Nonequilibrium soft and active matter: TD1

Department of Physics and Materials Science, University of Luxembourg

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1 Gaussian variables and equipartition

A. Prove the following properties of the Gaussian integrals for the variables $\mathbf{x} = \{x_1, \dots, x_N\}$:

$$\int d\mathbf{x} e^{-\mathbf{x}^2/(2a)} = (2\pi a)^{N/2}, \quad \int \mathbf{x}^2 d\mathbf{x} e^{-\mathbf{x}^2/(2a)} = Na(2\pi a)^{N/2}. \tag{1}$$

Correction. One can separate each of these integrals as

$$\begin{aligned} \int d\mathbf{x} e^{-\mathbf{x}^2/(2a)} &= \left[\int dx e^{-x^2/(2a)} \right]^N, \\ \int \mathbf{x}^2 d\mathbf{x} e^{-\mathbf{x}^2/(2a)} &= N \int dy y^2 e^{-y^2/(2a)} \left[\int dx e^{-x^2/(2a)} \right]^{N-1}. \end{aligned} \tag{2}$$

Using decomposition in terms of polar coordinates, we get

$$\left[\int_{-\infty}^{\infty} dx e^{-x^2/(2a)} \right]^2 = \iint_{-\infty}^{\infty} dx dy e^{-(x^2+y^2)/(2a)} = \int_0^{\infty} r dr \int_0^{2\pi} d\theta e^{-r^2/(2a)} = 2\pi a, \tag{3}$$

from which we deduce the first integral in (1). Moreover, we note that

$$\int_{-\infty}^{\infty} x^2 dx e^{-x^2/(2a)} = 2a^2 \frac{d}{da} \int_{-\infty}^{\infty} dx x^2 e^{-x^2/(2a)} = a\sqrt{2\pi a}, \tag{4}$$

from which we deduce the second integral in (1).

B. Consider the underdamped dynamics of a colloidal particle in a harmonic trap. Prove the equipartition theorem for the kinetic and potential energies.

Correction. Given the kinetic energy $K(\mathbf{v}) = m\mathbf{v}^2/2$ and the potential energy $U(\mathbf{x}) = k\mathbf{x}^2/2$, the steady state follows the Boltzmann distribution:

$$P_s(\mathbf{x}, \mathbf{v}) = \frac{e^{-(K(\mathbf{v})+U(\mathbf{x}))/T}}{Z}, \quad Z = \int d\mathbf{x} d\mathbf{v} e^{-(K(\mathbf{v})+U(\mathbf{x}))/T}. \tag{5}$$

The average of kinetic and potential energies reads

$$\langle K(\mathbf{v}) \rangle_s = \frac{\int K(\mathbf{v}) d\mathbf{v} e^{-K(\mathbf{v})/T}}{\int d\mathbf{v}' e^{-K(\mathbf{v}')/T}}, \quad \langle U(\mathbf{x}) \rangle_s = \frac{\int U(\mathbf{x}) d\mathbf{x} e^{-U(\mathbf{x})/T}}{\int d\mathbf{x}' e^{-U(\mathbf{x}')/T}}. \tag{6}$$

Using the integrals in (1), we deduce that, for d spatial dimensions, one gets the equipartition theorem:

$$\langle K(\mathbf{v}) \rangle_s = dT/2 = \langle U(\mathbf{x}) \rangle_s. \tag{7}$$

2 Itinerant oscillator model

A. Prove that the sum of Gaussian variables is a Gaussian variable.

Correction. For simplicity, we consider the case of $z = x + y$ (extension to the sum of higher number of Gaussian variables is straightforward), where x and y are Gaussian variables with distributions

$$P_x(x) \propto e^{-(x-\mu_x)^2/(2a_x)}, \quad P_y(y) \propto e^{-(y-\mu_y)^2/(2a_y)}. \tag{8}$$

The distribution of z reads

$$P_z(z) = \int dx dy \delta(x + y - z) P_x(x) P_y(y) = \int dx P_x(x) P_y(z - x). \tag{9}$$

yielding

$$\begin{aligned} P_z(z) &\propto \int dx \exp\left[- \frac{(x-\mu_x)^2}{2a_x} - \frac{(z-x-\mu_y)^2}{2a_y} \right] \\ &\propto \exp\left[- \frac{(z-\mu_x-\mu_y)^2}{(2(a_x+a_y)} \right] \int dx \exp\left[- \frac{(x-(a_x(z-\mu_y)+a_y\mu_x)/(a_x+a_y))^2}{2a_x a_y/(a_x+a_y)} \right] \\ &\propto \exp\left[- \frac{(z-\mu_x-\mu_y)^2}{(2(a_x+a_y)} \right]. \end{aligned} \tag{10}$$

B. Consider the following coupled Langevin dynamics:

$$\gamma \dot{x} = -k(x-y) + \eta_x, \quad \bar{\gamma} \dot{y} = -k(y-x) + \eta_y. \tag{11}$$

Give the statistics of the noise terms η_x and η_y to ensure that the steady state obeys the Boltzmann distribution $P_s(x, y) \propto \exp(-k(x-y)^2/(2T))$.

