8.08/8.S308 - Problem Set 4 - IAP 2025

Due before January 28 23:59

Anything marked as "graduate" count as bonus problems for undergraduate students.

1- Active spins on lattice

We consider an active particle on a square lattice in an arbitrary dimension d. The particle hops in a given direction at rate h and changes direction at rate α, picking its new direction among the $2d$ possibilities uniformly at random. Such a direction change is called a 'tumble'. The purpose of the next few questions is to compute the diffusivity of the particle. A trajectory of duration t can be decomposed into n successive runs, defined as the period between two tumbles. Note that the number n is itself a random variable, which fluctuates between different trajectories of the same duration t. During each run, the particle undergoes a displacement $\vec{a}_i$ along one of the lattice direction (the lattice spacing is taken equal to 1).

1.1) Draw a schematic trajectory with $n = 6$ for a two-dimensional lattice.

1.2) Show that, if the particle starts at the origin, its displacement $\vec{r}(t)$ at time t satisfies

$$\langle \vec{r}(t)^2 \rangle = \left\langle \sum_{i=1}^{n} \vec{a}_i^2 + 2 \sum_{i<j} \vec{a}_i \cdot \vec{a}_j \right\rangle \tag{1}$$

where brackets represent averages over many trajectories.

1.3) Using simple symmetry arguments, explain why $\langle \vec{a}_i \cdot \vec{a}_j \rangle = 0$ for $i \neq j$.

1.4) We now assume that $\langle \sum_{i=1}^{n} \vec{a}_i^2 \rangle \underset{t\to\infty}{\sim} \langle n \rangle \langle a^2 \rangle$, where $\langle n \rangle$ is the average number of run phases during a trajectory of length t and $\langle a^2 \rangle$ is the second moment of the run length. This is called the Wald identity; explain briefly the underlying asumption and why it is valid in the large time limit.

1.5) Compute the mean time between two tumbles. Deduce the mean number $\langle n \rangle$ of run phases during a large time t.

1.6) We now want to compute $\langle a^2 \rangle$. At any time, what is the probability that the next configuration change is a hopping event? A tumble? Show that the probability $P(a)$ that the particle covers a distance a during a run phase is given by

$$P(a) = \frac{\alpha h^a}{(\alpha + h)^{a+1}} \tag{2}$$

1.7) We introduce the generating function $G(z) = \sum_{a=0}^{\infty} z^a P(a)$. Compute $G(z)$, for $z < 1 + \alpha/h$, in terms of α, h and z.

1.8) Compute $G'(1)$ and $G''(1)$. Deduce the first and second moment of the run length a:

$$\langle a \rangle = \frac{h}{\alpha}; \qquad \langle a^2 \rangle = 2\frac{h^2}{\alpha^2} + \frac{h}{\alpha} \tag{3}$$

1.9) Using these results and Eq. (1), compute the diffusivity D as:

$$D \equiv \lim_{t\to\infty} \frac{1}{t} \frac{\langle \vec{r}(t)^2 \rangle}{2d}. \tag{4}$$

2- Rectification of bacterial density by anisotropic tumbles

Let us consider a self-propelled particle on a one-dimensional lattice of L sites with periodic boundary conditions (in the following, we silently identify site $L+1$ and site 1, as well as site 0 and site L). $P(i,+;t)$ and $P(i,-;t)$ are the probabilities to find the particle on site i going to the right and to the left, respectively. We silently omit the time dependency in the following and simply write $P(i,\pm)$. On site i, the particle may

- hop to the site $i+1$ at rate d_i^+ if it is in the right-going state.
- hop to the site $i-1$ at rate d_i^- if it is in the left-going state.
- change its orientation from right-going to left-going at rate α_i^+.
- change its orientation from left-going to right-going at rate α_i^-.

2.1) The configurations corresponding to having the particle at site i in a right-going or left-going states are noted $(i,+)$ and $(i,-)$, respectively. List all possible transitions into and out of configuration $(i,+)$ and the corresponding rates, and show that the evolution of $P(i,+)$ is given by the master equation

$$\partial_t P(i,+) = d_{i-1}^+ P(i-1,+) - d_i^+ P(i,+) + \alpha_i^- P(i,-) - \alpha_i^+ P(i,+) \tag{5}$$

What is the master equation yielding the evolution of $P(i,-)$?

