Blatt 5. Brownian Motion, Noise, and Fluctuations

The exercise marked by $\star$ and are challenge to think about, to be discussed when we discuss the solutions.

Problems

5.1. Brownian motion as a Markov process

For reference in this exercise the cumulants for Brownian motion are given in Appendix A of this exercise sheet. In another exercise we will show that Brownian motion is a Gaussian process, i.e., the probability distribution for Brownian motion is completely specified by the first two cumulants.

a) Show that the probabiltiy distribution $P(v,t|v_0,0)$ to find a velocity v at time t when it was v_0 at time 0 takes the form

$$P(v,t|v_0,0) = N(t)\ \exp\left[-\frac{\left(v - v_0\ \mathrm{e}^{-\lambda t}\right)^2}{\frac{2\,d}{\lambda}\left(1 - \mathrm{e}^{-2\lambda t}\right)}\right] ,$$

where $N(t)$ is an appropriate normalization of this conditional probability.
What is the appropriate normalization $N(t)$?
Hint: This expression assumes $\mathcal{C}_0(v,v) = 0$ and $\langle v_0 \rangle = v_0$. Why is this justified?

b) Under which condition on λ will Brownian motion become a Markov process for the velocities? What is special about the resulting conditional probability?

c) Adopt the limit $\lambda \to \infty$ at a fixed diffusion coefficient $D = d/\lambda^2$. Show that in this limit the probabiltiy distribution $P(x,t|x_0,0)$ to find the Brownian particle at position x at time t when it was at x_0 at time 0 takes the form

$$P(x,t|x_0,0) = (4\pi D t)^{-1/2}\ \exp\left[-\frac{(x - x_0)^2}{4\,D\,t}\right] . \tag{5.1}$$

d) Brownian motion is Markovian iff Eq. (5.1) satisfies the Chapman-Kolmogorov-criterion that for any set of times $t_1 < t_2 < t_3$ and positions x_1, x_2, x_3 one must have

$$P(x_3,t_3|x_1,t_1) = \int \mathrm{d}x_2\ P(x_3,t_3|x_2,t_2)\ P(x_2,t_2|x_1,t_1)$$

Verify that it holds!

5.2. Variance of positions in Brownian motion

In this exercise we derive the expression (A.1) for $\mathcal{C}_t(x,x)$ that is given in the appendix. We start from

$$x(t) = x_0 + \frac{v_0}{\lambda}\ \left(1 - \mathrm{e}^{-\lambda\,t}\right) + \int_0^t \mathrm{d}s_1\ \mathrm{e}^{-\lambda\,s_1}\ \int_0^{s_1} \mathrm{d}s_2\ A(s_2)\ \mathrm{e}^{\lambda\,s_2}$$

a) Introduce the function $W(s_1) = \int_0^{s_1} \mathrm{d}s_2 \; A(s_2) \, \mathrm{e}^{\lambda \, s_2}$ and use integration by parts to show that

$$x(t) = x_0 + \frac{v_0}{\lambda} \, \left(1 - \mathrm{e}^{-\lambda \, t}\right) + \lambda^{-1} \int_0^t \mathrm{d}s \, \left(1 - \mathrm{e}^{\lambda \, (s-t)}\right) \, A(s) \, . \tag{5.2a}$$

b) Use Eq. (5.2a) to evaluate

$$\mathcal{C}_t(x,x) = \left\langle \big(x(t) - \langle x(t) \rangle\big)^2 \right\rangle \, .$$

c) Show that in the limit of long times the resulting expression reduces to

$$\mathcal{C}_t(x,x) \simeq \left(\mathcal{C}_0(x,x) - \frac{D}{\lambda}\right) + \lambda^{-2} \, \left(\mathcal{C}_0(v,v) - \frac{d}{\lambda}\right) + 2 \, D \, t \tag{5.2b}$$

where we introduced the diffusion coefficient $D = d/\lambda^2$.
Provide an interpretation for the three contributions to this expression.

d) The result Eq. (5.2b) suggests that $\mathcal{C}_t(x,x)$ may take negetive values when $\mathcal{C}_0(x,x) = \mathcal{C}_0(v,v) = 0$ and small t.
What is wrong about this argument?
Find the expression that should rather be considered to discuss this special case of $\mathcal{C}_t(x,x)$.

