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Nonequilibrium Field Theories and Stochastic Dynamics
Sheet 4

Exercise 11 – Brownian particle in a gravitational field

Consider a Brownian particle in a gravitational potential $U(z) = mgz$.

a) *Fokker-Planck equation*

Write down the Fokker–Planck equation for $p(z, t|z_0, 0)$, the conditional probability density for the particle to be at height z at time t given it was at z_0 at $t = 0$, using the Stokes–Einstein relation. This equation is known as the Smoluchowski equation.

b) *Dimensionless Equation*

Show that the equation can be written in dimensionless form. Define $\ell := \frac{k_B T}{mg}$ as the characteristic length scale, and transform $z \mapsto x\ell$ and $t \mapsto D^{-1}\ell^2\tau$.

c) *Reflective boundaries*

We assume that there is a impenetrable floor at $x = 0$ that stops the particle from just drifting indefinitely towards $-\infty$. Show that the reflective boundary condition at $x = 0$ implies $\partial_x p(x, \tau)|_{x=0} + p(0, \tau) = 0$.

d) *Solution with reflective boundaries*

We now want to derive the solution of the dimensionless Fokker–Planck equation derived in exercise part b). Therefore, note that the initial condition is given by $p(x, 0|x_0, 0) = \delta(x - x_0)$.
To this end, we perform a substitution of the form $p(x, \tau) = u(x, \tau)e^{a\cdot(x-x_0)}e^{b\cdot\tau}$ to remove the drift terms from the Fokker–Planck equation.
How do you need to choose a and b to make sure that the drift term vanishes?
How do the initial condition and the boundary condition change by the substitution?

e) Solving this equation with the correct boundaries is a well known, but rather difficult, problem in the theory of heat conduction. This problem was first studied by M. Smoluchowski[1]. We will not perform the entire derivation here, but you can find it in the papers below[2]. Instead we will look at a simplified version of the problem that one obtains when reducing the boundary conditions to

$$\partial_x u|_{x=0} = 0$$

Show that using this as boundary conditions for $u(x, \tau)$ a solution to the corresponding equation for $p(x, \tau)$ is given by the function:

$$p(x, \tau|x_0, 0) = \frac{1}{2\sqrt{\pi\tau}}\left[\exp\left(-\frac{(x-x_0)^2}{4\tau}\right) + \exp\left(-\frac{(x+x_0)^2}{4\tau}\right)\right] \times \exp\left(-\frac{x-x_0}{2} - \frac{\tau}{4}\right). \tag{1}$$

Hint: Use the method of images to make sure your ansatz for $u(x, \tau)$ fulfills the boundary condition.

f) The solution of the full problem, with correct boundary conditions is given by

$$p(x, \tau|x_0, 0) = \frac{1}{2\sqrt{\pi\tau}}\left[\exp\left(-\frac{(x-x_0)^2}{4\tau}\right) + \exp\left(-\frac{(x+x_0)^2}{4\tau}\right)\right] \times \exp\left(-\frac{x-x_0}{2} - \frac{\tau}{4}\right) + A(x, \tau). \tag{2}$$

[1] "Drei Vorträge über Diffusion, Brownsche Bewegung und Koagulation von Kolloidteilchen", Phys. Zeits. 17:557 (1916)
[2] "Stochastic Problems in Physics and Atronomy" by S. Chandrasekhar in Rev. Mod. Phys. 15:1 (1943), "Sedimentation of Brownian Particles in a Gravitational Potential" by B. U. Felderhof in Journal of Statistical Physics 109:483-493 (2002), "Über Brownsche Molekularbewegung unter Einwirkung äußerer Kräfte und deren Zusammenhang mit der verallgemeinerten Diffusionsgleichung" by M. Smoluchowsky in Ann. d. Phys. 353:24 (1916)

Where we introduced the additional term

$$A(x, \tau) = \frac{1}{2} \exp(-x) \operatorname{erfc}\left(\frac{x + x_0 - \tau}{2\sqrt{\tau}} \right) . \tag{3}$$

You can verify that this is a solution of the original equation, where we added a suitably defined source term (you don't have to do it).

Show that this expressions now fulfills the correct boundary conditions obtained in exercise part c).

Additionally, show that with the term $A(x, \tau)$ the full solution converges to $p_{\text{eq}}(x) = e^{-x}$.

