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

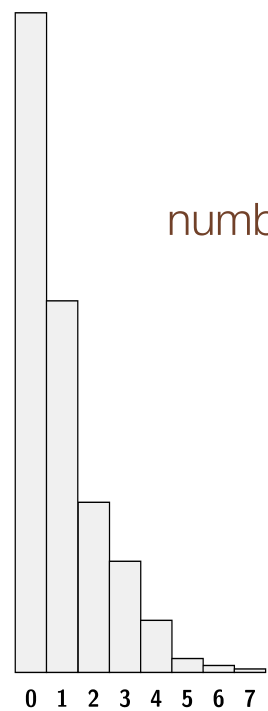
- Each site is an independent subsystem. The probability of a site having energy $\varepsilon_n$ is

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

# 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 |




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

Energy is flowing in and out of this site

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

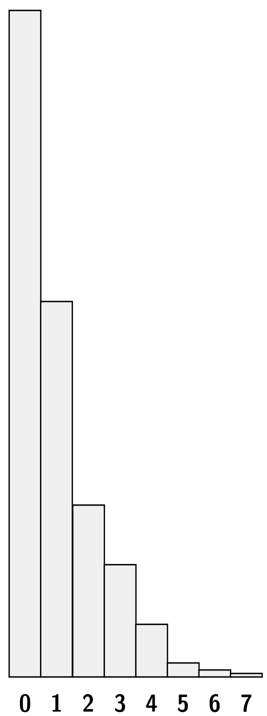
This is badly phrased: it should read the number of sites $N(n)$ with $n$ quanta of energy. The total number of sites is $N = \sum_{n=0}^{\infty} N(n) = 400$

# What is $N(n)$?

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

(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 |




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

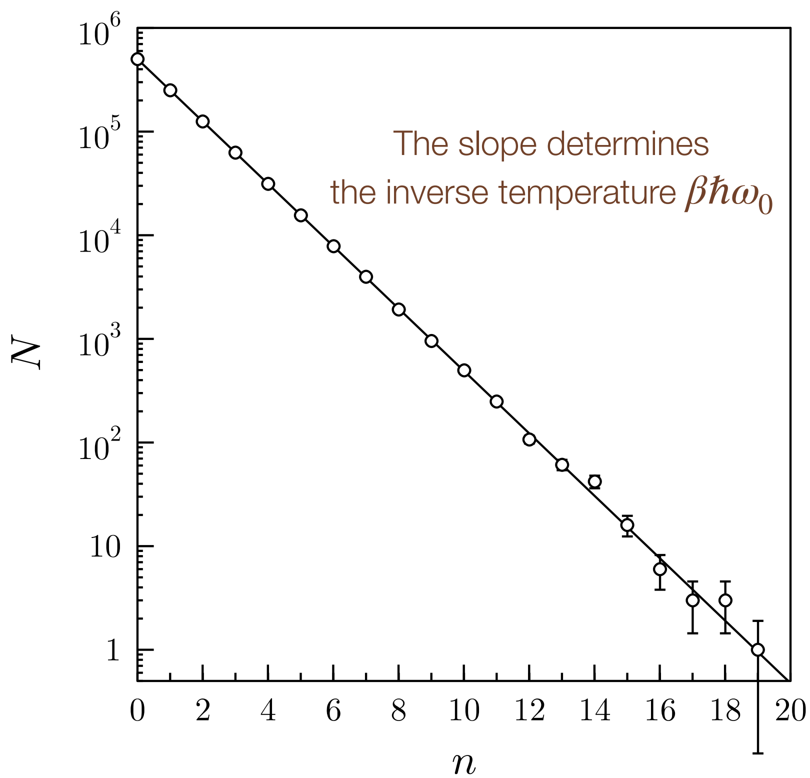
$$P(\varepsilon_n) \propto e^{-\beta\varepsilon_n} = e^{-n\beta\hbar\omega_0} = e^{-n\ln 2}$$

- 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!

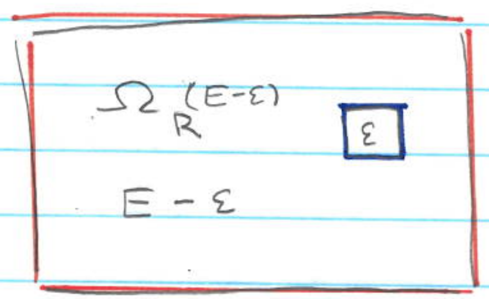
We found temperature in this problem $k_B T = \hbar\omega_0/\ln 2$ by counting possibilities!

# 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 <u>one</u> microstate with energy $\varepsilon$. 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 $\varepsilon$ 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:

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

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