Correction. Since x and y are linear combinations of η_x and η_y, then enforcing that η_x and η_y have Gaussian statistics ensures that the steady state $P_s(x, y)$ is Gaussian. Besides, at equilibrium, the fluctuation-dissipation theorem enforces the following noise correlations:

$$\langle \eta_x(t)\eta_x(0)\rangle = 2\gamma T\delta(t), \quad \langle \eta_y(t)\eta_y(0)\rangle = 2\bar{\gamma} T\delta(t), \quad \langle \eta_x(t)\eta_y(0)\rangle = 0. \tag{12}$$

Nonequilibrium soft and active matter: TD2

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1 From multiplicative to additive Langevin equations

A. Consider the following multiplicative Langevin equation:

$$\dot{x} = A(x(t)) + \eta, \quad \langle \eta(t)\eta(0)\rangle = 2B(x(t))\delta(t). \tag{1}$$

Give the corresponding Fokker-Planck equations for Stratonovitch and Itô conventions.

Correction. For Stratonovitch convention, we get

$$\partial_t P = \partial_x\left(A(x)P + \sqrt{B(x)}\partial_x(\sqrt{B(x)}P)\right), \tag{2}$$

and, for Itô convention, we get

$$\partial_t P = \partial_x(A(x)P + \partial_x(B(x)P)). \tag{3}$$

B. Find the appropriate change of variable $y = C(x)$ so that Eq. (1) reads

$$\dot{y} = D(y(t)) + \xi, \quad \langle \xi(t)\xi(0)\rangle = 2\delta(t), \tag{4}$$

where D can be expressed in terms of $\{A, B, C\}$.

Correction. Using Stratonovitch convention, we get $\dot{y} = (dC/dx)\dot{x}$, so that the dynamics of y reads

$$\dot{y} = (dC/dx)A(x(t)) + \xi, \quad \langle \xi(t)\xi(0)\rangle = 2(dC/dx)^2 B(x(t))\delta(t). \tag{5}$$

This implicitly assumes that the dynamics of x is interpreted with Stratonovitch convention. Choosing $(dC/dx)^2 B(x) = 1$, we deduce

$$D(y) = A(x)/\sqrt{B(x)} = A(C^{-1}(y))/\sqrt{B(C^{-1}(y))}, \tag{6}$$

where C^{-1} denotes the reciprocal of C, defined by $C(C^{-1}(x)) = x$.

C. Give the Fokker-Planck equation associated with Eq. (4). Prove that it is consistent with the Fokker-Planck equation associated with Eq. (1).

Correction. The Fokker-Planck equation for the distribution $P(y,t)$ reads

$$\partial_t P = \partial_y(D(y)P + \partial_y P). \tag{7}$$

The Fokker-Planck equation for the distribution $Q(x,t)$ obeys $Q(x,t)dx = P(y,t)dy$, yielding

$$Q(x,t) = (dy/dx)P(y,t) = P(y,t)/\sqrt{B(x)}. \tag{8}$$

Using that $\partial_y = \sqrt{B(x)}\partial_x$, we recover Eq. (2). This is consistent with the fact that we have used the Stratonovitch convention to get the dynamics of y.

2 Colloids close to a wall: Position-dependent damping

A. When a colloidal particle is immersed in a solvent close to a wall, the damping coefficient depends in its position. Give the corresponding Langevin equation for an external potential U, and the Fokker-Planck equation for an arbitrary temporal discretization.

Correction. For damping $\gamma(x)$ and potential U, the Langevin equation reads

$$\gamma(x(t)))\dot{x} = -dU/dx + \eta, \quad \langle \eta(t)\eta(0)\rangle = 2\gamma(x(t))T\delta(t). \tag{9}$$

With a discretization of the form

$$\begin{aligned} &x(t_n + \Delta t) - x(t_n) = (\Delta t/\gamma(x(t_n)))(dU/dx)(x(t_n)) + \sqrt{T\Delta t/\gamma((1-a)x(t_n) + ax(t_{n+1}))}\xi_n, \\ &\langle \xi_n \xi_m \rangle = 2\delta_{nm}, \end{aligned} \tag{10}$$

we get the following Fokker-Planck equation for the distribution $P(x,t)$:

$$\partial_t P = \partial_x \left[\left(\frac{1}{\gamma(x)} \frac{dU}{dx} - aT \frac{d}{dx} \frac{1}{\gamma(x)} \right) P + T\partial_x \left(\frac{P}{\gamma(x)} \right) \right]. \tag{11}$$

B. Find the appropriate discretization to ensure that the steady state is given by the Boltzmann distribution. Interpreting the dynamics with this discretization, write down the equation of motion in Itô convention.