Hint: The following relation may be useful:

$$\frac{\mathrm{d}}{\mathrm{d}x} \operatorname{erfc}(x) = -\frac{2e^{-x^2}}{\sqrt{\pi}} \tag{4}$$

g) *Solution with free boundaries*

Compare the above with the free solution obtained in the absence of a boundary.

Exercise 12 – Bistability in an autocatalytic reaction

Protein molecules consist of a chain of aminoacids. This chain folds into a very specific shape that determines the biological function of the protein. In many cases protein molecules need other protein molecules, sometimes of the same kind, to fold into the correct shape. In other cases, misfolded protein molecules can trigger the misfolding of other protein molecules of the same kind, as it is the case for amyloid fibers. In this exercise we study the influence of two protein molecules in shape X on one in shape Y. Those states can transform into each other by the following two reaction schemes:

$$X \underset{k_2}{\overset{k_1}{\rightleftarrows}} Y, \quad X + 2Y \overset{k_3}{\rightarrow} 3Y. \tag{5}$$

Let $n(t)$ be the number of proteins in state Y at time t and $m(t)$ be the number of proteins in state X. Since X and Y are only two different configurations of the same protein, the total number $N = n(t) + m(t)$ of proteins is conserved by these transformations.

The system is one example where we can find an exact solution for the stationary probability distribution of the number of proteins. In this exercise we want to compare different approximation methods among each other and with the exact solution.

a) *Master equation*

First, write down the Master equation for the probability $P(n, m, t)$ to have n proteins in state Y and m proteins in state X at time t. In a second step, use the protein number conservation to obtain a master equation depending only on n, t.

b) *Deterministic solution*

- Using the Master equation determine the time evolution of the mean $\langle n(t) \rangle$ and of $\langle n^2(t) \rangle$. Why can't you find a closed solution for these moments?

A first way to tackle this problem is to employ a so-called mean-field approximation, where correlations are neglected completely by assuming $\langle n^i(t) \rangle \overset{!}{=} \langle n(t) \rangle^i$ for all i.

- Use this ansatz to find an approximate equation for the evolution of the mean $y(t) = \langle n(t) \rangle$. Your result should read as:

$$\frac{\mathrm{d}y(t)}{\mathrm{d}t} = -k_2 y(t) + k_1(N - y(t)) + k_3 y(t)(y(t) - 1)(N - y(t)). \tag{6}$$

c) *Exact solution of the Master equation*

Now, we want to find an exact solution for the stationary probabilites $P_s(n)$. In order to do so, let us consider a general Master equation of the form

$$\partial_t P(n, t) = w_+(n-1)P(n-1, t) + w_-(n+1)P(n+1, t) - (w_+(n) + w_-(n))P(n, t). \tag{7}$$

- Assuming that $P_s(n) = 0 \; \forall n < 0$ and $n > N$ and $w_-(0) = 0$, derive a general solution for $P_s(n)$. Use that the stationary distribution here serves detailed balance between site n and $n + 1$ for all n. The resulting recursion can be solved using the boundary term at $n = 0$. Why does the stationary distribution obey detailed balance in this system?

- Convince yourself that the general solution to our problem is:

$$P_s(n) = \frac{P_s(0)}{k_2^n} \frac{N!}{(N-n)!n!} \prod_{m=0}^{n-1} (k_1 + k_3 m(m-1)) \tag{8}$$

where $n \in \{1, 2, \ldots, N\}$ and $P_s(0) + \sum_{n=1}^{N} P_s(n) = 1$.

d) *Fokker-Planck equation*

Another common approximation method is a Kramers-Moyal expansion.

- Using this expansion, derive the Fokker-Planck equation for this system from the master equation.
- What is the stationary solution (you don't need to solve the occuring integral explicitly)?
- What boundary conditions must be used?

Hint: Keep in mind that $P(n,t) = 0$ for $n < 0$ and $n > N$.

Exercise 13 – First passage times*

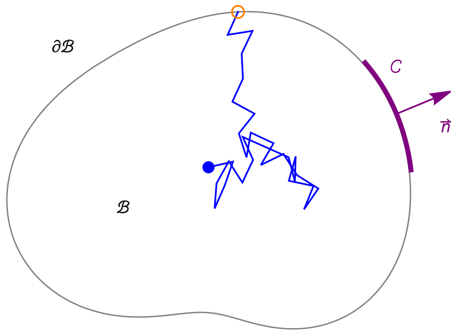

Figure 1: Sketch of a first passage time problem in 2D. A particle is starting at the blue point in the domain and hitting the boundary after some time.