2.2) We note $P(i)$ the probability to find the particle at site i, irrespectively of its direction. How are $P(i)$, $P(i,+)$, and $P(i,-)$ related mathematically? Show the evolution of $P(i)$ to be of the form

$$\partial_t P(i) = J_{i-1,i} - J_{i,i+1} \tag{6}$$

Give the expression of $J_{i,i+1}$ and its physical interpretation. If you were to simulate this system, how would you measure $J_{i,i+1}$?

2.3) We now consider the system in **steady state**. Show that the probability current is constant and that its value is given by

$$J = P(i,+)(d_i^+ + \alpha_i^+) - P(i,-)(d_i^- + \alpha_i^-) \tag{7}$$

2.4) *Graduate.* Express $P(i,+)$ as a function of $P(i-1,+)$, J and of the microscopic rates.

2.5) *Graduate.* We now consider a closed system of L sites ($d_1^- = d_L^+ = 0$). What is the value of J in the steady-state? Show that

$$\forall i \geq 2, \qquad P(i,+) = \left(\prod_{j=2}^{i} \frac{d_{j-1}^+}{d_j^-} \frac{d_j^- + \alpha_j^-}{d_j^+ + \alpha_j^+} \right) P(1,+); \qquad P(i,-) = \frac{d_i^+ + \alpha_i^+}{d_i^- + \alpha_i^-} P(i,+) \tag{8}$$

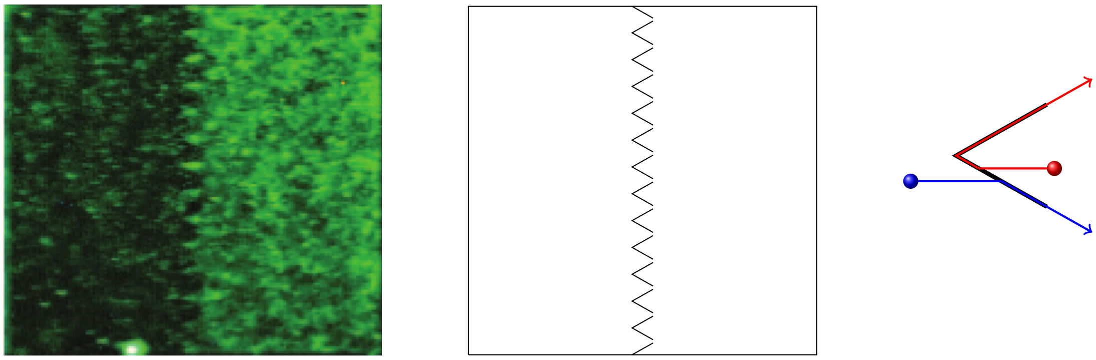

Figure 1: ***Left:*** *Steady-state density of bacteria in a cavity with asymmetric obstacles in the middle.* ***Center:*** *Sketch of the cavity. The distance between obstacles is larger than the size of the bacteria.* ***Right:*** *Description of the bacteria trajectories when they collide with an obstacle.*

2.6) *Graduate.* We consider a system with uniform, isotropic hoping rates $d_i^+ = d_i^- = d$. For $1 \leq i \leq \ell$ and for $\ell + h < i \leq L$, $\alpha_i^+ = \alpha_i^- = \alpha$. For $\ell < i \leq \ell + h$, on the other hand, we take $\alpha_i^+ = \alpha$ and $\alpha_i^- = \alpha + \varepsilon$. Compute $P(i,+)$, $P(i,-)$ and $P(i)$ for all i. Make a sketch of $\log P(i)$ as a function of i.

2.7) *Graduate.* In Fig. 1, the steady-state density distribution of bacteria swimming in a two-dimensional cavity containing at its center a one-dimensional line of asymmetric obstacles is shown. Explain this experimental result. (Feel free to model the experiment in any way you like.)

3- Zero-range process

We consider a one-dimensional lattice with L sites and periodic boundary conditions. N particles hop stochastically on the lattice and a configuration of the system is thus characterised by the occupancy numbers $\{\mathbf{n}\} \equiv (n_1, \ldots, n_L)$ for all sites. We consider $u(n)$ an arbitrary positive function of n such that $u(0) = 0$. With a rate $u(n_i)$, one particle on site i is transferred to site $i+1$, so that $n_i \to n_i - 1$ and $n_{i+1} \to n_{i+1} + 1$.

