Nonequilibrium & Active Systems

Exercises for understanding and training

PCS Master 2 program

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Contents

The sequence of sections follows the chapters of the lectures. Some of the problems will not be presented during the tutorials. Solutions to the problems will be posted at the end of each chapter. Questions on the exercises, before and/or after the live session devoted to solving them, are of course very welcome.

1 Equilibrium Statistical Dynamics

1.1 On and around molecular chaos, Kac's ring

This exercise is a translation of the Kac's ring subsection in the book by Dorfman [9]. It is a toy model illustrating the moelcular chaos hypothesis. In short, it is a toy model helpful in understanding what is at stake if we wanted to prove (instead of postulating) equilibrium statistical mechanics.

We consider a one-dimensional ring with N points, and thus N intervals, with periodic boundary conditions. Each interval between two points contains a ball, which is either black or white. At each time step, all balls shift their position by one unit clockwise. On a fraction of the sites, there exists and operator acting on the color of the ball that hops across the site in question by swapping its color before and after the hop. We are interested in the number of balls of each color after t steps. The number of white balls is $W(t)$ and the number of black balls is $B(t)$. The number of white and black balls right before an operator are denoted by $w(t)$ and $b(t)$. We also introduce $\Delta = B - W$.

1. Write the relationship between $B(t+1)$ and $B(t)$, $w(t)$, $b(t)$. Write a similar equation for $W(t+1)$.
2. Deduce a relationship between $\Delta(t+1)$, $\Delta(t)$, $b(t)$ and $w(t)$.
3. We now assume that the fraction of black or white balls that change color at time t equals the probability μ that an operator is present at a given site (that's the assumption that mimics molecular chaos). Implement this assumption and find $\Delta(t)$ as a function of $\Delta(0)$, μ and t.
4. Consider the time reversal transformation $t \to -t$ and consider the particular time $t_r = 2N$. Which properties of the system are broken by the explicit solution found in question 3?
5. We now consider an ensemble of Kac's rings with the same initial ball distribution, though the operators are distributed randomly over the different rings (drawn from the same probability distribution). For a given ring, let $\eta_i(t) = \pm 1$ according to whether a black/white ball lies just before site i, and let $\varepsilon_i = \pm 1$ according to whether there exists, or not, an operator at site i. Express $\Delta(t)$ as a function of the $\eta_i(t)$'s and relate $\eta_{i+1}(t+1)$ to $\eta_i(t)$.
6. Prove that
$$\langle \Delta(t) = \langle \varepsilon_1 ... \varepsilon_t \rangle \Delta(0) \tag{1}$$
where the average brackets $\langle \dots \rangle$ denote an ensemble average over all rings.
7. Show that for $0 \leq t \leq N$ the ensemble average $\langle \Delta(t) \rangle$ is the same as the $\Delta(t)$ found in question 3. What is happening for $2N \geq t \geq N+1$?

8. What lessons can one draw from the above calculations?

2 The Langevin Equation

2.1 Recipe for a Gaussian white noise

This is an exercise from Van Kampen's book [21]. The goal of this exercise is to show that a Gaussian white noise can be seen as the limiting process of a family of continuous time random signals. We consider a sequence of times t_i randomly distributed with a density ν along the time axis. Let the c_i be identically distributed independent random numbers, with zero average and finite moments, associated to each t_i. Finally, let $\psi(t)$ be a nonnegative function such that $\int \mathrm{d}x\psi(x) = 1$. We consider the random process

$$x(t) = \frac{1}{\sqrt{\nu}} \sum_i c_i \frac{1}{\tau} \psi(\frac{t - t_i}{\tau}) \tag{4}$$

Prove that in the

$$\tau \to 0, \qquad \nu \to \infty \tag{5}$$

limit, the process $x(t)$ is a Gaussian white noise. It may be useful to first determine the generating functional of $x(t)$.

2.2 A white, but non-Gaussian, noise

Consider the time interval $[0, t_{\text{obs}}]$ and the let $\eta(t) = \sum_{i=1}^{n} \ell_i \delta(t - t_i)$ be defined over that interval. Here n is a random integer drawn from a Poisson distribution with average νt_{obs} ($\nu > 0$ is a parameter). The ℓ_i's are random numbers drawn from a probability density $\pi(\ell)$ (to make things simpler, we'll assume $\langle \ell_i \rangle = 0$), and the t_i's are uniform random times in the $[0, t_{\text{obs}}]$ interval.

1. Show that the generating functional $G[h] = \langle \exp\left(\int_0^{t_{\text{obs}}} \mathrm{d}t h(t)\eta(t)\right)\rangle$ of the noise has the expression

$$G[h] = \exp\left[\nu \int_0^{t_{\text{obs}}} \mathrm{d}t \left(\langle \mathrm{e}^{h(t)\ell} \rangle_\pi - 1\right)\right] \tag{11}$$

   where $\langle \ldots \rangle_\pi = \int \mathrm{d}\ell \pi(\ell) \ldots$.

2. Show that $\langle \eta(t_1) \ldots \eta(t_n) \rangle_c = \nu \langle \ell^n \rangle_\pi \delta(t_1 - t_2) \ldots \delta(t_{n-1} - t_n)$.

3. Under which conditions (on ν and on the random numbers ℓ) does η become a Gaussian white noise?

4. Let $\Delta\eta = \int_t^{t+\Delta t} \eta(t')\mathrm{d}t'$. Express $\lim_{\Delta t \to 0} \frac{\langle \Delta\eta^k \rangle}{\Delta t}$ in terms of the moments of ℓ.

2.3 Translational Brownian motion

In the overdamped and Markov approximation, the Brownian motion of a particle in a bath is described by a stochastic differential equation of the form

$$\dot{x} = \sqrt{2\mu T}\eta,\ \langle \eta(t)\eta(t')\rangle = \delta(t-t') \tag{19}$$

where η is a Gaussian white noise. We work in one space dimension for simplicity.

1. What is the diffusion constant D of the particle? What would be the expression of D in higher space dimension if each component of the position independently evolved as in Eq. (19).

2. Is x a stationary process? Determine $\langle x(t)x(t')\rangle$.

3. In a variety if situations pertaining to mathematical finance [25], or the physics of disordered systems [6] or to nonequilibrium chemical processes [16], one is led to consider an observable z which is an exponential functional of a Brownian motion:

$$z(t) = \int_0^{+\infty} \mathrm{e}^{-t+gx(t)}\mathrm{d}t \tag{20}$$

   where g is a given constant. Determine $\langle z\rangle$ as a function of g and D (when $\langle z\rangle$ actually exists).

4. Determine $\langle z^2\rangle$ as a function of g^2D.

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2.4 Langevin equation for a classical magnet

In the book by Coffey and Kalmykov [4] a large section is devoted to the study of rotational Brownian motion. This applies to the modeling of mesoscopic magnets, electric dipoles, but also to liquid crystals or other elongated particles such as an E. coli bacterium. The physics of magnetism is of course of quantum origin, but it is possible to describe the thermal fluctuations of a small single domain of ferromagnetic particles using classical physics. Because information storage relies on the magnetic domains being able to retain their magnetization, in order to increase the amount of information stored, achieving ever smaller domains is of course a desired goal. However, for small enough domains, the possibility that thermal fluctuations actually destroy existing order cannot be overlooked [3, 5]. Hence the importance of understanding the interplay of thermal fluctuations with the dynamics of a single mesoscopic magnet.

In this problem, we first explore how rotational Brownian motion is described by a Langevin equation, and then we look at the specifics of the dynamics of a mesoscopic magnet.

1. Consider a particle characterized by its position $\mathbf{R}$ and by a unit vector $\mathbf{u}$ that fully characterizes its orientation in space. The particle is assumed to be in contact with a thermal bath, and it is in some external potential $V_0(\mathbf{R}, \mathbf{u})$ that may act both on the translational and rotational degrees of freedom. Under what assumptions can we write the effective dynamics of $\mathbf{R}$ as stochastic differential equation of the form

$$\frac{\mathrm{d}\mathbf{R}}{\mathrm{d}t} = -\mu \frac{\partial V_0}{\partial \mathbf{R}} + \sqrt{2\mu T}\boldsymbol{\eta} \tag{23}$$

where $\boldsymbol{\eta}$ is a Gaussian white noise with independent components, $\langle \eta^\mu(t)\eta^\nu(t')\rangle = \delta(t-t')$.

2. Let I be the inertia tensor of the particle and $\boldsymbol{\Omega}$ its rotation vector. Then the angular momentum $\mathbf{L} = I\boldsymbol{\Omega}$ evolves according to

$$\frac{\mathrm{d}\mathbf{L}}{\mathrm{d}t} = \boldsymbol{\Gamma}_0 + \boldsymbol{\Gamma}_b \tag{24}$$

where $\boldsymbol{\Gamma}_0$ and $\boldsymbol{\Gamma}_b$ are the torques exerted by the external operator and by the bath particles, respectively. Connect $\boldsymbol{\Gamma}_0$ to V_0.

