Aufgabe 11.1 Most probable distribution method

In the lecture we derived the Maxwell-Boltzmann distribution from a kinetic point of view. We saw that f_{MB} does not depend on the particular form of the molecular interactions. Being interested only in the distribution of a gas at equilibrium, we suspect that its law of distribution can be derived without consideration of its kinematics. We perform here the derivation of f_{MB} from a statistical point of view.

We start with the idea of the Gibbs ensemble by considering a gas of N particles confined in a volume V. In chapter 10 we saw that any state of the system can be represented by a point $(p,q) = (p_1, p_2, ..., p_{3N}, q_1, ..., q_{3N})$ in its phase space Γ. The ensemble of points corresponding to the same macroscopical conditions is called the representative volume of the system. At equilibrium, we assume that the system can be found in all the states corresponding to the same macroscopic conditions with equal probability. In other words, the density function defined in (10.5) is a constant on the representative volume of the system. If we fix the energy of the system between E and $E+\Delta$ with $\Delta \ll E$, the representative volume is a compact ensemble of points bounded by the energy surfaces E and $E+\Delta$. This is the so called microcanonical ensemble (10.8).

We now proceed as follows: We define the one-particle phase space μ, in which each particle occupies one point (p,q) corresponding to its state. Thus the distribution of points in μ defines the state of the whole system. Let us divide μ into K boxes each of volume $\omega = \Delta^3 p \Delta^3 q$. The discrete distribution function f_i is given by the number of particles N_i inside the ith box:

$$f_i = \frac{N_i}{\omega} \quad .$$

Averaging over the microcanonical ensemble, we have the equilibrium distribution function

$$f_{0i} = \frac{\langle N_i \rangle}{\omega} \quad ,$$

which satisfies the following conditions:

$$\sum_i^K N_i = N \quad , \quad \sum_i^K N_i \frac{p_i^2}{2m} = E \quad . \tag{1}$$

It is clear that there exists an ensemble of points $(p,q) \in \Gamma_{E,V,N}$ which define the same distribution function f_i, e.g. exchanging two particles, one from the ith box and the other from the jth box, leaves N_i and N_j unchanged. The idea now is to find the distribution function which corresponds to the largest volume in $\Gamma_{E,V,N}$. This gives us the most probable distribution function of the system. We make the assumption that this is nothing but the equilibrium distribution function f_{0i}. Practically we are looking for the set $\{N_i\}_1^K$ which gives the largest volume $\Omega\{N_i\} \in \Gamma_{E,V,N}$ such that the conditions (1) are satisfied.

1. Show that $\Omega\{N_i\} \propto N!/N_1!N_2!...N_K!$.

2. In the following we set

$$\Omega\{N_i\} \propto \frac{N!}{N_1!N_2!...N_K!} g_1^{N_1} g_2^{N_2} ... g_K^{N_K},$$

   where $g_1, g_2, ..., g_K$ are numbers that we put equal to unity at the end the calculation. Show that f_{0i} is nothing but the Maxwell-Boltzmann distribution.

   Hint: Maximize $\log \Omega\{N_i\}$ (why log?) with respect to N_i taking into account the conditions (1). Calculate f_{0i}.

3. The average of N_i over the microcanonical ensemble is given by

$$\langle N_j \rangle = \frac{\sum_{N_i} N_j \Omega\{N_i\}}{\sum_{N_i} \Omega\{N_i\}}.$$

   Taking $\langle N_j \rangle \approx N_{0j}$, show that the mean square fluctuation is given by

$$(\Delta N_j)^2 \equiv \langle N_j^2 \rangle - \langle N_j \rangle^2 = N_{0j}.$$

   Hint: Show that for $g_i \to 1$ one has

$$\langle N_j \rangle = g_i \frac{\partial}{\partial g_i} \sum_{N_i} \Omega\{N_i\}.$$

4. The probability of any set $\{N_j\}$ to be realized is given by

$$\mathcal{P}\{N_j\} = \frac{\Omega\{N_j\}}{\sum_{N_i} \Omega\{N_i\}}.$$

   Give the schematic plot of $\mathcal{P}\{N_j\}$ as a function of N_j/N and show that the assumption $\langle N_j \rangle \approx N_{0j}$ is reasonable.

   Hint: Express $\Delta(N_j/N)$, what happens for large N ?

Aufgabe 11.2 Ideal paramagnet

Consider a system of N magnetic moments $\boldsymbol{\mu}$ (classical and non-interacting moments). We apply a magnetic field $\boldsymbol{H} = H\hat{\boldsymbol{z}}$ in which the moments can only be parallel or anti-parallel to it. The energy for each moment is then given by $E_\sigma = -\boldsymbol{\mu H} = -\sigma\mu H$ with $\sigma = \pm 1$.

1. Calculate the total average energy and the specific heat of the system.

   Hint: Express the Maxwell-Boltzmann distribution of the system in which $\beta^{-1} = k_B T$ and calculate the average energy for one moment $\langle E_\sigma \rangle$. The average value of a quantity A over the microcanonical ensemble is given by $\langle A \rangle = \sum_i A_i f_{0i} / \sum_i f_{0i}$ where we sum over all the degrees of freedom.

2. Calculate the avarage projection along the z-axis of the magnetic moment $\boldsymbol{\mu}$ and the magnetisation M of the system. For the limit $\beta\mu H \ll 1$ (Curie-law), show that both the magnetization M and the magnetic susceptibility $\chi = (\partial M/\partial H)$ are proportional to the inverse temperature: $M(T), \chi(T) \propto \beta \propto T^{-1}$. Furthermore you should show that the magnetization M saturates in the opposite limit.

3. Plot the specific heat and the magnetic susceptibility in dimensionless values (for example with Mathematica) and show that they decrease exponentially at low temperature. What does this mean in terms of degrees of freedom?