Consider a particle in a finite domain $\mathcal{B}$ with boundary $\partial\mathcal{B}$ whose stochastic dynamics is described by the (forward) Fokker-Planck equation

$$\partial_t p(\mathbf{x}, t|\,\mathbf{x_0}, t_0) = -\partial_i \left[A_i(\mathbf{x}) p(\mathbf{x}, t|\,\mathbf{x_0}, t_0)\right] + \frac{1}{2}\partial_i\partial_j \left[B_{ij}(\mathbf{x}) p(\mathbf{x}, t|\,\mathbf{x_0}, t_0)\right], \tag{9}$$

where the drift vector A and the diffusion matrix B are considered to be time-independent. We would like to investigate the following question: When will a particle starting somewhere in the domain $\mathcal{B}$ first arrive at any point on the boundary $\partial\mathcal{B}$ of the domain? Problems of this type are called *first passage time* problems (see Fig. 1 for an illustration).

a) To answer this question, we first consider the *survival probability* defined as

$$S(\mathbf{x}, t) = \int_{\mathcal{B}} \mathrm{d}\mathbf{x}'\, p(\mathbf{x}', t|\,\mathbf{x}, t_0) \tag{10}$$

which is the probability that a particle starting at time t_0 at a position $\mathbf{x}$ inside the domain $\mathcal{B}$ remains inside the domain (at least) until time $t > t_0$. Argue why $p(\mathbf{x}', t|\,\mathbf{x}, t_0)|_{\mathbf{x}' \in \partial\mathcal{B}} = 0$ corresponds to absorbing boundary conditions, and why we need to impose them here.

Hint: To understand why this is an absorbing boundary condition, you might want to compare it to the case where $p(\mathbf{x}', t|\,\mathbf{x}, t_0)|_{\mathbf{x}' \in \partial\mathcal{B}} =$ const. > 0.

Hint: Also note that S depends on the initial *position of the particle, which we usually denote by $\mathbf{x_0}$ – we omit the subscript for simplicity.*

b) As $A(\mathbf{x})$ and $B(\mathbf{x})$ are time-independent, we choose $t_0 = 0$ in the following. Show that the survival probability obeys a *backward Fokker-Planck equation*

$$\partial_t S(\mathbf{x}, t) = A_i(\mathbf{x})\partial_i S(\mathbf{x}, t) + \frac{1}{2} B_{ij}(\mathbf{x})\, \partial_i\partial_j S(\mathbf{x}, t)\,. \tag{11}$$

Hint: Why can we use that $p(\mathbf{x}', t|\,\mathbf{x}, 0) = p(\mathbf{x}', 0|\,\mathbf{x}, -t)$? Which equation does $p(\mathbf{x}', 0|\,\mathbf{x}, -t)$ obey?

c) *Moments for the first passage time*

Derive the probability distribution $w(t)$ for the time T when the particle leaves $\mathcal{B}$ (or, equivalently, first arrives at the boundary $\partial\mathcal{B}$). We call T the *first passage time* and $w(t)$ the *first passage time probability density* or analogously to previous problems *waiting time distribution.*

Show that for the n-th moment of the first passage time the following relation holds:

$$T_n(\mathbf{x}) := \langle t^n \rangle = n \int_0^\infty \mathrm{d}t\; t^{(n-1)} S(\mathbf{x}, t) \tag{12}$$

d) *Mean first passage time*

Using the result from the previous parts, derive for the *mean* first passage time $T(\mathbf{x}) := T_1(\mathbf{x})$:

$$A_i(\mathbf{x})\partial_i T(\mathbf{x}) + \frac{B_{ij}(\mathbf{x})}{2}\partial_i\partial_j T(\mathbf{x}) = -1 \tag{13}$$

What kind of problem/equation have we derived now? What is the condition on $T(\mathbf{x})$ for $\mathbf{x} \in \partial\mathcal{B}$?

e) *Example: 1D random walk*

Now we focus on a one-dimensional problem without drift, $A = 0$, and uniform diffusion $B = 2D = \text{const}$. Assume that the domain is given by an interval of length L, i. e. $\mathcal{B} = [0, L]$. Solve Eq. (13) for the mean first passage time $T(x)$ and interpret your result.

Hint: It is helpful to think about the case $x = L/2$ to check your result.

f) In the part above, we discussed the first passage time for a random walker. Can you think about other real-life applications where the concept of first passage times is an interesting quantity?

Your solutions should be handed in by uploading them to Moodle by **Wednesday, 28^{th} of May 2025, 10:00 am**.