5.3. Covariance of position and velocity for Brownian motion

a) Determine the covariance

$$\mathcal{C}_t(x,v) = \big\langle \big(x(t) - \langle x(t) \rangle\big) \, \big(v(t) - \langle v(t) \rangle\big) \big\rangle \, .$$

b) Compare the result to the variance $\mathcal{C}_t(v,v)$. What do you observe?

c) For an equilibrated velocity ensemble, where $\mathcal{C}_0(v,v) = 0$, the asymptotics for large and small times becomes

$$\mathcal{C}_t(x,v) \simeq \begin{cases} dt/\lambda & \text{for} \quad \lambda \, t \ll 1 \, , \\ d/\lambda^2 & \text{for} \quad \lambda \, t \gg 1 \, . \end{cases}$$

What does this mean physically?
Which interpretation does this suggest for the diffusion coefficient $D = d/\lambda^2$?

5.4. Noise spectrum for measured noise

The relation between the fluctuations $\alpha(t)$ of an observable $\Omega(t)$, and the flucutations $\alpha_{\text{out}}(t)$ in the measured signal $\Omega_{\text{out}}(t)$ can be expressed through a filter, $K(t)$,

$$\alpha_{\text{out}}(t) = \int_{-\infty}^t K(t-s) \, \alpha(s) \, \mathrm{d}s \, .$$

a) Causality implies that $K(t) = 0$ for $t < 0$. What does this imply for the integral

$$\int_{-\infty}^{\infty} K(t-s) \, \alpha(s) \, \mathrm{d}s \, ?$$

b) Let $\alpha(\omega)$ and $\alpha_{\text{out}}(\omega)$ be the Fourier transforms of $\alpha(t)$ and $\alpha_{\text{out}}(t)$. Show that

$$\alpha_{\text{out}}(\omega) = k(\omega)\ \alpha(\omega)\,.$$

Determine $k(\omega)$.

c) Let $G(x)$, $x \in \{\alpha(t), \alpha_{\text{out}}(t)$ be the average noise intensity

$$G(x) = \lim_{T\to\infty} \frac{1}{2T} \int_{t_0-T}^{t_0+T} |x|^2 \, \mathrm{d}t\,.$$

Under which condition will $G(x)$ *not* depend on t_0? Show that

$$G(\alpha_{\text{out}}) = |k(\omega)|^2\ G(\alpha)\,.$$

d) For an ideal measurement one would like to approach $G(\alpha_{\text{out}}) = G(\alpha)$ as closely as possible. What does this imply for the filter function $K(t)$?

5.5. Fluctuation relations

In 1999 Lebowitz and Spohn established a very powerful symmetry relation that holds for fluctuations in stochastic dynamics.[1] It applies to fluctuations of the observable $\sigma^j_k = \ln\big(r^j_k / r^k_j\big)$ for a Markov process with dynamically reversible transition rates r^j_k between the states j and k. Let $\tau(t)$ we a trajectory of this process, and $\Sigma(\tau, t)$ the value observed when σ^j_k is integrated along the trajectory. Then the theorem states that the cumulant generating function, $Z(\mathbf{q})$, for the cumulants of the distribution of $\Sigma(\tau, t)$ obeys the symmetry

$$Z(\mathbf{q}) = Z(\mathbf{1} - \mathbf{q}) \tag{5.5a}$$

where $\mathbf{1}$ is the vector whose entries are all one.

