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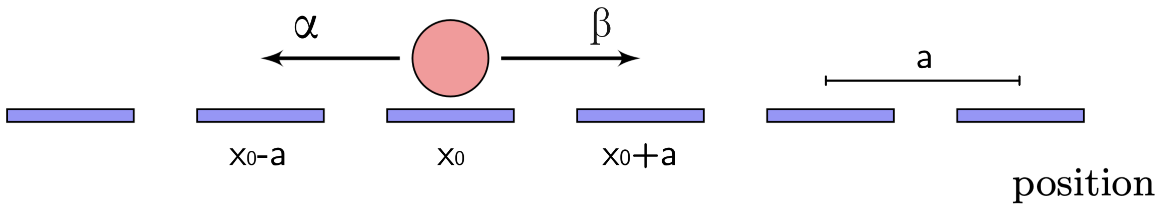
Nonequilibrium Field Theories and Stochastic Dynamics
Sheet 1

Exercise 3 – One-dimensional Random Walker

One of the most basic stochastic processes is the so-called random walker. Consider a particle on a one-dimensional, discrete lattice with lattice spacing a (see sketch). The particle hops one lattice site to the left with rate α and one lattice site to the right with rate β. The random variable $X(t)$ labels the position of the particle at time t and takes values in $\{0, \pm a, \pm 2a \dots\}$. We are interested in the probability distribution $\text{Prob}\{X(t) = x \mid X(0)\} =: P(x, t|x_0, 0)$, i. e. the probability of finding the particle at position x at time t under the condition that the particle was at site x_0 at time $t_0 = 0$.



a) Write down the probability that the particle jumps forward/backward in the time interval $[t, t + dt]$. Based on the jumping probabilities, write down an equation for the probability distribution $P(x, t + \mathrm{d}t|x_0, 0)$ to find the particle at position x at time $t + \mathrm{d}t$ in terms of the probability distribution at time t. Expand the resulting equation for small $\mathrm{d}t$ to obtain a difference equation for the probability distribution $P(x, t|x_0, 0)$. Your result should read

$$\partial_t P(x, t) = \alpha P(x + a, t) + \beta P(x - a, t) - (\alpha + \beta)P(x, t) \; . \tag{1}$$

An equation of this form for the time evolution of the probabilities is called *master equation*.

b) Use the master equation to derive an ordinary differential equation (ODE) for the average position of the particle, $\langle X \rangle(t)$, and for the variance $\text{Var}(X)(t) = \langle X^2 \rangle(t) - \langle X \rangle^2(t)$. Solve both ODEs for the initial condition that the particle is at position x_0 at time $t_0 = 0$.

c) The moment-generating function $M(z, t)$ is defined as

$$M(z, t) := \sum_{x \in a\mathbb{Z}} e^{zx} P(x, t) \; . \tag{2}$$

Obtain the time evolution equation for it. Why is it simpler to solve this equation than the master equation? Solve for $M(z, t)$, assuming that the particle at $t_0 = 0$ was at position x_0. Calculate $\langle X \rangle(t)$ and $\text{Var}(X)(t)$ from the solution of $M(z, t)$ and verify your result from part **b)**.

d) As a naive approximation of the master equation with discrete jumps, consider the continuum limit of the 1D random walker. Assuming that the step size a becomes small and hence the variable x continuous, expand the master equation around $P(x, t|x_0, t_0 = 0)$ up to second order in a and obtain a partial differential equation for $P(x, t|x_0, t_0 = 0)$.
Aside: Note that this approximation only makes sense when the coefficients in front of the derivatives remain finite in the continuum limit as $a \to 0$, which is not always the case. In the course of the lecture, we will make this so-called Kramers-Moyal expansion more formal and recognize its truncated form as the Fokker-Planck equation.

Exercise 4 – One-dimensional Random Walker: Numerics*

This exercise is optional, but we encourage you to try it, especially if you have little experience with programming. We have put a short guide on how to use Python and Jupyter on Moodle. That material and the solution to this exercise will be covered in the central tutorial next week (Wednesday, 07.05.2025, 14:00 s.t., room A348). If you run into problems with the numerical parts of the exercise, please ask the tutors or your fellow students for help. Note that part ***a)-b)*** *does not require numerical calculations.*

Here we will revisit the problem of a one-dimensional random walker with forward hopping rate β and backward hopping rate α as discussed in the previous exercise, but approach the problem numerically.

a) In the lecture you have discussed the basic concept of the fixed time step and the Gillespie algorithm. Recapitulate the idea behind the algorithms in your own words. What are the major differences?

b) Use the waiting time distribution

$$w(t) = \nu \exp(-\nu t) \tag{3}$$

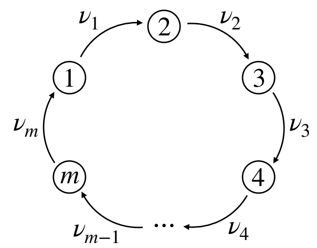
which you derived in the lecture to show that the fixed time step algorithm converges to the correct solution in the limit of small Δt

c) Implement the fixed time step algorithm for the one dimensional random walker defined in the Exercise 3. Measure the mean and the variance of the particle position. Compare your numerical results to your analytic results from Exercise 3. Play with the time step Δt to observe how it affects your results.

d) Implement the Gillespie algorithm for the one dimensional random walker defined in the Exercise 3. What do you have to take care about when you measure observables (e.g. the mean particle position) as a function of time?

Exercise 5 – Cyclic m-step process

Consider a cyclic m-step process where the states $1, 2, \ldots, m$ are passed through in sequential order with the reaction rates $\nu_i = 1/\tau_i$, as shown on the scheme below.



The individual transitions $i \xrightarrow{\nu_i} (i+1)$ are assumed to be statistically independent. The reaction times T_i of each transition are random variables, which we assume to be distributed exponentially:

$$\text{Prob}\{T_i = t\} = w_i(t) = \nu_i e^{-\nu_i t} \; . \tag{4}$$

a) Show that the mean and the variance of the total time $T = \sum_{i=1}^{m} T_i$ required to complete the chemical cycle are given by

$$\langle T \rangle = \sum_{i=1}^{m} \tau_i =: \tau, \quad \text{Var}[T] = \sum_{i=1}^{m} \tau_i^2 \; . \tag{5}$$

Hint: You can use known results for the exponential distribution from the lecture.

b) Restrict the analysis to the case of identically distributed reaction times with $\tau_i = \tau/m$, and show that

$$\langle T \rangle = \tau \quad \text{and} \quad \text{Var}[T] = \frac{\tau^2}{m} \; . \tag{6}$$

Why, heuristically, does the variance scale as $\sim 1/m$? What does this imply for $m \gg 1$?

c) Consider now the case where one of the m transitions (say, ν_i) is *rate-limiting*. That means, on average, the i-th reaction takes much longer than any of the others (or $\forall j \neq i: \ \tau_j \ll \tau_i \approx \tau$). Show that

$$\langle T \rangle = \tau \quad \text{and} \quad \mathrm{Var}[T] \approx \tau^2 \ . \tag{7}$$

What if there are k rate-limiting reactions, each with mean reaction time $\approx \tau/k$? What actually determines the variance of T?

Your solutions should be handed in by uploading them to Moodle by **Wednesday, 7$^{\text{th}}$ May 2025, 10:00 am**.