3. When interested in the statistics of $\mathbf{R}$ and $\mathbf{u}$, it is possible to replace the individual degrees of freedom of the bath particles by the combination of a deterministic contribution and a random one. In your opinion, how does the average torque created by the bath, $\langle \boldsymbol{\Gamma}_b \rangle_b$, connect to the angular degrees of freedom? You should work within the Markov approximation where the time scale of the bath degrees of freedom is much shorter than any relevant time scale related to the particle of interest.

4. Let $\boldsymbol{\xi} = \boldsymbol{\Gamma}_b - \langle \boldsymbol{\Gamma}_b \rangle_b$. What can you say about the statistics of $\boldsymbol{\xi}$? How about $\langle \xi^\mu(t)\xi^\nu(t')\rangle$?

5. Express $\frac{\mathrm{d}\mathbf{u}}{\mathrm{d}t}$ in terms of $\boldsymbol{\Omega}$ and $\mathbf{u}$.

6. Find a Langevin equation for $\mathbf{u}$ within the approximation in which the time scale τ_{inertia} related to inertia is also much shorter than any relevant time scale related to the particle of interest. Write the stochastic differential equation for $\mathbf{u}$ in the form

$$\frac{\mathrm{d}\mathbf{u}}{\mathrm{d}t} = \text{deterministic term } + \underbrace{\boldsymbol{\lambda}}_{\text{noise term with zero mean}} \tag{25}$$

What is the amplitude of the correlations of $\boldsymbol{\lambda}$ in terms of $\mathbf{u}$?

7. Assuming one can manipulate $\mathbf{u}$ as if it were a smoothly differentiable function, does your equation respect the $\mathbf{u}^2 = 1$ constraint?

8. We now get back to the magnetic problem of interest and consider a magnet with dipole $\mathbf{m} = m_0\mathbf{u}$ in some external field $\mathbf{B}$ (m_0 is fixed). The energy is $V_0 = -\mathbf{m} \cdot \mathbf{B}$. Translational degrees of freedom are not included in the description. Express $\boldsymbol{\Gamma}_0$ in terms of $\mathbf{m}$ and $\mathbf{B}$.

3 Stochastic Calculus

3.1 Differential calculus likes Stratonovich discretization

Consider a Langevin equation $\frac{\mathrm{d}x}{\mathrm{d}t} = A + B\xi$, where ξ is a Gaussian white noise with correlations $\langle \xi(t)\xi(t')\rangle = \delta(t-t')$. The multiplicative noise B is understood with the α discretization rule, namely according to

$$\Delta x = x(t+\Delta t) - x(t) = A(x(t) + \alpha \Delta x)\Delta t + B(x(t) + \alpha \Delta x)\Delta\xi,\ \Delta\xi = \int_t^{t+\Delta t} \mathrm{d}t' \xi(t') \quad (30)$$

In the above equation, in the rhs, the first term is of order Δt while the second one is of order $\sqrt{\Delta t}$.

1. Justify the above statement and show that an equivalent discretization reads

$$\Delta x = B(x(t))\Delta\xi + (A(x(t)\Delta t + \alpha B'(x(t))B(x(t))\Delta\xi^2) + \mathcal{O}(\Delta t^{3/2}) \quad (31)$$

2. Let $x \mapsto f(x)$ be an arbitrary function. Let $F(t) = f(x(t))$. Show that $\Delta F = F(t+\Delta t) - F(t)$ can be expressed as

$$\Delta F = B\Delta\xi f'(x(t)) + (A(x(t))\Delta t + \alpha B'(x(t))B(x(t))\Delta\xi^2) f'(x(t)) + \frac{1}{2}B^2(x(t))\Delta\xi^2 f''(x(t)) \quad (36)$$

   up to $\mathcal{O}(\Delta t^{3/2})$ terms.

3. If regular differential calculus was allowed, one could actually write that $\frac{\mathrm{d}F}{\mathrm{d}t} = f'\frac{\mathrm{d}x}{\mathrm{d}t}$, and hence that $\frac{\mathrm{d}F}{\mathrm{d}t} = f'A + f'B\xi$. Assuming this Langevin equation is written with an α' discretization rule, show that

$$\Delta F = f'B\Delta\xi + f'A\Delta t + \alpha'(f'B)'B\Delta\xi^2 + \mathcal{O}(\Delta t^{3/2}) \quad (39)$$

   where all functions are evaluated at time t.

4. What are the conditions on α and α' for the two expressions found in **2** and **3** for ΔF to match, irrespective of the function f?

5. Why is it legitimate to use differential calculus when working with the Stratonovich convention?

3.2 How "natural" is Stratonovich calculus?

In physics, a Langevin equation is always the result of a series of approximations. An obvious approximation is the existence of a diffusive limit, in which the typical length scale governing the evolution of the system is larger than the scale involved in its various changes throughout time (the size of the jump is smaller than the typical size of the process). But even before that diffusive limit, lies the Markov approximation, which is based on the separation of time scales between the (fast) ones characterizing the bath and entering the source of noise, and the (slow) ones related to the system of interest whose degrees of freedom are modeled. In the limit where memory effects induced by the time-correlations of the bath can be discarded, one gets a Markov approximation. In this exercise, we want to explore how an evolution equation with a noise displaying time correlations naturally leads, in the limit where these correlations are short-ranged, to a Langevin equation expressed in the Stratonovich discretization. This exercise echoes Sec. **IX.7** of Van Kampen's book [21].

1. Let $\Delta(t) = \frac{1}{2\tau}\mathrm{e}^{-|t|/\tau}$. Show that Δ converges to the δ distribution when $\tau \to 0$. It may be useful to consider $\int \mathrm{d}t \Delta(t) f(t)$ for an arbitrary function f in the $\tau \to 0$ limit.

2. Determine $\int_{t_0}^{t_0+\Delta t} \mathrm{d}s\mathrm{d}s' \Delta(s-s')$ at finite τ for t_0 and $\Delta > 0$ that are fixed. Determine the asymptotic behavior of that quantity in the $\tau \to 0$ and $\Delta t \to 0$ limits. Discuss the importance of the order of limits.

   Let $x(t)$ be a function evolving according to the following equation

   $$\frac{\mathrm{d}x}{\mathrm{d}t} = A(x(t)) + B(x(t))\eta(t) \tag{47}$$

   where η is a Gaussian process with time correlations $\langle \eta(t)\eta(t')\rangle = \Delta(t-t')$. Here A and B are arbitrary smooth functions of x.

3. Let $\Delta x = x(t_0+\Delta t) - x(t_0)$ for $\Delta t > 0$, t_0 and $x(t_0) = x_0$ being given. Explain why, at fixed $\tau > 0$, the process $x(t)$ remains a smoothly differentiable function (a physicist's argument would be to show that Δx is of order Δt, instead of being of order $\sqrt{\Delta t}$ in a standard Langevin equation).

4. Prove that $\lim_{\Delta t \to 0} \lim_{\tau \to 0} \frac{\langle \Delta x \rangle}{\Delta t} = A(x_0) + \frac{1}{2}B'(x_0)B(x_0)$.

5. Consider the α discretized Langevin equation $\dot{x} = A + B\eta$ where η is a white (delta correlated) noise. How should we choose α in order to recover the predictions of Eq. (47) in the $\tau \to 0$ limit?

3.3 Playing around with stochastic calculus

We consider a particle with position $\mathbf{r}$ evolving under the action of an external force field $\mathbf{F}(\mathbf{r})$ in contact with a thermal bath at temperature T:

$$\frac{\mathrm{d}\mathbf{r}}{\mathrm{d}t} = \mathbf{F} + \sqrt{2T}\boldsymbol{\eta} \tag{50}$$

where the space components $\eta^\mu(t)$ of $\boldsymbol{\eta}$ are independent white noises with unit variance: $\langle \eta^\mu(t)\eta^\nu(t')\rangle = \delta^{\mu\nu}\delta(t-t')$.

1. Let $W(t) = \int_0^t \mathrm{d}t \mathbf{F}\cdot\frac{\mathrm{d}\mathbf{r}}{\mathrm{d}t}$. What is the direct physical meaning of W? Explain in what sense W is the work exerted by the particle on its surrounding thermostat.

2. Write a stochastic evolution for W (aka Langevin equation) that couples to $\mathbf{r}$. If you did it right, this equation features a multiplicative noise. Write the equation in both the Ito and the Stratonovich forms.