3.1) Consider a configuration $\{\mathbf{n}\}$. What are the configurations $\{\mathbf{n}'\}$ connected to $\{\mathbf{n}\}$ by a single-particle displacement? What are the corresponding transition rates from $\{\mathbf{n}\}$ to $\{\mathbf{n}'\}$ and from $\{\mathbf{n}'\}$ to $\{\mathbf{n}\}$?

3.2) Explain the principle of detailed balance for a model with a discrete set of configurations. Can this model satisfy detailed balance? Show that the master equation can be written as

$$\partial_t P(\{\mathbf{n}\}) = \sum_{k=1}^{L} [u(n_{k-1}+1) P(\{n_{k-1}+1, n_k - 1\}) - u(n_k) P(\{\mathbf{n}\})] \tag{9}$$

where $\{n_{k-1}+1, n_k - 1\}$ is the configuration obtained from $\{\mathbf{n}\}$ by adding a particle at site $k-1$ and substracting a particle from site k.

3.3) We look for a factorized steady-state:

$$P(\{\mathbf{n}\}) = Z_{L,N}^{-1} \prod_{k=1}^{L} f(n_k) \tag{10}$$

Show that a sufficient condition for (10) to be a solution of Eq. (9) is

$$u(n_{k-1}+1)\frac{f(n_{k-1}+1)}{f(n_{k-1})} = u(n_k)\frac{f(n_k)}{f(n_k-1)} \tag{11}$$

Explain why this imposes both left-hand side and right-hand side to be equal to a constant λ independant of n_k and n_{k-1}.

3.4) We assume $\lambda = f(0) = 1$ without loss of generality. Compute $f(n_k)$ and show that

$$P(\{\mathbf{n}\}) = Z_{L,N}^{-1} \prod_{k=1}^{L} \prod_{j=1}^{n_k} \frac{1}{u(j)}\ , \tag{12}$$

where $Z_{L,N}^{-1}$ is a normalization constant.

3.5) Show that

$$Z_{L,N} = \sum_{\{\mathbf{n}\}} \prod_{k=1}^{L} f(n_k)\delta(\sum_{i=1}^{L} n_i - N) \tag{13}$$

where $\delta(p=0) = 1$ and $\delta(p \neq 0) = 0$.

3.6) *Graduate.* Let $p(n)$ be the (marginal) probability that n particles are at site 1, irrespectively of the other occupancy numbers, but given that there are N particles in total. Show that

$$p(n) = f(n)\frac{Z_{L-1,N-n}}{Z_{L,N}} \tag{14}$$

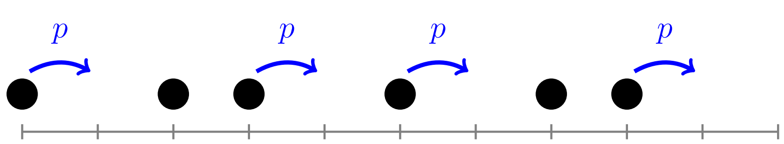

Figure 2: *In a TASEP, all particles hop forward at rate p provided the arrival site is empty. (Conversely, all the particles could be hoping towards the left.)*

3.7) *Graduate.* We now consider the following mapping, valid for periodic boundary conditions, from a lattice with L sites and N particles to a lattice with $N+L$ sites and L particles. Each *site* of the system 1 corresponds to a *particle* of the system 2. The occupancy number of site i in system 1 then corresponds to the number of empty sites between the $(i-1)^{\text{th}}$ particle and the i^{th} particle in system 2. Draw two configurations of your choice, that you find illustrative, for $L = 6$ and $N = 5$. Show that if system 1 is a zero-range process with $u(n) = p$, then the system 2 corresponds to a TASEP. To do so, one will represent all possible representative transitions in one system and the corresponding transitions in the second system.

3.8) *Graduate.* Consider the TASEP illustrated in Figure 2. Write down the master equation for a system of $M = N + L$ sites and N particles. Show that in steady state, all configurations have equal probability. Given the mapping discussed at the question 3.7, is this compatible with (12)?