

# Complementary Statistical Physics

## Homework Set 1: Brownian Motion

This problem set reviews microscopic and Brownian time scales, free diffusion, random walks, first-passage processes, Brownian motion under external forces, relaxation in a confining potential, and data-driven identification of stochastic dynamics. Show the essential steps in each analytical calculation. For numerical problems, state the parameters used and explain how the numerical results are compared with the analytical predictions.

### Useful notation and relations

For overdamped one-dimensional Brownian motion in a potential  $U(x)$ ,

$$\dot{x} = -\mu \frac{dU}{dx} + \sqrt{2D} \xi(t),$$

where

$$\langle \xi(t) \rangle = 0, \quad \langle \xi(t) \xi(t') \rangle = \delta(t - t').$$

The corresponding Fokker-Planck equation is

$$\frac{\partial \rho}{\partial t} = \frac{\partial}{\partial x} \left[ \mu \frac{dU}{dx} \rho \right] + D \frac{\partial^2 \rho}{\partial x^2},$$

At thermal equilibrium,

$$D = \mu k_B T.$$

### A. Brownian time scales and free diffusion

#### Problem 1. Microscopic and Brownian time scales

Consider a spherical Brownian particle of radius

$$R = 1 \mu\text{m}$$

suspended in air at room temperature and atmospheric pressure. For order-of-magnitude estimates use

$$d = 3 \times 10^{-8} \text{ cm}, \quad v_{\text{th}} = 5 \times 10^4 \text{ cm s}^{-1}, \\ n = 3 \times 10^{19} \text{ cm}^{-3}, \quad \eta = 1.8 \times 10^{-4} \text{ P}, \quad \rho_p = 1 \text{ g cm}^{-3}.$$

**a)** Estimate the duration  $\tau$  of one molecule-particle interaction from

$$\tau \sim \frac{d}{v_{\text{th}}}.$$

**b)** The molecular flux incident on a unit area is approximately

$$j \simeq \frac{n v_{\text{th}}}{4}.$$

Use this result to estimate the total rate of molecular impacts on the surface of the Brownian particle and hence the mean interval  $\tau'$  between the beginnings of successive molecular interactions.

c) Estimate the Brownian momentum-relaxation time

$$\tau_p = \frac{m}{\gamma},$$

using

$$m = \frac{4}{3}\pi R^3 \rho_p, \quad \gamma = 6\pi\eta R.$$

d) Compare the three time scales and verify the hierarchy

$$\tau' \ll \tau \ll \tau_p.$$

Explain physically why the interval  $\tau'$  between the beginnings of successive molecular interactions can be much shorter than the duration  $\tau$  of one individual interaction.

## Problem 2. Free one-dimensional diffusion

A free Brownian particle moves on the whole real axis. Its probability density satisfies

$$\frac{\partial \rho(x, t)}{\partial t} = D \frac{\partial^2 \rho(x, t)}{\partial x^2}, \quad -\infty < x < \infty,$$

with the initial condition

$$\rho(x, 0) = \delta(x).$$

a) Solve the Fokker–Planck equation and determine  $\rho(x, t)$ .

b) Verify explicitly that the solution remains normalised for every  $t > 0$ .

c) Plot  $\rho(x, t)$  as a function of  $x$  for several values of  $t$ .

d) Calculate the moments

$$\langle x^n(t) \rangle = \int_{-\infty}^{\infty} x^n \rho(x, t) dx.$$

Determine separately the result for odd and even  $n$ .

e) In particular, determine  $\langle x(t) \rangle$  and  $\langle x^2(t) \rangle$ , and identify the mean-square displacement.

## Problem 3. Random walk on a two-dimensional square lattice

Consider a random walker on an infinite two-dimensional square lattice with lattice spacing  $a$ . Initially,

$$(x_0, y_0) = (0, 0).$$

At every discrete time step the walker jumps by one lattice spacing to one of the four nearest-neighbour sites, each with probability  $1/4$ .

a) Generate  $M$  independent trajectories containing  $N$  jumps each.

b) Calculate the ensemble-averaged mean-square displacement

$$\langle r_N^2 \rangle = \langle x_N^2 + y_N^2 \rangle.$$

c) Plot  $\langle r_N^2 \rangle$  as a function of  $N$  and determine its dependence on  $N$ .

d) If one lattice step corresponds to a time interval  $\Delta t$ , write

$$t = N\Delta t$$

and compare the result with the two-dimensional Brownian-motion relation

$$\langle r^2(t) \rangle = 4Dt.$$

Determine the diffusion coefficient  $D$  in terms of  $a$  and  $\Delta t$ .

e) For a sufficiently large value of  $N$ , construct a histogram of the  $x$ -coordinates of the walkers and compare its shape with the Gaussian distribution predicted by the continuum diffusion equation.

## B. First-passage processes

### Problem 4. First passage to a point

A free one-dimensional Brownian particle starts at

$$x(0) = 0.$$

Let  $a > 0$  be a fixed target position. Determine the probability density  $f_a(t)$  such that

$$f_a(t) dt$$

is the probability that the particle reaches  $x = a$  for the first time between  $t$  and  $t + dt$ .

a) Derive  $f_a(t)$ .

b) Verify that

$$\int_0^\infty f_a(t) dt = 1.$$

c) Determine the large- $t$  behaviour of  $f_a(t)$ .

d) Calculate the mean first-passage time

$$\langle T \rangle = \int_0^\infty t f_a(t) dt.$$

Does the fact that the particle reaches  $x = a$  with probability one imply that the mean first-passage time is finite?