3. Let $\mathscr{V} = \frac{\mathbf{r}^2}{2}$. Write a stochastic evolution for $\mathscr{V}$ that couples to $\mathbf{r}$. Write the equation in both the Itō and the Stratonovich forms. From this equation deduce that the pressure of an ideal gas of N identical Langevin particles is $P = NT/V$. (Hint: Think of the particle being trapped in a closed box of volume V and of $\mathbf{F}$ as being the force exerted by the wall.

4. First consider the conservative case where we have $\mathbf{F} = -\boldsymbol{\nabla} V$ (here V depends on $\mathbf{r}$ only). Write a stochastic evolution for V that couples to $\mathbf{r}$. Write the equation in both the Itō and the Stratonovich forms.

5. Second, consider $\mathbf{F} = -\boldsymbol{\nabla} V + \mathbf{f}$, where the force $\mathbf{f}$ stands for a (possibly time dependent) additional force (like that of an operator performing some action on the system). Between t and $t+\mathrm{d}t$, V varies by $\mathrm{d}V = V(\mathbf{r}(t+\mathrm{d}t)) - V(\mathbf{r}(t))$. Show that it is possible to write $\mathrm{d}V = \delta W + \delta Q$, where $\delta W = \mathbf{f}\cdot\frac{\mathrm{d}\mathbf{r}}{\mathrm{d}t}\mathrm{d}t$. What is the microscopic mechanical meaning of δQ? Does this relationship ring any bell?

3.4 Particle in contact with a thermostat

Our interest goes to a particle with unit mass in contact with a thermostat at temperature T and with friction coefficient γ. The velocity v of the particle evolves according to a Langevin equation

$$\frac{\mathrm{d}v}{\mathrm{d}t} = F \tag{65}$$

where the force F reads $F = -\gamma v + \sqrt{2\gamma T}\xi$, with ξ a Gaussian white noise with correlations $\langle \xi(t)\xi(t')\rangle = \delta(t-t')$. Let $E(t) = \frac{1}{2}v^2(t)$ be the particle's kinetic energy.

1. Write the evolution equation for the probability $p(v,t)$ that the particle has velocity v at time t.

2. Write a Langevin equation for $E(t)$ that couples to ξ.

3. Let t_0 be a given time at which the energy is $E(t_0)$ and let Δt be an infinistesimal time duration. Find $\frac{\langle E(t_0+\Delta t) - E(t_0)\rangle}{\Delta t}$ as a function of γ and of T.

4. What's the stationary value of $\langle v^2 \rangle = T$? Was that expected?

5. We define $W(t) = \int_0^t \mathrm{d}t\sqrt{2\gamma T}\xi v$. Can you endow W with some physical meaning? In the evolution equation for E found in **2**, not only does $\frac{\mathrm{d}W}{\mathrm{d}t}$ appear, but also some additional contribution the physical meaning of which will be given.

6. We set out to determine the large time behavior of the pdf of W. Write an evolution equation for the probability $p(v, W, t)$ that the particle has velocity v at time t, and that $W(t) = W$.

7. Fourier transform the equation found in **6** with respect to W, and prove that $\hat{p}(v, \lambda, t) = \int \mathrm{d}W \mathrm{e}^{-\lambda W} p(v, W, t)$ evolves according to

$$\partial_t \hat{p} = \text{part with no explicit dependence in } \lambda + \gamma T(\lambda^2 v^2 - \lambda)\hat{p} + 2\gamma T\lambda \partial_v(v\hat{p}) \quad (89)$$

8. Prove that $\hat{p}(v, \lambda, t) = \mathrm{e}^{t\psi(\lambda)}\mathrm{e}^{-av^2}$ is a solution. Express both a and ψ in terms of T, γ and λ.

9. Justify that the probability to get a value W at large times behaves as $P(W, t) \simeq \mathrm{e}^{t\pi(W/t)}$, where the function $\pi(w)$ will be related to $\psi(\lambda)$.

10. Qualitatively plot $\pi(w)$ as a function of w. Does this function possess any remarkable symmetry property? Comment on your finding.

4 The Fokker-Planck Equation

4.1 Heat flux in a two particle system

We consider two coupled, overdamped particles connected to two different thermal baths at temperatures T_1 and T_2, evolving according to

$$\dot{x}_1 = -\mu_1 \partial_{x_1} V(x_1 - x_2) + \sqrt{2\mu_1 T_1}\eta_1,\ \dot{x}_2 = -\mu_2 \partial_{x_2} V(x_1 - x_2) + \sqrt{2\mu_2 T_2}\eta_2 \quad (105)$$

where the Gaussian whites noises η_1 and η_2 are independent,

$$\langle \eta_i(t)\eta_j(t')\rangle = \delta_{ij}\delta(t - t'),\ i = 1, 2 \quad (106)$$

The temperatures T_1 and T_2 are not necessarily equal.

1. Let $A(x_1(t), x_2(t))$ be a physical quantity of interest. Explain why

$$\langle A \rangle = \int \mathrm{d}y_1 \mathrm{d}y_2 A(y_1, y_2)\langle \delta(y_1 - x_1(t))\delta(y_2 - x_2(t))\rangle \quad (107)$$

2. Find an evolution equation for the average $p(y_1, y_2, t) = \langle \delta(y_1 - x_1(t))\delta(y_2 - x_2(t)) \rangle$.

3. The coupling between the two systems is achieved by means of a quadratic potential $V(x_1 - x_2) = \frac{k}{2}(x_1 - x_2)^2$. Show that the dynamics of $z = x_1 - x_2$ is given by

$$\dot{z} = -\mu k z + \sqrt{2\mu T}\xi,\ \langle \xi(t)\xi(t') \rangle = \delta(t - t') \tag{110}$$

where ξ is a Gaussian white noise. Express μ and T in terms of known parameters.

4. What is the steady-state distribution $q(z)$ of z? Is it an equilibrium one?

5. Show $q(y_1 - y_2)$ is a stationary solution of the equation derived in question 2. Is this an acceptable solution?

6. How would you define the heat Q_1 received by particle 1 from the thermal bath at T_1?

7. Show that in the steady-state we have $\langle \frac{\mathrm{d}Q_1}{\mathrm{d}t} \rangle = -\langle \frac{\mathrm{d}Q_2}{\mathrm{d}t} \rangle$, and comment on this result.

4.2 Nonequilibrium driving of a single particle

Consider an overdamped Langevin equation for a particle with position $\mathbf{r}(t)$ evolving according to $\dot{\mathbf{r}} = -\partial_{\mathbf{r}} V + \sqrt{2T}\boldsymbol{\eta}$, where V is a given external potential, and where $\boldsymbol{\eta}$ is a Gaussian white noise with independent components, $\langle \eta_i(t)\eta_j(t') \rangle = \delta_{ij}\delta(t - t')$. We are working in a space of dimension d.

1. Write the Fokker-Planck equation for the probability density p ($p(\mathbf{x}, t)\mathrm{d}^d x = \mathrm{Prob}\{\mathbf{x} \leq \mathbf{r}(t) \leq \mathbf{x} + \mathrm{d}\mathbf{x}\}$).

2. Check by whatever means you like that the process is in equilibrium.

3. As a mathematical game (for now), suppose that we add a force $\delta\mathbf{F} = -A\partial_{\mathbf{r}} V$, where A is a d-dimensional skew symmetric matrix, so that now $\dot{\mathbf{r}} = -(\mathbf{1} + A)\partial_{\mathbf{r}} V + \sqrt{2T}\boldsymbol{\eta}$. Write the new Fokker-Planck equation and find out whether p_B is a stationary solution or not.

4. Show that with this extra force the stationary-state is not an equilibrium one. What is, in your opinion, the advantage of using such a fictitious and unphysical dynamical evolution, if any?

4.3 Gallavotti-Cohen theorem for a driven particle

A Brownian particle is subjected to both conservative force $-\partial_{\mathbf{r}} V$ and to nonconservative ones $\mathbf{f}$ and it evolves according to $\dot{\mathbf{r}} = -\partial_{\mathbf{r}} V + \mathbf{f} + \sqrt{2T}\boldsymbol{\eta}$ where $\boldsymbol{\eta}$ is a Gaussian white noise with independent components, $\langle \eta_i(t)\eta_j(t') \rangle = \delta_{ij}\delta(t - t')$

1. Let W such that $\frac{\mathrm{d}W}{\mathrm{d}t} \overset{1/2}{=} \mathbf{F} \cdot \dot{\mathbf{r}}$, with $\mathbf{F} = -\partial_{\mathbf{r}} V + \mathbf{f}$. What is the physical meaning of W? Rewrite $\frac{\mathrm{d}W}{\mathrm{d}t}$ in Itō form.

