The Micro-canonical Algorithm

- The preceding discussion leads to the algorithm
- We have a system (E.g. N two state atoms) with total energy E (e.g. $E = N\Delta\bar{n}$) 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: Two State System

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

- Take N two level atoms with N_1 of them excited: $E = N_1\Delta = N\Delta\bar{n}$ with $\bar{n} = N_1/N$. The number in the ground state is $N_0 = N - N_1$ or $N_0 = N(1-\bar{n})$. $\bar{n}$ is the mean number of quanta of energy per site $\bar{n} < 1$. We found

$$\frac{S(E)}{k_B} = \ln\Omega = -N_0 \ln\frac{N_0}{N} - N_1 \ln\frac{N_1}{N}$$

$$= N\left[-(1-\bar{n})\ln(1-\bar{n}) - \bar{n}\ln\bar{n}\right]$$

- As the energy increases $E = N\Delta\bar{n}$ increases

- Then Differentiating we can express $\bar{n}$ in terms of T

$$\frac{1}{T} = \frac{\partial S}{\partial E} = \frac{1}{N\Delta}\frac{\partial}{\partial\bar{n}} Nk_B\left[-(1-\bar{n})\ln(1-\bar{n}) - \bar{n}\ln\bar{n}\right]$$

do it in HW!

$$\frac{1}{k_BT} = \frac{1}{\Delta}\ln\left(\frac{1-\bar{n}}{\bar{n}}\right)$$

- For $\bar{n} = 1/4$ we find $k_BT = \Delta/\ln 3$

- We can now solve for $\bar{n}$ (in Homework)

$$\bar{n} = \frac{1}{e^{\Delta/kT} + 1} = \frac{e^{-\Delta/kT}}{1 + e^{-\Delta/kT}}$$

- This a agrees with the canonical approach (i.e. Partition Fcn

$$\bar{n} = \frac{N_1}{N} = \text{probality to be in excited state}$$

Previously we found

$$\boxed{P_1 = \frac{e^{-\Delta/kT}}{Z_1} = \frac{e^{-\Delta/kT}}{1 + e^{-\Delta/kT}}}$$

Comments

- Clearly the canonical approach (the partition fcn way) is easier. But we didn't derive it. We relied on an intuitive notion of temperature, and postulated the probability $P_r \propto e^{-\varepsilon_r/kT}$ =

- The temperature is just a parameter in the in the Boltzmann Probality P_r which is adjusted to reproduce the energy of the system.

- In the next section we will derive the Boltzmann factor from the $S(E)$