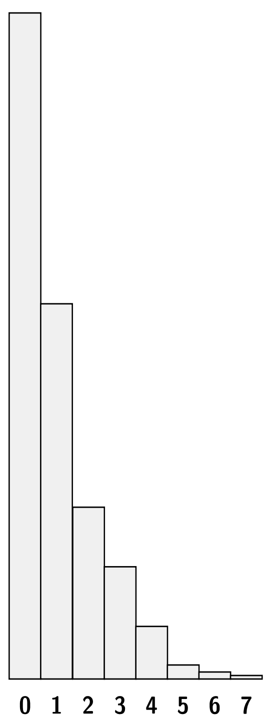
A typical histogram of the number quanta is shown above: What is $N(n)$?

What is $N(n)$?

(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

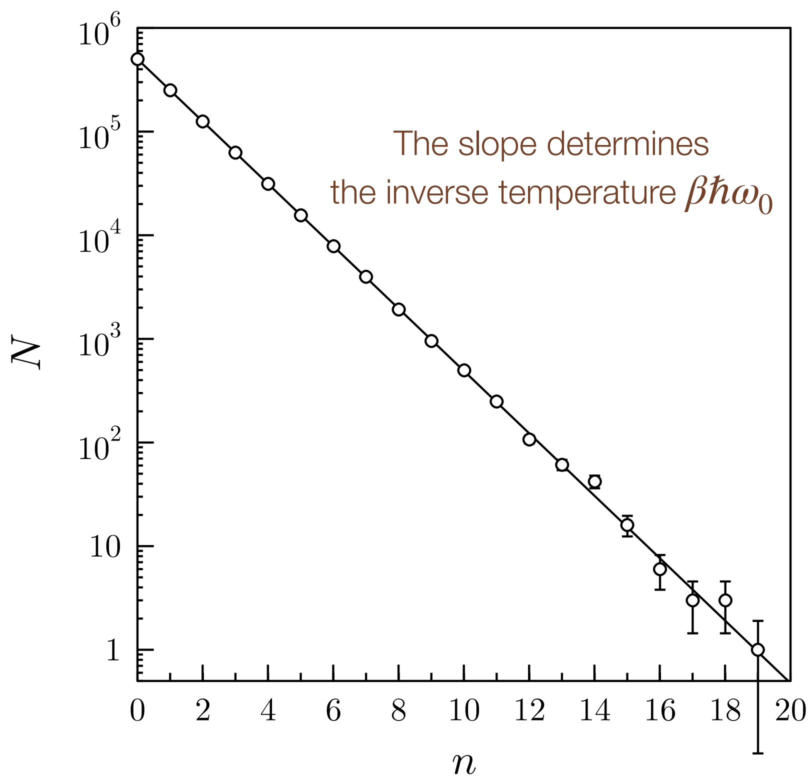
$$P(\varepsilon_n) \propto e^{-\beta\varepsilon_n} = e^{-n\beta\hbar\omega_0} = e^{-n\ln 2}$$

- 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

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!

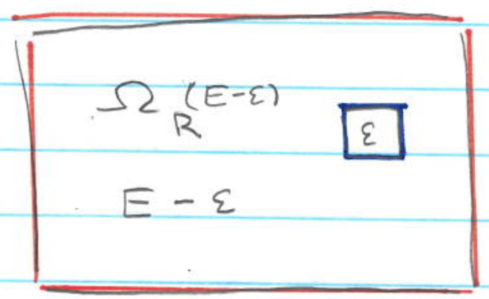
We found temperature in this problem $k_B T = \hbar\omega_0 / \ln 2$ by counting possibilities!

The Boltzmann Factor

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

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

- 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 one microstate with energy ε. The remaining system has energy $E-\varepsilon$. The probability of this configuation is

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

(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

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

- 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:

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

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