Stochastic Processes — Tutorial 9

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Exercise 1 *Escape by diffusion to the boundaries of a 1d interval*

We consider unbiased diffusion on the interval $\mathcal{I} = [0, L]$ for a random walk that is started at $x_0 \in \mathcal{I}$. The probability density $\rho(x,t)$ to find a walker at time t at a position x obeys the Fokker-Planck equation

$$\partial_t \rho(x,t) = D\, \partial_x^2 \rho(x,t)$$

(a) What are the boundary conditions? What are the initial conditions? Is the probability density $\rho(x,t)$ normalized on the interval $\mathcal{I}$?

(b) We consider

$$C_n(x) = \int_{\mathbb{R}} \mathrm{d}t\; t^n\; \rho(x,t)$$

to extract information concerning the probability to leave the interval to the left and right and the moments of the according waiting times. Show that $C_n(x)$ is the solution of the differential equation

$$D\, \partial_x^2 C_n(x) = \begin{cases} -n\, C_{n-1}(x) & \text{for} \quad n > 0 \\ -\delta(x - x_0) & \text{for} \quad n = 0 \end{cases}$$

(c) Find $C_0(x)$ by integration of the differential equation, and use the resulting expression to determine the probabilities to leave to the left and right, respectively. How do they depend on the starting position?

(d) Determine $C_1(x)$. Use it to determine the mean waiting time for escape to the left and right, respectively.

Exercise 2 *Model H for phase separation*

Model H describes the evolution of the composition of an incrompressible binary fluid that comprises A and B molecules. For simplicity we assume that A and B molecules have the same physical properties (volume, mass, etc). In appropriate units the free energy $F(T,V,\rho)$ takes the form

$$F(T,V,\rho) = \frac{V}{4}\, \rho^2\; \left(\rho^2 + 2\, b(T)\right)\,. \tag{2a}$$

(a) Show that $F(T, V, \rho)$ is convex for $b(T) > 0$ and that it has two minima at the compositions $\pm\rho_c = \pm\sqrt{-b(T)}$ when $b(T) < 0$. According to the Maxwell construction the latter prescribe the composition of two coexisting phases.

(b) In the following we consider systems with a spatially uniform temperature where $b(T) < 0$. The mixture can then be characterized in terms of the scaled density $\varrho(\vec{x}, t) = \rho(\vec{x}, t)/\rho_c$ and the energy density

$$f(\varrho(\vec{x}, t)) = \frac{F(T, V, \varrho(\vec{x}, t))}{V\ \rho_c^2} = \frac{\varrho^4(\vec{x}, t)}{4} - \varepsilon^2$$

For a d-dimensional system the free energy takes the form

$$\mathcal{F}(T, V, [\rho(\vec{q}, t)]) = \int_V \mathrm{d}^d q\ \left[f(\varrho(\vec{q}, t)) - \varepsilon^2\ \left|\nabla\varrho(\vec{x}, t)\right|^2 \right] \tag{2b}$$

What is the effect of the term involving ε^2? Show that Eq. (2b) reduces to Eq. (2a) when the composition is spacially uniform.

(c) The local density ϱ is a conserved quantity that obeys the continuity equation

$$\partial_t \rho(\vec{q}, t) = -\nabla \cdot \vec{J}$$
$$\text{with current} \quad \vec{J} = -\frac{D_0}{2}\ \nabla \left(\frac{\delta f(\varrho)}{\delta\varrho} - \varepsilon^2\ \Delta\varrho \right)$$

Proof the following two assertions about this dynamics:
1. The overall concentration is invariant in a system with inpenetrable walls, i.e.

$$0 = \frac{\mathrm{d}}{\mathrm{d}t} \int_V \mathrm{d}^d q\ \varrho(\vec{q}, t)$$

2. The total free energy is a strictly decaying function until the system has reached a state where the current vanishes everywhere in space, i.e.,

$$0 \geq \frac{\mathrm{d}}{\mathrm{d}t} \mathcal{F}[\varrho]$$

and the equality holds only if $\vec{J}(\vec{x}, t) = 0$ for all $\vec{x} \in V$.[1]

(d) Show that the current takes the form

$$\vec{J} = D(\varrho(\vec{x}, t))\ \nabla\varrho(\vec{x}, t) \quad \text{with} \quad D(\varrho(\vec{x}, t)) = D_0\ \frac{3\varrho^2 - 1}{2}\,.$$

Hence, D_0 is the equilibrium diffusion coefficient.
However, in the range $-3^{-1/2} < \varrho < 3^{-1/2}$ the generalized diffusion coefficient $D(\varrho(\vec{x}, t))$ takes negative values. What does this imply for the stability of spatially uniform solutions?

[1](optional) The current vanishes when $\varrho(\vec{x})$ is either spatially uniform, or when it takes the form $\varrho(\vec{x}) = \operatorname{atanh}(\vec{k} \cdot \vec{x})$ with a constant vector $\vec{k}$ of appropriate length.

Exercise 3 *The Kramer's problem with a harmonic trap*

We consider the evolution of an ensemble of particles that diffuse in harmonic trap centered at $x = 0$ that has a cutoff to the right at a distance L from its center. The starting point of the discussion will be the evolution equation for the particle density, $\rho(x, t)$,

$$\partial_t \rho(x,t) = \gamma\, \partial_x (x\, \rho(x,t)) + D\, \partial_x^2 \rho(x,t) \tag{3a}$$

with initial condition

$$\rho(x, t = 0) = \delta(x - x_0) \tag{3b}$$

(a) Show that this initial condition will evolve into a Gaussian with time-dependent width

$$\rho(x,t) = \frac{1}{2\pi w(t)}\ \exp\left[-\frac{x^2}{2\, w(t)}\right] \tag{3c}$$

Insert Eq. (3c) into the Fokker-Planck equation, Eq. (3a) and show that

$$w(t) = \frac{D}{\gamma}\ \left(1 - \mathrm{e}^{-\gamma\, t}\right)$$

(b) The exit to the right can be taken into account by considering the constraint density

$$c(x,t) = \rho(x,t) - rho(2L - x, t)$$

(This strategy follows the use of image charges to account for grounded surfaces in electrodynamics.) The flux out of the trap will amount then to the current of the constraint density at $x = L$. Show that it takes the form

$$F(L,t) = J(L,t) = \gamma\, x\, c(x,t)\ \frac{2\, \mathrm{e}^{-2\gamma t}}{\mathrm{e}^{2\gamma t} - \mathrm{e}^{-2\gamma t}}$$

Plot the γt dependence of this function for different values of $\gamma x^2/D$.

(c) The expectation values for the moments of the waiting time till a particle escapes are related to the derivative of the Laplace transform

$$F(L,s) = \int_0^\infty \mathrm{d}t\, \mathrm{e}^{-st}\ F(L,t) \tag{3d}$$

of $F(L,t)$. Unfortunately, this function can not be determined in a closed form. However, the leading order dependence of the waiting time $\langle t \rangle$ on L can be obtained by adopting the substitution $t \to z = 1/w(t)$. This transformation turns $\exp(-x^2/2\, w(t))$ again into a Gaussian in the new variable z. As a consequence the dominant L dependence can be pulled out of the integral in Eq. (3d). What does this imply for the L-dependence of the waiting time?