2. Write a Fokker-Plank equation for $p(\mathbf{r}, W, t)$. For $z \in \mathbb{C}$, determine an evolution equation for $\hat{p}(\mathbf{r}, z, t) = \int \mathrm{d}W \mathrm{e}^{-zW} p(\mathbf{r}, W, t)$ by identifying the operator $\mathbb{H}(z)$ such that $\partial_t \hat{p} = -\mathbb{H}\hat{p}$.

3. Verify that for z real we have $\mathbb{H}(z)^\dagger = \mathbb{H}(T^{-1} - z)$.

4. Let $P(W, t) = \int \mathrm{d}^d r p(\mathbf{r}, W, t)$ be the probability density to observe W. Show that if $\pi(w) = \lim_{t\to+\infty} \frac{1}{t} \ln P(w\, t, t)$ exists, then it must verify $\pi(w) - \pi(-w) = \beta w$.

5. Explain why the second law of thermodynamics amounts to $\langle W \rangle > 0$. Is there any truth/meaning to that statement at the level of fluctuating trajectories (without the averaging)?

5 Thermal ratchets and stochastic engines

5.1 Stochastic Stirling engine

A colloidal particle is in contact with a thermostat at temprature T and controled by optical tweezers imposing an external potential $V(\mathbf{r}) = k\frac{\mathbf{r}^2}{2}$ where $\mathbf{r}$ is the position of the particle. The particle is first equilibrated at temperature T_c within a trap characterized by a stiffness k_c. The stiffness is then varied to $k_h > k_c$ during an isothermal transformation. The next step is to increase the temperature up to T_h at fixed k_h. Then during an isothermal transformation the stiffness is brought back to k_c and the final step is, at fixed stiffness, to cool the system back to T_c.

1. Draw this cycle in a $(k, \langle x^2 \rangle)$ plane assuming that after each transformation each state is an equilibrium one. Why is this machine an engine?

2. Show that the efficiency $\mathcal{E}$ of the engine is expressed, in terms of T_c, T_h and $a = \frac{k_h}{k_c} > 1$ as
$$\mathcal{E} = \frac{(T_h - T_c)\ln a}{T_h - T_c + T_h \ln a} \tag{136}$$

3. Compare with the Carnot efficiency.

4. As implemented in [18], the thermal bath is now replaced with a bath of bacteria. Explain why it is reasonable to consider that the effective dynamics of the passive colloidal particle now becomes an active dynamics, say of the form $\dot{\mathbf{r}} = -\mu k \mathbf{r} + v_0 \mathbf{u}$, with $\mathbf{u}$ a unit vector that decorrelates exponentially fast over a time scale τ inherited from the motion of the bacteria ($\langle \mathbf{u}(t) \cdot \mathbf{u}(t') \rangle = \mathrm{e}^{-\frac{|t-t'|}{\tau}}$).

To make calculations easier, we now work in one space dimension.

5. If the above assumption is correct, the system is now far from equilibrium and temperature is an undefined concept. In the steady-state of the activated colloid (at fixed

k), we define $T_{\rm act}$ as $T_{\rm act} = k\langle x^2\rangle_{\rm ss}$. We can also define another energetic scale $T_{\rm diff} = v_0^2\tau/\mu$. What is the physical meaning of $T_{\rm diff}$. Show that

$$\frac{T_{\rm act}}{T_{\rm diff}} = \frac{1}{1+\Omega\tau} \tag{137}$$

where Ω is a function of k and μ to be determined.

6. The same cycle as before is now implemented. What is the new efficiency if isothermal processes are now replaced with iso-$T_{\rm act}$ processes? How about using $T_{\rm diff}$ instead?

6 Active particles

6.1 A run-and-tumble particle in an external potential

Finding the steady-state of an active particle in some external potential is a challenge on its own. For an RTP in one space dimension, some progress can be made. We begin by reviewing what happens for an RTP in some external confining potential V. The equation of motion for our RTP with position $r(t)$ is

$$\dot{r} = -\mu V'(r) + v_0 u \tag{138}$$

where $\mu > 0$ is the particle's mobility, $v_0 > 0$ and $u = \pm 1$ is a telegraphic noise flipping at a rate $(2\tau)^{-1}$.

1. What is the scaling limit for v_0 and τ that ensures that the steady-state of the particle is an equilibrium state of the Boltzmann form $P_{\rm eq}(r) \propto {\rm e}^{-\beta V(r)}$. Express β in terms of v_0, μ and τ.

2. Express the steady-state probability $P_{\rm ss}(r)$ in term of V.

3. Consider for this question only the particular case of a non-confining periodic potential. Is a steady particle current possible?

4. At fixed β but when $\tau \to 0$, the steady-state distribution can be cast in the form

$$P_{\rm ss}(x) \propto {\rm e}^{-\beta V_{\rm eff}(x)},\ V_{\rm eff}(x) = V(x) + \tau\delta V(x) + O(\tau^2) \tag{146}$$

Find δV as a functional of V.

6.2 An active particle in a quadratic well

We consider an active particle with position $\mathbf{r}$ evolving according to $\dot{\mathbf{r}} = \mathbf{v}(t) - \mu k\mathbf{r}$, where $\mathbf{v}$ is a self-propulsion velocity and μ is the particle's mobility. For mathematical simplicity we shall focus on the one-dimensional case.

1. When $v(t) = v_0 u(t)$, with v_0 fixed and $u(t) = \pm 1$ a telegraph process with flipping rate $\frac{1}{2\tau}$, the particle can travel a distance λ at most away from the origin. Express λ as a function of μ, k and v_0.

2. Write an evolution equation for the probability $p(x, u, t)$ to find the particle at position x with orientation u. Find $\langle u(t)u(t')\rangle$ as a function of t, t' and τ.

3. What is the steady-state probability $P_{ss}(x)$ to find the particle at a distance x? Express $P_{ss}(x)$ in terms of x, λ and in terms of the run length $\ell = v_0\tau$.

For the rest of this exercise we focus on an Active Ornstein-Uhlenbeck particle instead of a Run-and-Tumble one.

4. When the statistics of the self-propulsion force $v(t)/\mu$ is not of the run-and-tumble type, because the velocity amplitude can fluctuate, one usually writes that $v(t) = v_0 u$ where u evolves according to

$$\frac{\mathrm{d}u}{\mathrm{d}t} = -\frac{u}{\tau} + \sqrt{2a}\eta(t) \tag{149}$$

where η is a Gaussian white noise with correlations $\langle \eta(t)\eta(t')\rangle = \delta(t - t')$. Choose a so that $\langle u(t)u(t')\rangle$ is the same as in question 2 for a run and tumble particle.

5. Write the new Fokker-Planck equation for $p(x, u, t)$. Find the steady-state distribution $p_{ss}(x, u)$ and then $P_{ss}(x)$.

6. Is the process $(x(t), u(t))$ out of equilibrium? Is the process $x(t)$ out of equilibrium?

6.3 A one-dimensional run-and-tumble particle close to a hard wall

We consider a run-and-tumble particle in one-space dimension effectively confined between $x = 0$ and $x = L$, because at these positions an infinitely steep hard wall prevents the particles from going any further. Of course, the concept of a hard wall at $x = 0$ or at $x = L$ is an idealization. For instance, we can think of the left hard-wall at $x = 0$ as resulting from an external potential $V(x) = U_0 \mathrm{e}^{-x/\sigma}$ when $\sigma \to 0^+$ (which we assume throughout).

1. What is the smallest abscissa $\lambda(\sigma)$ at which the particle can be found?

2. Write the coupled master equations for $P_\pm(x) = P_{ss}(x, u = \pm)$. Integrate the latter equations between λ and $\lambda(1-\varepsilon)$ where $\varepsilon > 0$ is for now arbitrary. Take the $\sigma \to 0^+$ limit first, and then the $\varepsilon \to 0^+$ limit, and show that the solution P_- must possess a singular $\delta(x)$ component.

3. The hard-wall limit is now understood. Assuming that $P_+(x) = a + b\delta(L-x)$ and that $P_-(x) = c + d\delta(x)$, find the constants a, b, c and d as functions of L and $\ell = v_0\tau$.

4. Consider now two mutually excluding particles on a ring of size L. Find the steady-state probabilities $P_{\pm,\pm}(r)$ that particle 2 is a distance r to the right of particle 1.

7 Exam, 17/01/2023, 3 hours

7.1 One, and then two, oscillators

This problem considers one, and then two coupled oscillators. Consider first a single harmonic oscillator with position $x(t)$ in contact with one thermostat evolving according to the overdamped Langevin equation

$$\frac{\mathrm{d}x}{\mathrm{d}t} = -x + \sqrt{2T}\eta \tag{163}$$

where the mobility has been set to unity (which fixes the time unit), the temperature T is given, and η refers to a Gaussian white noise with correlations $\langle \eta(t)\eta(t')\rangle = \delta(t-t')$.