⋆ a) Take a look into the Lebowitz/Spohn paper, and provide a qualitative argument why the theorem holds.
Hint: The proof is easier when one rather considers the observable

$$\omega^j_k = \ln \frac{p_j r^j_k}{p_k r^k_j}\,,$$

where p_j is the steady-state probability density of state p_j.
Where does this help? Why is it admissible?

b) Verify that Equation (5.5a) entails the following fluctuation relation for the probability $P(\Sigma, t)$ to find the value Σ for $\Sigma(\tau, t)$:

$$\lim_{t\to\infty} \ln \frac{P(\Sigma, t)}{P(-\Sigma, t)} = \Sigma\,. \tag{5.5b}$$

c) Check that the fluctuation relation (5.5b) holds trivially for

[1] Joel L. Lebowitz and Herbert Spohn: *A Gallavotti-Cohen-Type Symmetry in the Large Deviation Functional for Stochastic Dynamics.* Journal of Statistical Physics **95** (1999) 333–365.

- the displacement in a random walk on a line with probabilities r and l to take a step to the right and left, respectively. Steps are taken at integer times and $r + l < 1$.
- the displacement in a random walk on a line with rates r and l to take a step to the right and left, respectively.
- a Gaussian distribution.

d) Provide a sketch of the distribution and provide a geometric interpretation of the fluctuation relation.

5.6. Estimating the diffusive displacement

In 1879 Nageli[2] dismissed the role of molecular collisions as origin of Brownian motion. In this exercise we revisit his argument that is based on his estimate of the speed, $U_B \simeq 1\,\mu\text{m/s}$, of a Brownian particles with a diameter of about $R_B \simeq 2\,\mu\text{m}$.

a) According to Stokes' law the friction force on a solid spherical particle is

$$F_S = 6\pi\, R_B\, \rho_s\, \nu_s\, U_B$$

where ρ_s and ν_s are the density and the kinematic viscosity of the surrounding fluid, respectively. For water they take the values $\rho_s \simeq 1 \times 10^3\,\text{kg}\,\text{m}^{-3}$ and $\nu_s \simeq 1 \times 10^{-6}\,\text{m}^2/\text{s}$. Show that for these parameters the damping takes the value $\lambda \simeq 1 \times 10^6\,\text{s}^{-1}$.
Bonus: Note that smaller particles have a larger damping. Which radius will result in the damping $\lambda \simeq 1 \times 10^7\,\text{s}^{-1}$ that was quoted in the lecture?

b) When the particle is at thermal equilibrium it should have a velocity U_E

$$\frac{1}{2}\,\frac{4\pi\rho_B R_B^3}{3}\,U_E^2 = \frac{3}{2}\,k_B\,T$$

Estimate U_E for a particle that has roughly the same density as water.

c) Assume that water molecules have an effective radius of about $R_w \simeq 4 \times 10^{-10}\,\text{m}$. What would the momentum balance

$$M_B U_B \simeq M_w U_w$$

imply about typical verlocity U_B for our Brownian particle when it collides with water molecules in thermal equilibrium?

d) Show that the diffusion coefficient takes a value of the order to $D \simeq 1 \times 10^{-13}\,\text{m}^2/\text{s}$, and calculate the diffusive displacement $\Delta X(t) = 2\,D\,t$ for time intervals $t = 0.1, 1.0, 10, 100\,\text{s}$.

e) Compare now Nageli's estimate of $U = 1 \times 10^{-6}\,\text{m}\,\text{s}^{-1}$ to the velocity $U_t = \Delta X(t)/t$.
What does this imply about the time and space resolution of Nageli's observation?
Observe also that $U_E > U_t > U_P$. Why would one expect this relation?

[2] K. von Nageli, Sitzungsberichte der Königlich Bayrischen Akademie der Wissenschaften München, Mathematisch-physikalische Klasse **9** (1879) 389–453.

A Cumulants for Brownian Motion

Velocity

$$v(t) = v_0\, \mathrm{e}^{-\lambda\, t} + \int_0^t \mathrm{d}s\; A(s)\; \mathrm{e}^{\lambda\,(s-t)}$$

$$\begin{aligned}
\text{with}\;\;\text{velocity}\quad & v(t) \quad \text{at time } t \\
& v_0 \quad \text{at initial time } 0 \\
\text{relaxation rate}\quad & \lambda \\
\text{random forces}\quad & A(t) \\
\text{where}\quad & \langle A(t) \rangle = 0 \\
\text{where}\quad & \langle A(t_1)\, A(t_2) \rangle = 2\, d\, \delta(t_1 - t_2)
\end{aligned}$$

Expectation

$$\mathcal{C}_t(v) = \langle v(t) \rangle = \langle v_0 \rangle\; \mathrm{e}^{-\lambda\, t} + \int_0^t \mathrm{d}s\; \langle A(s) \rangle\; \mathrm{e}^{\lambda\,(s-t)} = \langle v_0 \rangle\; \mathrm{e}^{-\lambda\, t}$$

Starting from its initial value $\langle v_0 \rangle$ the expectation decays exponentially to zero.