### Problem 5. Escape from a finite interval

A Brownian particle diffuses freely in the interval

$$0 < x < L,$$

with absorbing boundaries at  $x = 0$  and  $x = L$ . The particle starts at

$$x = x_0, \quad 0 < x_0 < L.$$

- a)** Let  $q(x_0)$  be the probability that the particle reaches  $x = L$  before it reaches  $x = 0$ . Derive the differential equation satisfied by  $q(x_0)$ , apply the appropriate boundary conditions, and determine  $q(x_0)$ .
- b)** Let  $T(x_0)$  be the mean time required to reach either boundary for the first time. Derive the differential equation satisfied by  $T(x_0)$  and solve it subject to

$$T(0) = T(L) = 0.$$

- c)** Determine the initial position  $x_0$  for which the mean exit time is maximal, and determine this maximal mean exit time.

## C. Brownian motion under external forces

### Problem 6. Brownian sedimentation in a constant gravitational field

Let the  $x$ -axis point vertically upward. A Brownian particle of mass  $m$  moves on the whole real axis in the gravitational potential

$$U(x) = mgx.$$

Initially,

$$x(0) = x_0.$$

- a)** Write the corresponding Fokker–Planck equation and solve it for

$$\rho(x, 0) = \delta(x - x_0).$$

- b)** Determine the mean position  $\langle x(t) \rangle$  and the variance

$$\sigma^2(t) = \langle [x - \langle x(t) \rangle]^2 \rangle.$$

- c)** Plot  $\rho(x, t)$  for several values of  $t$ . Identify separately the systematic gravitational drift and the diffusive broadening of the distribution. Does the system on the whole real axis possess a normalisable equilibrium distribution? Explain.

### Problem 7. Brownian particle in a harmonic trap

A Brownian particle moves in the harmonic potential

$$U(x) = \frac{1}{2} \kappa x^2.$$

At  $t = 0$ ,

$$\rho(x, 0) = \delta(x - x_0).$$

- a)** Write the corresponding Fokker–Planck equation and show that the probability distribution remains Gaussian.
- b)** Determine the time-dependent mean  $\langle x(t) \rangle$  and variance

$$\sigma^2(t) = \langle [x - \langle x(t) \rangle]^2 \rangle.$$

c) Determine the long-time probability distribution and show that it agrees with the Boltzmann distribution

$$\rho_{\text{eq}}(x) \propto \exp \left[ -\frac{U(x)}{k_B T} \right].$$

Identify the characteristic relaxation time of the trapped Brownian particle.

## D. AI-assisted identification of Brownian dynamics

### Problem 8. Inferring Brownian dynamics from trajectory data

Two accompanying datasets, A and B, contain ensembles of trajectories  $x(t)$  generated by two unknown one-dimensional stochastic processes. Assume that each process can be described by

$$\dot{x} = A(x) + \sqrt{2D} \xi(t),$$

where

$$\langle \xi(t) \rangle = 0, \quad \langle \xi(t) \xi(t') \rangle = \delta(t - t').$$

The drift  $A(x)$  and diffusion coefficient  $D$  are unknown.

**a) AI-assisted model identification.** Provide each dataset to a generative-AI system and ask it to determine whether the data are most consistent with

$$A(x) = 0, \quad A(x) = v, \quad \text{or} \quad A(x) = -\lambda x.$$

For each dataset, ask the AI to identify the most likely model, estimate the relevant parameter or parameters, and state which statistical properties of the trajectory data support its conclusion. Include the prompt and the AI response in your submission.

**b) Independent determination of drift and diffusion.** For a short time interval  $\Delta t$ , define

$$\Delta x = x(t + \Delta t) - x(t).$$

Divide the observed range of  $x$  into small intervals. For a bin centred at  $x$ , collect all increments  $\Delta x_i$  whose initial position lies in that bin. If  $N_x$  such increments are found, define

$$\langle \Delta x \mid x \rangle = \frac{1}{N_x} \sum_{i=1}^{N_x} \Delta x_i.$$

Estimate the drift from

$$A(x) \simeq \frac{\langle \Delta x \mid x \rangle}{\Delta t},$$

and estimate the diffusion coefficient from the fluctuations about this mean,

$$D(x) \simeq \frac{1}{2\Delta t} \frac{1}{N_x} \sum_{i=1}^{N_x} [\Delta x_i - \langle \Delta x \mid x \rangle]^2.$$

Plot the numerical estimates of  $A(x)$  and  $D(x)$ . Fit the measured drift to the three candidate forms above and determine which model gives the best description of each dataset. Estimate the corresponding parameter  $\nu$  or  $\lambda$ . Determine whether  $D(x)$  is consistent with a constant diffusion coefficient.

**c) Independent test of the fitted model.** Using the parametric model and parameter values obtained in part (b), derive the predicted time dependence of the ensemble mean

$$\langle x(t) \rangle$$

and the variance

$$\sigma^2(t) = \langle [x(t) - \langle x(t) \rangle]^2 \rangle.$$

Determine these two quantities directly from the supplied trajectories and compare them with the theoretical predictions. Decide whether the model inferred from the short-time increments in part (b) also describes the longer-time evolution of each dataset. Finally, compare your conclusion and parameter estimates with those proposed by the AI in part (a).