1. Let t_0 be some arbitrary time and $\Delta t > 0$. Let $\Delta\eta = \int_{t_0}^{t_0+\Delta t} \mathrm{d}t\eta(t)$. Determine $\langle \Delta\eta\rangle$ and $\langle \Delta\eta^2\rangle$ as functions of Δt.

2. Given an initial value $x(t_0)$, we study the process $x(t)$ over the $[t_0, t_0+\Delta t]$ time interval. We denote by $\Delta x = x(t_0+\Delta t) - x(t_0)$. Express the $\langle \Delta x\rangle$ and $\langle \Delta x^2\rangle$ averages in terms of $x(t_0)$ and Δt to leading order in $\Delta t \to 0$.

3. Deduce the Fokker-Planck equation for the probability density $p(x,t)$ ($p(x,t)\mathrm{d}x = \mathrm{Prob}\{x \le x(t) \le x + \mathrm{d}x\}$).

4. Determine $\langle x\rangle$ and $\langle x^2\rangle$ in the steady-state.

5. What is the steady-state probability density $p_{\mathrm{ss}}(x)$?

6. Explain why $p_{\mathrm{ss}}(x)$ is not just a stationary distribution, but that it is actually an equilibrium one.

7. Consider now the local fluctuating elastic energy $\varepsilon(t) = \frac{x^2}{2}$ stored in the oscillator. The Langevin equation for ε can be written in the form

$$\frac{\mathrm{d}\varepsilon}{\mathrm{d}t} = -2\varepsilon + T + 2\sqrt{T\varepsilon}\eta \tag{167}$$

   This is a Langevin equation with multiplicative noise. Explain in a few words why there is an ambiguity, and specify the correct way of understanding Eq. (167). Determine $\langle\varepsilon\rangle$ in equilibrium.

8. We now couple the particle to two heat baths with temperatures T_c and T_h

$$\frac{\mathrm{d}x}{\mathrm{d}t} = -x + \sqrt{T_c}\eta_c + \sqrt{T_h}\eta_h \tag{170}$$

   where η_c and η_h are δ correlated independent Gaussian white noises. Show that even if $T_h \ne T_c$ the oscillator is in equilibrium at some temperature T_{eff} to be given in terms of T_c and T_h.

Consider now two interacting oscillators with positions x and y coupled as follows:

$$\frac{\mathrm{d}x}{\mathrm{d}t} = -x - k(x-y) + \sqrt{2T_c}\eta_c,\ \frac{\mathrm{d}y}{\mathrm{d}t} = -y - k(y-x) + \sqrt{2T_h}\eta_h \tag{171}$$

where $k > 0$ is a spring constant.

9. Let $V(x,y) = \frac{x^2}{2} + \frac{y^2}{2} + \frac{k}{2}(x-y)^2$. Show that the vector $\mathbf{r}(t) = \begin{pmatrix} x(t) \\ y(t) \end{pmatrix}$ evolves according to $\frac{\mathrm{d}\mathbf{r}}{\mathrm{d}t} = -\partial_{\mathbf{r}} V + \sqrt{2}\boldsymbol{\xi}$ where $\boldsymbol{\xi}$ stands for a Gaussian white noise matrix. Specify the correlation matrix of $\boldsymbol{\xi}(t)$.

10. For a given initial condition $\mathbf{r}(0)$ and a given arrival state $\mathbf{r}(t_{\text{obs}})$ after a time t_{obs}, the probability to observe a given time realization $\mathbf{r}(t)$ connecting $\mathbf{r}(0)$ to $\mathbf{r}(t_{\text{obs}})$ is denoted by $\mathscr{P}[\mathbf{r} : 0 \to t_{\text{obs}}]$. Fill in the ... in the following formula:

$$\begin{aligned}\mathscr{P}[\mathbf{r} : 0 \to t_{\text{obs}}] = \exp&\left[-\frac{1}{T_c}\int_0^{t_{\text{obs}}} \mathrm{d}t \underbrace{\ldots}_{\text{something not depending on } T_c}\right] \\ \times \exp&\left[-\frac{1}{T_h}\int_0^{t_{\text{obs}}} \mathrm{d}t \underbrace{\ldots}_{\text{something not depending on } T_h}\right]\end{aligned} \tag{172}$$

11. On what condition on T_c and T_h can a constant $\beta > 0$ be found such that $p_{\text{eq}}(\mathbf{r}) = \mathrm{e}^{-\beta V(\mathbf{r})}/Z$ is actually an equilibrium distribution (or, in other terms, that the process $\mathbf{r}(t)$ is an equilibrium process)? In what follows, whatever that condition is, it is not assumed to hold.

12. Write the Fokker-Planck equation governing the evolution of the probability density of x and y, denoted by $p(\mathbf{r}, t)$.

13. The stationary solution of the Fokker-Planck equation reads

$$p_{\text{ss}}(\mathbf{r}) = \frac{1}{Z}\exp\left[-\frac{a}{2}(x^2+y^2) - bxy\right],\ a = \frac{2(1+k)}{T_c + T_h} \tag{173}$$

where Z is some normalization constant. The constant b is uglier, and given only for your curiosity,

$$b = -\frac{k(T_c+T_h) + \sqrt{8T_c^2 + 16kT_c^2 + 9k^2T_c^2 - 8T_cT_h - 16kT_cT_h - 6k^2T_cT_h + k^2T_h^2}}{2T_c(T_c+T_h)} \tag{174}$$

How do we know, before any calculation, and even before writing the Fokker-Planck equation, that the stationary solution $p_{\text{ss}}(\mathbf{r})$ is a Gaussian?

14. Express the stationary distribution of x, denoted by $q(x)$, in terms of a, b and x (normalization is not asked for, and do not use the explicit expressions of a or b).

15. Consider the generalized Langevin equation

$$\frac{\mathrm{d}x}{\mathrm{d}t} = -(k+1)x(t) - \int_{-\infty}^{t} \mathrm{d}t' M(t-t')x(t') + \sqrt{2}\chi(t) \tag{175}$$

with $M(\tau) = k^2 \mathrm{e}^{-(k+1)\tau}$ and χ is a Gaussian but colored noise. Write the time correlations of χ so that the statistical properties of x evolving according to Eq. (175) are, in the steady-state, equivalent to those of x evolving as in question 171. Verify that for $k = 0$ your result matches what you expect in that limit.

16. Is the $x(t)$ process alone, as described in Eq. (175), an equilibrium one? Even if you can't reach a conclusion, at least outline a calculation that would give the answer to that question.

7.2 Brownian Carnot engine

In a 2016 article, the authors managed to subject an individual colloidal particle to the famous Carnot engine sequence (isothermal compression, adiabatic compression, isothermal expansion, adiabatic expansion). This has required to overcome a number of experimental and theoretical challenges. We won't cover experimental aspects here (related in particular to temperature control), and we will take as our starting point a colloidal particle evolving in one space dimension in an external potential $U(x,t) = \kappa(t)\frac{x^2}{2}$ and whose Hamiltonian is given by $H = \frac{p^2}{2m} + U(x,t)$, $p = m\dot{x}$ being the momentum of the particle and m its mass.

1. The first question is how to define an adiabatic process at the mesoscale. This was done in a 2015 article. This goes in two steps. First, for a constant value of κ, and in thermal equilibrium at temperature T, establish that

$$\langle x^2 \rangle = \frac{T}{\kappa} \tag{178}$$

2. Second, compute the canonical partition function Z as a function of h (yes, Planck's constant), m, β and κ. Find the free energy and the entropy of the particle. Explain why a possible definition of an adiabatic process is one in which the ratio $\frac{T^2}{\kappa}$ remains a constant.

3. The equation of motion for the colloid is $m\ddot{x} = -\gamma\dot{x} - \partial_x U + \sqrt{2\gamma T}\eta$ where γ is the friction coefficient of the colloid in the solvent. What is the physical meaning of $F_b = -\gamma\dot{x} + \sqrt{2\gamma T}\eta$?

4. Between t and $t+\mathrm{d}t$ the particle changes its position by $\mathrm{d}x$ and the stiffness is varied by an external operator by an amount $\mathrm{d}\kappa$. The energy H varies by $\mathrm{d}H$. Show that if δQ stands for the heat received by the particle then $\mathrm{d}H = \delta W + \delta Q$, where $\delta W = \frac{1}{2}x^2\mathrm{d}\kappa$. What is the interpretation of δW?

5. We also need to define a time-dependent temperature $T_{\rm eff}$. This is done by setting $T_{\rm eff}(t) = \kappa(t)\langle x^2(t)\rangle$. If the protocol were not quasistatic it would differ from the bath temperature (but we stick to quasistatic protocols). Determine, during an isothermal compression at fixed $T_{\rm eff} = T$ in which the stiffness goes from κ_1 to $\kappa_2 > \kappa_1$, the average work $\langle W\rangle$ received by the colloid as a function of κ_1 and κ_2 and $T_{\rm eff}$.

