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 $$\Omega(q) = \frac{(N+q-1)!}{q!\,(N-1)!}$$

(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

$$\boxed{\bar{n} = \frac{1}{e^{\hbar\omega_0/kT} - 1}}$$

$\longleftarrow$ 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

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