Variance

$$\begin{aligned}
\mathcal{C}_t(v,v) &= \left\langle (v(t) - \langle v(t) \rangle)^2 \right\rangle = \left\langle \left((v_0 - \langle v_0 \rangle)\; \mathrm{e}^{-\lambda t} + \int_0^t \mathrm{d}s\; A(s)\; \mathrm{e}^{\lambda\,(s-t)} \right)^2 \right\rangle \\
&= \left\langle (v_0 - \langle v_0 \rangle)^2 \right\rangle\; \mathrm{e}^{-2\lambda t} + 2\, \mathrm{e}^{-\lambda t} \int_0^t \mathrm{d}s\; \left\langle (v_0 - \langle v_0 \rangle) A(s) \right\rangle\; \mathrm{e}^{\lambda\,(s-t)} + \left\langle \left(\int_0^t \mathrm{d}s\; A(s)\; \mathrm{e}^{\lambda\,(s-t)} \right)^2 \right\rangle \\
&= \mathcal{C}_0(v,v)\; \mathrm{e}^{-2\lambda t} + \int_0^t \mathrm{d}s_1\; \mathrm{e}^{\lambda\,(s_1-t)} \int_0^t \mathrm{d}s_2\; \mathrm{e}^{\lambda\,(s_2-t)}\; \langle A(s_1)\; A(s_2) \rangle \\
&= \mathcal{C}_0(v,v)\; \mathrm{e}^{-2\lambda t} + 2\, d \int_0^t \mathrm{d}s_2\; \mathrm{e}^{2\,\lambda\,(s_2-t)} \\
&= \left(\mathcal{C}_0(v,v) - \frac{d}{\lambda} \right)\; \mathrm{e}^{-2\lambda t} + \frac{d}{\lambda}
\end{aligned}$$

Starting from ints initial value $\mathcal{C}_0(v,v)$ the variance decays exponentially to the value d/λ.

Position

$$x(t) = x_0 + \int_0^t \mathrm{d}s\; v(s) = x_0 + \frac{v_0}{\lambda}\; \left(1 - \mathrm{e}^{-\lambda\, t}\right) + \int_0^t \mathrm{d}s_1 \int_0^{s_1} \mathrm{d}s_2\; A(s_2)\; \mathrm{e}^{\lambda\,(s_2-s_1)}$$

Expectation

$$\mathcal{C}_t(x) = \langle x(t) \rangle = \langle x_0 \rangle + \frac{\langle v_0 \rangle}{\lambda} \, \left(1 - \mathrm{e}^{-\lambda\, t}\right)$$

When the expectation of the velocity in the initial ensemble vanishes, $\langle v_0 \rangle = 0$, the expectation of the position remains constant at $\langle x_0 \rangle$. Otherwise, it decays exponentially to its asymptotic value $\langle x_0 \rangle + \langle v_0 \rangle / \lambda$.

Variance

$$\begin{aligned} \mathcal{C}_t(x,x) &= \left\langle \left(x(t) - \langle x(t) \rangle\right)^2 \right\rangle \\ &= \mathcal{C}_0(x,x) + \frac{\left(1 - \mathrm{e}^{-\lambda\, t}\right)^2}{\lambda^2} \, \left(\mathcal{C}_0(v,v) - \frac{d}{\lambda}\right) + \frac{2\, d}{\lambda^3} \left(\lambda\, t - \left(1 - \mathrm{e}^{-\lambda\, t}\right)\right) \end{aligned} \tag{A.1}$$

The derivation and interpretation is given as an 5.1.