6. Explain why, during the same isothermal compression, the average heat $\langle Q\rangle$ received by the colloid is $-\langle W\rangle$.

7. In Fig. 1, the four steps of the Carnot cycle are depicted (left) and the force-stiffness curve is shown. How can you see that this cycle is indeed a motor cycle? Without computing anything explicitly, express the efficiency ε of the motor in terms of the average works $\langle W_i\rangle$ received during each of the four steps ($i = 1, \dots, 4$).

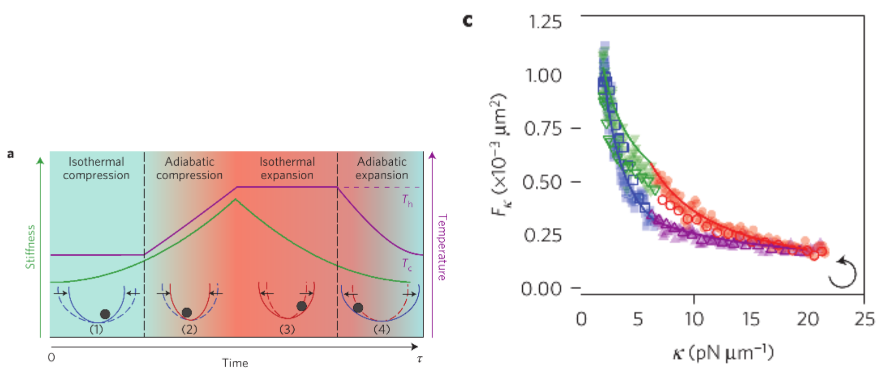

Figure 1: Left: a sketch of the cycle undergone by the colloidal particle. Right: Experimental data showing the measured spring force as a function of the applied stiffness.

8. Give a rough numerical estimate of the work that can be extracted from such a cycle.

7.3 Quasistatic cooling

Think of a colloidal particle with position $X(t)$ embedded in some thermal bath that imposes a temperature T. Such a particle is described by a Langevin equation. We ask ourselves (following a 1990 article) how this equation is affected (if at all) when the temperature of the bath is slowly modified (T becomes a time-dependent function $T(t)$) so that, at each time, the sytem has time to equilibrate at the new temperature (the bath-colloid energetic exchanges are sufficiently fast for this to be true). The external potential $V(X)$ is *a priori* arbitrary.

1. Write a Langevin equation for an overdamped or underdamped colloid (your choice) in the Markov limit. Replace T in your Langevin equation with the time-dependent function $T(t)$. Write the corresponding Fokker-Planck equation.

2. If $\lim_{t\to+\infty} T(t) = T_f$ (T_f is a constant) what is the steady-state distribution $p_{\rm ss}(X)$? Is it an equilibrium distribution?

In principle a Langevin equation results from coarse-graining out the degrees of freedom of the bath. We consider a specific model in which the Hamiltonian of the colloidal particle (coordinates X and P, mass M) and of the bath particles (coordinates x_i and p_i, unit mass $m = 1$) evolve according to a set of deterministic, Hamiltonian-like, equations.

$$H = \frac{P^2}{2M} + V(X) + \sum_i \left[\frac{p_i^2}{2} + \frac{k}{2}(x_i - X)^2\right] \tag{179}$$

3. Write the equations of motion for the coordinates x_i and p_i of the bath particles if, when decoupled from the colloid, their Hamilonian were $\sum_i \left[\frac{p_i^2}{2} + \frac{k_i}{2}x_i^2\right]$.

Because we now drive the system out of equilibrium by modifying the state of the bath, we now postulate new equations of motion for the bath particles. In the absence of the colloidal particle, these now read

$$\dot{x}_i = p_i + \alpha(t)x_i,\ \dot{p}_i = -k_i x_i + \beta(t)p_i \tag{180}$$

where $\alpha(t)$ and $\beta(t)$ are time-dependent functions, and where $k_i > 0$ is a spring constant. In the absence of the colloid, the bath particles are independent.

4. What is the condition on α and β under which these equations can be the result of some Hamiltonian dynamics for the bath alone?

5. Write an evolution equation for the probability density $f(x_i, p_i, t)$ that particle i of the bath is at position x_i with momentum p_i:

$$\partial_t f = -\partial_{x_i}[(p_i + \alpha(t)x_i)f] - \partial_{p_i}[\ldots] \tag{181}$$

The equations in Eq. (180) are a deterministic process, so that the equation for f has no second order derivative.

6. We now ask that the equation for f has the time-dependent solution

$$f(x_i, p_i, t) = \sqrt{k_i}\frac{1}{2\pi T(t)} \mathrm{e}^{-\frac{1}{T(t)}\left[\frac{p_i^2}{2} + \frac{k_i}{2}x_i^2\right]} \tag{183}$$

Express the functions $\alpha(t)$ and $\beta(t)$ in terms of $T(t)$ so that this specific form of f with a time-dependent temperature is indeed a solution. Why do we impose this specific form on f?

In the presence of the colloidal particle, the equations of motion for the bath coordinates become:

$$\dot{x}_i = p_i + \alpha(t)x_i,\ \dot{p}_i = -k_i(x_i - X) + \beta(t)p_i \tag{184}$$

where α and β are adjusted so that the condition of the previous question is fulfilled. For the colloidal particle, the equations of motion are

$$\dot{X} = P/M,\ \dot{P} = -V'(X) + \sum_i k_i(x_i - X) \tag{185}$$

7. Describe as precisely but as concisely as possible how you would proceed to arrive at a Langevin equation for X and P alone. Do not write any calculation; instead, explain which calculation you would like to do.

8. The latter Langevin equation, with one more assumption on the k_i's, reads

$$\dot{P} = -\gamma\left(\frac{P}{M} - \frac{1}{2}X\frac{\dot{T}}{T}\right) - V'(X) + \sqrt{2\gamma T(t)}\eta(t) \tag{186}$$

   where η is a Gaussian white noise with δ correlations. How does the Gaussian statistics of η come about?

9. Simplify the equation in the overdamped limit. Is the latter well-justified for a colloid in water?

10. Comment on how universal the extra term appearing in the Langevin equation for a process equilibrated with a bath at varying temperature is.

7.4 Sedimentation of run-and-tumble particles

We work in two space dimensions and we denoted by y the vertical coordinate. We consider a sedimenting run-and-tumble particle whose dynamics is given by

$$\dot{\mathbf{r}} = v_0\mathbf{u}(t) - v_s\mathbf{e}_y \tag{188}$$

where v_s is, up to the particle's mobility, the amplitude of the gravitional force mg, and v_0 is the bare self-propulsion speed of the active particle. The unit vector $\mathbf{u}(t)$ is a random variable that reorients stochastically with a rate $\frac{\alpha}{2\pi}$. When a jump occurs, its orientation θ is replaced by θ' chosen uniformly in $[0, 2\pi[$. We assume that a wall (the bottom of the container) localized at $y = 0$ imposes at late time a flux-free steady state and we consider (for simplicity) periodic boundary condition along the $\mathbf{e}_x$ direction.

1. The probability density $p(\theta, t)$ that $\mathbf{u}$ point in the θ direction evolves according to

$$\partial_t p = \frac{\alpha}{2\pi}\int_0^{2\pi} \mathrm{d}\theta' p(\theta', t) - \dots \tag{189}$$

   Fill in the ... and explain the physical origin of both terms appearing in the right-hand side of that equation.

2. Determine $\langle \mathbf{u}(0)\cdot\mathbf{u}(t)\rangle$ as a function of α and t.

3. Write an evolution equation for the probability $p(x,y,\theta,t)$ to find the particle at position $\mathbf{r}=(x,y)$ with orientation θ. Verify that $p(\theta,t)=\int \mathrm{d}x\mathrm{d}y p(x,y,\theta,t)$ indeed evolves as you found at the previous question.

4. We look for a steady-state solution in the form $p_{\rm ss}(x,y,\theta)=\rho(y)f(\theta)$ where $\int_0^{2\pi}\mathrm{d}\theta f(\theta)=1$. Show that such a solution can exist iff

$$\frac{\rho'(y)}{\rho(y)}=\alpha\frac{2\pi f(\theta)-1}{2\pi f(\theta)(v_s-v_0\sin\theta)} \tag{192}$$

5. Let $\lambda=-\frac{\rho'(y)}{\rho(y)}$. Why is λ a constant? What is its sign?

6. Find $f(\theta)$ as a function of v_s, v_0, α and λ.

7. Using the normalization condition on f (and possibly a change of variable $w=\tan\frac{\theta}{2}$), find the expression of λ in terms of v_0, v_s and α.

