Active Matter Physics

Prepare the solutions for the seminar on 2024.4.17

Exercise Sheet 1

1.1

Consider a system of N ideal particles that are distinguishable and which are distributed on m energy levels such that the total energy is fixed by E. The amount of energy levels m for $N \gg 1$ is chosen such that the number of particles, n_i, that can be found on the ith level ($i = 1, \cdots, m$) fulfills $1 \ll n_i \ll N$. In this task, we assume that the energy differences between two adjacent energy levels are all equal. An example for $N = 6$, $m = 3$, and $E = 4a$ with a the energy difference between two adjacent energy levels is shown in Figure 1.

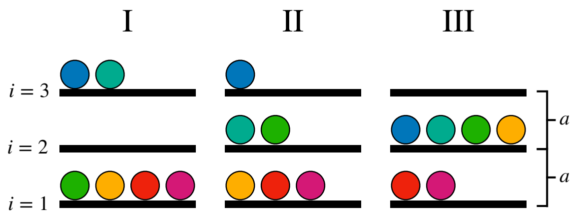

Figure 1: Possible distributions of $N = 6$ particles on $m = 3$ energy levels such that the total energy is $E = 4a$. The number of possible arrangements of these six particles for the setup I is $\omega_{\mathrm{I}} = 15$. For the setups II and III the number of such arrangements is $\omega_{\mathrm{II}} = 60$ and $\omega_{\mathrm{III}} = 15$, respectively.

- Back to the general case, calculate the number of possibilities ω to distribute these N particles on the m energy levels for a fixed arrangement (cf. Figure 1).

A single realization of this distribution is called a configuration. The total number of these configurations Ω is related to the probability to find the system in a particular configuration via

$$P_j = 1/\Omega \qquad (j = 1, \cdots, \Omega) \tag{1}$$

according to the principle of equal *a priori* probability. Hence, ω/Ω is the probability to find the system in a given distribution.

- Calculate the probability distribution $n_i(\epsilon_i)$ that maximizes ω by means of a variational approach, i.e., by infinitesimally increasing the number of particles n_i that can be found in the ith energy level and by calculating how ω changes then:

  $$n_i \to n_i + \mathrm{d}n_i \Rightarrow \ln(\omega) \to \ln(\omega) + \mathrm{d}(\ln(\omega)). \tag{2}$$

  The variable ϵ_i is hereby the energy of a particle in the ith energy level. The natural logarithm of ω is maximized and not ω directly as this unveils technical benefits. Such an approach is valid for large values of ω. For the calculation you may use the following recipe:

  – State the two side conditions that hold for this system and calculate their variation with respect to n_i.

  – Expand the total differential $\mathrm{d}(\ln(\omega)) = \mathrm{d}(\ln(\omega(\{n_i\}_{i=1}^m)))$ in general terms of $\{\mathrm{d}n_i\}_{i=1}^m$. Which general condition holds for $\mathrm{d}(\ln(\omega))$ in this maximization task?

  – Add to the previous function of $\mathrm{d}(\ln(\omega))$ the variations of the two side conditions with Lagrange multipliers α and $-\beta$.

– As these two Lagrange multipliers can be chosen freely, they will be chosen such that those terms are set to zero in $\mathrm{d}(\ln(\omega))$ that belong to $i = 1, 2$. What does this then mean for those terms in $\mathrm{d}(\ln(\omega))$ that belong to $i \geq 3$?

– Use the result for ω from the first bullet point as well as Strinling's formula:

$$\ln(n!) \approx n \ln(n) - n \tag{3}$$

to calculate the probability distribution $n_i(\epsilon_i)$.

– For the determination of the Lagrange multipliers, you can make the following assumptions:

$$\sum_{i=1}^{m} \mathrm{e}^{-\beta\epsilon_i} \to \int_0^\infty \mathrm{e}^{-\beta\epsilon} \mathrm{d}\epsilon, \tag{4}$$

$$\sum_{i=1}^{m} \epsilon_i \mathrm{e}^{-\beta\epsilon_i} \to \int_0^\infty \epsilon \mathrm{e}^{-\beta\epsilon} \mathrm{d}\epsilon \tag{5}$$

which hold, since we considered equidistant energy differences.

1.2

Consider an agent that can switch between two states 1 and 2 as, for example, a person being healthy (state 1) or sick (state 2) or a chemical reaction taking place such as an atom of sodium that is not bound (state 1) or bound to a chlorine atom (state 2). Furthermore, assume the rates at which the agent changes its state, i.e., $\pi(1 \to 2)$ and $\pi(2 \to 1)$ to be constant. Starting at some initial time t_0, the probabilities of finding the agent in state 1 or 2 at time t are $P_1(t)$ and $P_2(t)$, respectively.

- Determine which processes contribute to the probability $P_1(t + \mathrm{d}t)$ of finding the agent in state 1 at time $t + \mathrm{d}t$.
- Derive the master equations for the given system.
- Solve the system of master equations using the initial conditions $P_1(t = t_0) = P_1(t_0)$ and $P_2(t = t_0) = P_2(t_0)$.
- Verify that the stationary distributions satisfy the detailed balance condition.

1.3

Consider N indistinguishable ideal particles that are freely moving in a box of volume V, i.e., their energy is given by

$$\epsilon(\mathbf{r}, \mathbf{p}) = \begin{cases} \frac{\mathbf{p}^2}{2m} & \mathbf{r} \in V, \\ \infty & \text{else}, \end{cases} \tag{6}$$

where m is the mass of a particle.

- Calculate the canonical partition function of a single particle and express it in terms of the thermal de-Broglie wavelength λ_β given via

$$\lambda_\beta = \sqrt{\frac{\beta h^2}{2\pi m}}. \tag{7}$$

(Hint: Do not forget the unit "volume" h^3 in this continuous situation.)

- Using the Boltzmann distributed particle density $n(\mathbf{r}, \mathbf{p})$ calculate the number of particles $N(p)$ with momentum in the range of p and $p + \mathrm{d}p$.
- Employing the previous result calculate the number of particles $N(v)$ with velocities in the range of v and $v + \mathrm{d}v$ which is the familiar Maxwell–Boltzmann velocity distribution.