Number of Configurations, Entropy, The Shannon Formula

- Consider N independent atoms, each of which can be in one of two states, 1 and 2 with probability P_1 and P_2, $P_1 + P_2 = 1$

1 2 2 2 1 2 2 1 2 1 2 2

- Suppose there N_1 atoms in state 1 and N_2 atoms in state 2. The number of configurations with this partition of N into N_1, N_2 is

$$\Omega = \frac{N!}{N_1!\,N_2!} \qquad N_1 + N_2 = N$$

- For large N, $N_1 = NP_1$ and $N_2 = NP_2$. Then lets find Ω for N large

$$\ln \Omega = \ln N! - \underline{\ln N_1! - \ln N_2!} \qquad N_1 + N_2 = N$$

$$= (N \ln N - \cancel{N}) - \left(\sum_{i=1}^{2} N_i \ln N_i - \cancel{N_i}\right)$$

write as $\sum_i N_i \ln N$ since $\sum N_i = N$

Then

$$\ln \Omega = \sum_i N_i (\ln N - \ln N_i)$$

So

$$\boxed{\ln \Omega = -\sum_i N_i \ln N_i/N}$$

Finally noting that $N_i/N = P_i$ for N large

$$\boxed{\ln \Omega = N\left(-\sum_i P_i \ln P_i\right)}$$

Comments:

- $\ln \Omega$ is known as the entropy of the ensemble of atoms, and will be called $S = NS_1$

Important

- ★ $\ln \Omega$ increases linearly in the number of sites by an amount $S_1 = -\sum_i P_i \ln P_i$ per site.

  This means Ω grows exponentially in the number of sites, increasing by a factor e^{S_1} for every site added.

  S_1 is the entropy per site, and $-\sum_i P_i \ln P_i$ is the Shannon formula for it

Examples

- Suppose $P_1 = 1$ and $P_2 = 0$

$$S_1 = -\sum P_i \ln P_i = -1 \ln 1 + 0 \ln 0 = 0$$

In this case

$$\ln \Omega = 0 \quad \text{or} \quad \Omega = 1, \quad \text{of course since}$$

the only configuration is $|\ |\ |\ |\ |\ |\ |$ all ones

- Suppose $P_1 = P_2 = \frac{1}{2}$

$$S_1 = -\sum_i P_i \ln P_i = -\frac{1}{2}\ln\frac{1}{2} - \frac{1}{2}\ln\frac{1}{2} = \ln 2$$

This also makes sense for each site added, the atom can be in one of two states @ equal weight So the number of configurations is, $\Omega = e^{N \ln 2} = 2^N$

A Generalizion

- These formulas generalize to more than two states. For 3 states for example, A, B, C:

$$\Omega = \frac{N!}{N_1! N_2! N_3!} \qquad \ln \Omega = -\sum_{i=1}^{3} N_i \ln N_i / N$$

And

$$\boxed{\ln \Omega = N \left(-\sum_{i=1}^{3} P_i \ln P_i \right)}$$

If $P_1 = P_2 = P_3 = 1/3$ (i.e. equal weights)

$$\ln \Omega = N \sum_{i=1}^{3} -\frac{1}{3} \ln \frac{1}{3} = N \ln 3$$

So $\ln \Omega$ grows linearly with N, while Ω grows as

$$\Omega = 3^N$$