8. When $v_s=0$, we consider $R^2(t)=\langle(\mathbf{r}(t)-\mathbf{r}(0))^2\rangle$. For $t\gg 1$, show that $\frac{\mathrm{d}R^2}{\mathrm{d}t}=4T$ where the coefficient T will be expressed in terms of α and v_0. What is the physical meaning of T?

9. In the $v_s\ll v_0$ limit, one expects a barometric Boltzmann-like behavior for ρ, in the form $\rho(y)\propto \mathrm{e}^{-\beta mgy}$. Prove this behavior for $v_s\ll v_0$ and specify the expression of β in terms of v_0 and α.

8 Exam, 12/01/2024, 3 hours

8.1 Relaxing towards equilibrium

The motion of a particle in one space dimension is described by its position $x(t)$. At the initial time $t=0$, $x(t)=x_0$. The particle's position evolves according to an overdamped Langevin equation $\dot{x}=-V'(x)+\sqrt{2T}\eta$, where V is a confining potential and where η is a Gaussian white noise with correlations $\langle\eta(t)\eta(t')\rangle=\delta(t-t')$.

1. Write an evolution equation for the probability density $p(x,t)$ to find the particle at position x at time t.

2. Find the stationary solution $p_{\rm ss}(x)$ of the previous equation in terms of V, T, up to a normalization constant.

3. The probability to observe a given realization of $x(t)$ over the time window $[0,t_{\rm obs}]$, starting from x_0, is given, in the Stratonovich discretization, by

$$\mathscr{P}[x(t);t\in[0,t_{\rm obs}];x(0)=x_0]=\exp\left[-\int_0^{t_{\rm obs}}\mathrm{d}t\left(a(\dot{x}+V'(x))^2+bV''\right)\right] \tag{197}$$

Express the a and b constants in terms of the parameters of the problem.

4. Assuming that x_0 is now sampled from the steady-state distribution p_{ss}, what is the probability $\mathscr{P}[x(t); t \in [0, t_{\text{obs}}]]$ to observe a given realization of $x(t)$ over the time window $[0, t_{\text{obs}}]$?

5. Determine the ratio $\frac{\mathscr{P}[x(t);t\in[0,t_{\text{obs}}]]}{\mathscr{P}[x(t_{\text{obs}}-t);t\in[0,t_{\text{obs}}]]}$. What does this number tell you about the process $x(t)$ when x_0 is sampled from p_{ss}?

In what follows, x_0 will remain fixed and is not sampled from any distribution.

6. Write a Langevin equation for the energy $V(t) = V(x(t))$ of the particle (this equation of course couples to $x(t)$). Make sure you specify the discretization scheme of the corresponding equation.

7. Explain why, at zero temperature, and for a convex function V, the dynamics leads the particle to a minimum of the potential.

8. When $V(x) = \frac{1}{2}kx^2$, express $\langle V(t)\rangle$ in terms of $V(x_0)$, k, T and t (here the initial state is not sampled, it is fixed at x_0).

9. The long time limit of $\langle V(t)\rangle$ in question 8 could have been guessed ahead of time. How?

We now assume that at $t = 0$ the system is in equilibrium (and thus that x_0 is sampled accordingly).

10. Determine $\langle V(0)^2\rangle_{\text{eq}}$ in equilibrium in terms of k and T.

11. We consider the correlation function $C(t) = \langle V(t)V(0)\rangle - \langle V(t)\rangle\langle V(0)\rangle$. Show that $C(t) = \frac{T^2}{2}\mathrm{e}^{-2kt}$.

12. We now ask about how a slight perturbation in the temperature of the bath affects the system's behavior. To measure this quantity, we consider $R(t-t') = \frac{\delta\langle V(t)\rangle}{\delta T(t')}$ where the temperature T is varied by an infinitesimally small amount δT at a time $t' < t$. Explain carefully how R can be connected to C without carrying out any additional calculation.

8.2 Linear response without perturbation, in or out of equilibrium

The connection between the response of an equilibrium system to some infinitesimal external perturbation to its unperturbed fluctuations is well-understood in terms of the fluctuation-dissipation theorem. Linear response coefficients can however also be defined out of equilibrium. This problem is about finding a clever way to access the linear response coefficients, in or out of equilibrium.

Let's begin with a particle with position $x(t)$ in one space dimension evolving according to the following overdamped Langevin equation:

$$\frac{\mathrm{d}x}{\mathrm{d}t} = F(x, \lambda) + \sqrt{2T}\eta \tag{200}$$

where the particle's mobility has been set to unity, η is a Gaussian white noise with correlations $\langle \eta(t)\eta(t')\rangle = \delta(t - t')$. The force field $F(x, \lambda)$ felt by the particle depends on some external parameter λ.

1. Let $q(t, \lambda)$ be a random process such that $q(0, \lambda) = 0$ and $\frac{\mathrm{d}q}{\mathrm{d}t} \stackrel{0}{=} \frac{1}{\sqrt{2T}}\partial_\lambda F\eta$. Rewrite $\frac{\mathrm{d}q}{\mathrm{d}t}$ in a Stratonovich-discretized form.

2. Let $A(x(t_{\mathrm{obs}}))$ be a given physical quantity depending on the position at time $t_{\mathrm{obs}} > 0$ (but A is assumed to exhibit no explicit λ-dependence). Write the average of A in the form of a path-integral over a single field $x(t)$, using the Itō discretization scheme.

3. Express $\partial_\lambda\langle A\rangle$ in terms of an average involving A and q.

We now consider $A = \dot{x}$ and $F(x, \lambda) = -\frac{\mathrm{d}V}{\mathrm{d}x} + \lambda$, where V is a periodic potential landscape.

4. What can you say about $\langle \dot{x}\rangle$ when $\lambda = 0$ (this is a qualitative question, no calculations asked)?

5. We now consider $\mu = \left.\frac{\partial\langle\dot{x}\rangle}{\partial\lambda}\right|_{\lambda=0}$. Without any further calculation, what is the argument that allows you to relate μ to $D = \lim_{t\to+\infty} \frac{\langle(x(t)-x(0))^2\rangle}{2t}$? And what exactly is that connection between μ and D?

Up until now, we have assumed the temperature T of the bath to remain constant. We now allow T to vary (slowly) as a function of time, and we assume the equation of motion is simply generalized to

$$\frac{\mathrm{d}x}{\mathrm{d}t} = F(x, \lambda) + \sqrt{2T(t)}\eta \tag{208}$$

6. How is the answer to question 3 modified if one pays attention to the time-dependence of $T(t)$?

7. Under what generic conditions on $T(t)$ and/or the periodic landscape $V(x)$ should we expect that $\langle\dot{x}\rangle \neq 0$ when $\lambda = 0$?

8. Show that the mobility of the particle can be obtained as the steady-state average of some observable, regardless of the system being in or out of equilibrium.

8.3 Actively climbing over an energy barrier

Self-propelled particles are micron-sized entities (whether bacteria or synthetic colloids) that use energy from their environment to convert it into motion. Energy is then dissipated instead of being returned to the environment (as would be the case for a passive colloid undergoing Brownian motion). There are various ways of modelling the motion of such a particle. One of them is to describe it by means of an overdamped Langevin equation with a colored noise,

$$\frac{\mathrm{d}\mathbf{r}}{\mathrm{d}t} = -\boldsymbol{\nabla} V(\mathbf{r}) + \sqrt{2T}\boldsymbol{\eta} \tag{209}$$

where $\boldsymbol{\eta}$ is a Gaussian noise whose spatial components η^μ have correlations $\langle \eta^\mu(t)\eta^\nu(t')\rangle = \delta^{\mu\nu}\Delta(t-t')$ with $\Delta(t) = \frac{\mathrm{e}^{-|t|/\tau}}{2\tau}$ and where τ is a time scale expressing the persistent nature of the motion. A natural question that arises is whether such a particle hops over a potential barrier faster or slower than its equilibrium counterpart. We will explore this question in one space dimension in the limit where T is small with respect to the relevant potential energy scale.

1. Explain why, as $\tau \to 0$, the function $\Delta(t)$ becomes a distribution $\Delta(t) = a\delta(t) + b\tau^2\delta''(t) + O(\tau^4)$, where a and b are constants to be determined.

2. Let G such that $\int \mathrm{d}t_2\, G(t_1-t_2)\Delta(t_2-t_3) = \delta(t_1-t_3)$. Show that for $\tau \to 0$, G becomes a distribution, $G(t) = a\delta(t) + c\tau^2\delta''(t) + O(\tau^4)$, where c is a constant to be determined.

3. Show that as $\tau \to 0$ one recovers an equilibrium process for $x(t)$. In physics, it is meaningless to write $\tau \to 0$, as one should instead write $\tau \ll \tau'$ where τ' is some other time scale. What is the physical meaning and physical origin of τ'?

