

Thermodynamics and Statistical Mechanics Lecture 2

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Statistical Physics

Statistical physics is a framework for translating from the microscopic model of a system to its macroscopic properties.

$$\langle X \rangle = \sum_i P_i X_i$$

What this says is that the expectation value of X of the system is equal to the weighted sum of the values of X summed over all micro-states.

Microcanonical Ensemble

The microcanonical ensemble represents a closed system with fixed energy. It is not always the easiest to calculate but is the simplest in principle. The probability of it can be represented by the following equation.

$$P_i = \frac{1}{N(E)}$$

Canonical Ensemble

The canonical ensemble describes a system in thermal contact with a bath. Temperature and particle numbers are fixed, but the bath and the system can share and exchange energy. The probability distribution for this ensemble is the Boltzmann distribution and is as follows.

$$P_i = \frac{1}{Z} e^{\frac{-E_i}{kT}}$$

Grand Canonical Ensemble

The grand canonical ensemble describes a system that can allow thermal and particle exchange between the system and the bath. Temperature and a "chemical potential" are fixed. The probability distribution of this system is the Gibbs distribution and is as follows.

$$P_i = \frac{1}{Z} e^{-\frac{E_i - \mu N_i}{kT}}$$

Ensemble Selection Although it might seem like we would choose the ensemble that matches our system the best, but with large samples all of these ensembles and their respective distributions lead to the same physical results. We choose the ensemble that is easiest to use with our system.

Thermodynamics

Thermodynamics is the science of macroscopic heat and energy transfer. Historically, it was developed from a few empirical rules before statistical mechanics became a thing. In such a closed system, E and N are fixed.

Microcanonical Ensemble Revisited

Let's look a little bit deeper into the microcanonical ensemble. $\Omega(E)$ will be the number of micro-states and is also known as the **Multiplicity Function**. If we wanted to know the probability of a certain micro-state n , it would be related to the reciprocal of the multiplicity function.

$$P_n = \frac{1}{\Omega(E)}$$

Example We have a system of N spin-1/2 particles.

$$E = \sum_{i=1}^N \epsilon_i = -B \sum_{i=1}^N s_i = -B \left(\frac{1}{2} (N_u - N_d) \right) = -BM = -NBm$$

$\frac{1}{2}(N_u - N_d)$ will be the total magnetization of the system and $m = \frac{M}{N}$ is the magnetization density, an intensive quantity.

$$\Omega(N_u) = \binom{N}{N_u} = \frac{N!}{N_u!(N - N_u)!}$$

Finding Ω will the come down to solving that equation which can be simplified using **Stirling's Approximation** which is as follows.

$$\ln(N!) = N \ln(N) - N + O(\ln(N))$$