Active Matter Physics

Prepare the solutions for the seminar on 2025.5.8

Exercise Sheet 2

2.1

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

$$\epsilon(\mathbf{r}, \mathbf{p}) = \begin{cases} \frac{\mathbf{p}^2}{2m} & \mathbf{r} \in V, \\ \infty & \text{else}, \end{cases} \tag{1}$$

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

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

  (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.

2.2

(Background: detailed balance equation

$$\pi(i) \cdot P(i \to j) = \pi(j) \cdot P(j \to i) \tag{3}$$

where $P(i \to j)$ is the probability of jumping from state i to j, i.e., $P(i \to j) = P(X_t = j | X_{t-1} = i)$. π_i and π_j are the probabilities of being in state i and j in equilibrium.)

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.

2.3

Consider a biased random walk on a discrete lattice with $L+1$ sites and for all $1 \leq i \leq L-1$ the transition probabilities:

$$\pi(i \to j) = \begin{cases} p & \text{if } j = i+1 \\ q & \text{if } j = i-1 \\ 0 & \text{otherwise} \end{cases} \quad . \tag{4}$$

For the boundaries, it holds that

$$\pi(0 \to j) = \begin{cases} p & \text{if } j = 1 \\ q & \text{if } j = 0 \\ 0 & \text{otherwise} \end{cases} \quad \text{and} \quad \pi(L \to j) = \begin{cases} p & \text{if } j = L \\ q & \text{if } j = L-1 \\ 0 & \text{otherwise} \end{cases} \quad , \tag{5}$$

i.e., the random walker stays where it is if it tries to move below 0 or above L (reflecting boundary conditions).

- Calculate the stationary probability $P(0)$ using the detailed balance condition.
- Consider the explicit case of $L = 2$ and $p = 1 - q = 1/3$. Write down the transition matrix and the transition graph of this process (cf., for example, Markov chains). Calculate the stationary probability distribution $P = (P(0), P(1), P(2))$ for this case. Is the process reversible (i.e., is the detailed balance condition fulfilled)?
- In another setting a random walker obtains the following transition matrix:

  $$\Pi = (\pi(i \to j))_{i,j\in\{0,1,2\}} = \begin{pmatrix} 0 & 2/3 & 1/3 \\ 1/3 & 0 & 2/3 \\ 2/3 & 1/3 & 0 \end{pmatrix} . \tag{6}$$

  Write down its transition graph. Calculate the stationary probability distribution via the ansatz $P \cdot \Pi \stackrel{!}{=} P$. Is this random walker in detailed balance?