4. In the absence of the external potential V, determine the mean-square displacement of the particle after a duration t in terms of T, t and τ. Briefly discuss the various regimes that are observed.

Henceforth we work in one space dimension and we consider a potential landscape displaying a minimum V_m at x_m and a maximum V_M at x_M. We denote by $\Delta V = V_M - V_m$ and we ask about the typical time it take a particle starting from x_m to reach x_M. visits a given position starting from some other position and some other value of u.

5. Show that the probability of observing a given realization of the position x is proportional to $\mathrm{e}^{-\frac{1}{4T}\int \mathrm{d}t_1\mathrm{d}t_2(\dot{x}+V')(t_1)G(t_1-t_2)(\dot{x}+V')(t_2)}$.

6. Show that the probability of observing a given realization of the position x is proportional to $\mathrm{e}^{-\frac{1}{T}S[x]}$ where S is independent of T and is given by

$$S[x] = \frac{1}{4}\int \mathrm{d}t \left[(\dot{x} + V')^2 + d\tau^2(\ddot{x} + \dot{x}\,V'')^2 + O(\tau^4)\right] \tag{214}$$

where the constant d is to be determined.

7. What is, at low temperature and at $\tau = 0$, for a trajectory starting from x_m and ending at x_M, the evolution equation for the most likely path $x_c^{(0)}(t)$?

8. Show that the probability to observe such a trajectory decays as $\mathrm{e}^{-\frac{V_M - V_m}{T}}$ when $\tau = 0$ and as $T \to 0$.

9. For τ small but nonzero, we find that the most likely path x_c picks up a τ^2 contribution: $x_c(t) = x_c^{(0)}(t) + \tau^2 2V'(x_c^{(0)})V''(x_c^{(0)})$. Show that the energy barrier is effectively increased (explain the calculation you'd like to carry out if you had plenty of time).

8.4 A chiral active particle

In the living world, some self-propelled particles are chiral. The motion of such a particle, in two space dimensions, is sometimes modeled by the following equation:

$$\frac{\mathrm{d}\mathbf{r}}{\mathrm{d}t} = \mu\mathbf{F} + v_0\mathbf{u} \tag{217}$$

where $\mathbf{u} = \cos\theta\mathbf{e}_x + \sin\theta\mathbf{e}_y$ is a unit vector, μ is the particle's mobility, and $\mathbf{F}$ is some externally applied force. The chirality appears through the equation governing the dynamics of $\mathbf{u}$:

$$\frac{\mathrm{d}\theta}{\mathrm{d}t} = \omega + \sqrt{2D_r}\eta \tag{218}$$

where $D_r > 0$ and $\omega > 0$ are constants, while η is a Gaussian white noise with correlations $\langle\eta(t)\eta(t')\rangle = \delta(t - t')$. The chirality arises from the presence of a nonzero ω.

1. Write an evolution equation for the probability density $p(\mathbf{r}, \theta, t)$ to find the particle at location $\mathbf{r}$ with orientation θ.

For the remainder of the exercise, we work with $\mathbf{F} = \mathbf{0}$.

2. Show that $\frac{\mathrm{d}}{\mathrm{d}t}\langle\mathbf{u}\rangle = \omega\langle\mathbf{e}\rangle - D_r\langle\mathbf{u}\rangle$, where $\mathbf{e} = -\sin\theta\mathbf{e}_x + \cos\theta\mathbf{e}_y$.

3. Find a similar equation for the evolution of $\langle\mathbf{e}\rangle$.

4. Explain why, at fixed initial orientation $\mathbf{u}(0)$, one obtains $\langle\mathbf{u}\rangle(t) = \cos\omega t \mathrm{e}^{-D_r t}\mathbf{u}(0) + \mathrm{e}^{-D_r t}\sin\omega t\mathbf{e}(0)$.

5. What is the long time diffusion constant of the chiral active particle (in the absence of an external force) as a function of D_r and of ω? Comment on the qualitative effect of ω.

References

[1] Adrian Baule and Peter Sollich. Optimal escape from metastable states driven by non-gaussian noise. *arXiv preprint arXiv:1501.00374*, 2015.

[2] Ludovic Berthier. Efficient measurement of linear susceptibilities in molecular simulations: Application to aging supercooled liquids. *Physical review letters*, 98(22):220601, 2007.

[3] Hans-Benjamin Braun and H Neal Bertram. Nonuniform switching of single domain particles at finite temperatures. *Journal of applied physics*, 75(9):4609–4616, 1994.

[4] William Coffey and Yu P Kalmykov. *The Langevin equation: with applications to stochastic problems in physics, chemistry and electrical engineering*, volume 27. World Scientific, 2012.

[5] William T Coffey and Yuri P Kalmykov. Thermal fluctuations of magnetic nanoparticles: Fifty years after brown. *Journal of Applied Physics*, 112(12):121301, 2012.

[6] Alain Comtet, Cécile Monthus, and Marc Yor. Exponential functionals of brownian motion and disordered systems. *Journal of applied probability*, 35(2):255–271, 1998.

[7] Leticia F Cugliandolo, Giuseppe Gonnella, and Isabella Petrelli. Effective temperature in active brownian particles. *Fluctuation and Noise Letters*, 18(02):1940008, 2019.

[8] Sara Dal Cengio, Demian Levis, and Ignacio Pagonabarraga. Linear response theory and green-kubo relations for active matter. *Physical Review Letters*, 123(23):238003, 2019.

[9] Jay Robert Dorfman. *An introduction to chaos in nonequilibrium statistical mechanics*. Number 14. Cambridge University Press, 1999.

[10] Eric Fournié, Jean-Michel Lasry, Jérôme Lebuchoux, and Pierre-Louis Lions. Applications of malliavin calculus to monte-carlo methods in finance. ii. *Finance and Stochastics*, 5:201–236, 2001.

[11] Eric Fournié, Jean-Michel Lasry, Jérôme Lebuchoux, Pierre-Louis Lions, and Nizar Touzi. Applications of malliavin calculus to monte carlo methods in finance. *Finance and Stochastics*, 3:391–412, 1999.

[12] Futoshi Futami, Issei Sato, and Masashi Sugiyama. Accelerating the diffusion-based ensemble sampling by non-reversible dynamics. In *International Conference on Machine Learning*, pages 3337–3347. PMLR, 2020.

[13] Xuefeng Gao, Mert Gurbuzbalaban, and Lingjiong Zhu. Breaking reversibility accelerates langevin dynamics for non-convex optimization. *Advances in Neural Information Processing Systems*, 33:17850–17862, 2020.

[14] Cristian Giardina, Jorge Kurchan, and Frank Redig. Duality and exact correlations for a model of heat conduction. *Journal of mathematical physics*, 48(3):033301, 2007.

[15] Cristian Giardina, Jorge Kurchan, Frank Redig, and Kiamars Vafayi. Duality and hidden symmetries in interacting particle systems. *Journal of Statistical Physics*, 135(1):25–55, 2009.

[16] D Gredat, I Dornic, and JM Luck. On an imaginary exponential functional of brownian motion. *Journal of Physics A: Mathematical and Theoretical*, 44(17):175003, 2011.

[17] C Kipnis, C Marchioro, and E Presutti. Heat flow in an exactly solvable model. *Journal of Statistical Physics*, 27(1):65–74, 1982.

[18] Sudeesh Krishnamurthy, Subho Ghosh, Dipankar Chatterji, Rajesh Ganapathy, and AK Sood. A micrometre-sized heat engine operating between bacterial reservoirs. *Nature Physics*, 12(12):1134, 2016.

[19] Wenlong Mou, Yi-An Ma, Martin J Wainwright, Peter L Bartlett, and Michael I Jordan. High-order langevin diffusion yields an accelerated mcmc algorithm. *J. Mach. Learn. Res.*, 22:42–1, 2021.

[20] Grzegorz Szamel. Evaluating linear response in active systems with no perturbing field. *Europhysics Letters*, 117(5):50010, 2017.

[21] Nicolaas Godfried Van Kampen. *Stochastic processes in physics and chemistry*, volume 1. Elsevier, 1992.

[22] Patrick B Warren and Rosalind J Allen. Malliavin weight sampling for computing sensitivity coefficients in brownian dynamics simulations. *Physical review letters*, 109(25):250601, 2012.

[23] Patrick B Warren and Rosalind J Allen. Malliavin weight sampling: a practical guide. *Entropy*, 16(1):221–232, 2013.

[24] Xiao-Lun Wu and Albert Libchaber. Particle diffusion in a quasi-two-dimensional bacterial bath. *Physical review letters*, 84(13):3017, 2000.

[25] Marc Yor and Marc Yor. *Exponential functionals of Brownian motion and related processes*, volume 112. Springer, 2001.