The Microcanonical Ensemble

1 Defects in a crystal: microcanonical ensemble

In a perfect crystal, atoms occupy the sites of a periodic lattice (cubic, for example). Some atoms may leave their equilibrium position to occupy so-called interstitial sites (located, for example, between two atoms) but with an energy penalty of $+dE$.

A crystal contains 10^{24} atoms capable of occupying interstitial sites, and $dE = 0.1$ eV. We create a population of interstitial sites with a total energy of 4000 J. This system is isolated from the outside.

We observe the state of one of the atoms. What is the probability of observing it in its interstitial position?

For an isolated system in equilibrium, all accessible microstates are equally likely.
Firstly, we observe that $E = 4000J \implies \frac{4000J}{0.1eV} = 2.5 \times 10^{23}$ atoms occupy interstitial sites.
So, the probability that an atom occupies an interstitial site is $\frac{2.5\times10^{23}}{10^{24}} = \frac{1}{4}$.

2 Density fluctuations in an ideal gas

A 1 liter bottle contains one mole of gas, and it is well isolated from the outside. This gas is assumed to be ideal, which means that, if we neglect the force of gravity, the energy is independent of the positions of the gas molecules.

At a given instant, we look at a small volume of the bottle which is a cube of side 0.01 micron. What is the probability that there are no molecules in this volume?

Again, we have an isolated system in equilibrium, so all accessible microstates are equally likely.

Let X_i be a random variable denoting the position of particle i. We suppose the X_i are independent are identically distributed.

We know that X_i follows a **uniform distribution** over the bottle's volume because the energy is independent of the positions of the gas molecules.

By independence, the probability that there are no molecules in this volume is the product of the probabilities that each individual particle is not in the volume.

$$\left(1 - \left(\frac{0.01\mu m}{10^5\mu m}\right)^3\right)^{6.022\times10^{23}} \leq e^{-6.022\times10^{16}} \approx 10^{-260}$$

We used the inequality

$$(1-x)^n \leq e^{-nx}$$

which is true for $n \geq 1$ and $-1 \leq x \leq 1$.

3 Genetic information and the brain

The human DNA contains approximately 3 billion base pairs. The human brain contains approximately 10^{11} neurons, each being connected to approximately 410^3 synapses.

We assume, for simplification, that synapses can only be of two types, excitatory or inhibitory. Is there enough information in the DNA to encode the state of each synapse?

We shall compute the quantity of information in both channels of information using Shannon's entropy.

The human DNA is made out of pairs of bases A-T or C-G which we'll suppose are equally likely. We have

$$H_1 = \sum_{\text{pair}} \frac{1}{2} \log(2) = \frac{3 \cdot 10^9}{4} \log(2) \approx 2,26 \cdot 10^8$$

Now, suppose each one of the two types of synapses are equally likely, we have

$$H_2 = \sum_{synapse} \frac{1}{2} \log(2) = \frac{10^{11} \cdot 410^3}{2} \log(2) \approx 2,07 \cdot 10^{18}$$

Thus, we conclude that there is not enough information in the human DNA to encode the state of each synapse.