Correction. One recovers the proper steady state $P_s \propto \exp(-U/T)$, which is independent of $\gamma(x)$, for $a = 1$. It is sometimes called anticipating convention (or anti-Itô convention), which is neither Stratonovitch nor Itô convention. To turn the dynamics from anti-Itô to Itô convention, one needs to a spurious drift term as

$$\gamma(x(t)))\dot{x} = -(d/dx)(U + T\ln\gamma) + \eta. \tag{12}$$

Nonequilibrium soft and active matter: TD3

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1 From Kramers to Smoluchowski equation: Multiscale approach

A. Consider the underdamped dynamics of a colloidal particle subject to a potential U:

$$m\ddot{x} = -\gamma\dot{x} + dU/dx + \eta, \quad \langle\eta(t)\eta(0)\rangle = 2\gamma T\delta(t). \tag{1}$$

Give the corresponding Fokker-Planck equation in the space of position x and velocity $v = \dot{x}$, also known as the Kramers equation, and prove that the Maxwell-Boltzmann distribution is the stationary solution.

Correction. The dynamics can be written as

$$\dot{x} = v, \quad m\dot{v} = -\gamma v - dU/dx + \eta, \tag{2}$$

yielding

$$\left[\partial_t + v\partial_x + \frac{1}{m}\frac{dU}{dx}\partial_v\right]P = \frac{\gamma}{m}\partial_v\left[\left(v + \frac{T}{m}\partial_v\right)P\right]. \tag{3}$$

The stationary solution is $P_s \propto \exp[-(mv^2/2 + U(x))/T]$.

B. Consider the following change of variables:

$$x \to x/\ell, \quad v \to v\sqrt{m/T}, \quad t \to t\sqrt{T/m}/\ell, \quad U \to U/T \tag{4}$$

where ℓ is a characteristic lengthscale (*e.g.*, particle size). Give the corresponding Fokker-Planck equation in terms of these non-dimensional units.

Correction. Introducing $\varepsilon = \sqrt{mT}/(\gamma\ell)$, we get

$$\varepsilon\Big[\partial_t + v\partial_x + (dU/dx)\partial_v\Big]P = \partial_v\Big[(v + \partial_v)P\Big]. \tag{5}$$

C. Consider the following expansion of the distribution $P(x, v, t)$ at small $\varepsilon = \sqrt{mT}/(\gamma\ell)$:

$$P(x, v, t) = \sum_{i=0}^{\infty}\varepsilon^i P_i(x, v, t), \quad t = \sum_{i=0}^{\infty}\varepsilon^i t_i. \tag{6}$$

Give the corresponding equations for P_0, P_1 and P_2. What is the physical significance of ε?

Correction. The small parameter ε is the Reynolds number, which compares inertial and viscous effects. To order ε^i for $i \in \{0, 1, 2\}$, we get

$$\begin{aligned}
\partial_v\Big[(v + \partial_v)P_0\Big] &= 0, \\
\partial_v\Big[(v + \partial_v)P_1\Big] &= \Big[\partial_{t_0} + v\partial_x + (dU/dx)\partial_v\Big]P_0, \\
\partial_v\Big[(v + \partial_v)P_2\Big] &= \Big[\partial_{t_0} + v\partial_x + (dU/dx)\partial_v\Big]P_1 + \partial_{t_1}P_0.
\end{aligned} \tag{7}$$

D. Derive the solution for P_0 and P_1. This requires enforcing the following solubility condition: the equations for P_0, P_1 and P_2 must remain valid when integrating with respect to v.

Correction. The solution for P_0 reads

$$P_0(x,v,t) = c_0(x,t)\exp(-v^2/2), \tag{8}$$

and, after substituting in the P_1 equation, we get

$$\partial_v\Big[(v+\partial_v)P_1\Big] = \exp(-v^2/2)\Big[\partial_{t_0} + v(\partial_x + (dU/dx))\Big]c_0(x,t). \tag{9}$$

Integrating this equation with respect to v leads to $\partial_{t_0}c_0 = 0$, hence c_0 is a function of x and $\bar{t} = t - t_0$ The solution for P_1 follows as

$$P_1(x,v,t) = \exp(-v^2/2)\Big[c_1(x,t) - v(\partial_x + (dU/dx))c_0(x,\bar{t})\Big], \tag{10}$$

and, after substituting in the P_2 equation, we get

$$\begin{aligned}\partial_v\Big[(v+\partial_v)P_2\Big] = \exp(-v^2/2)\Big[&\partial_{t_0}c_1 + \partial_{t_1}c_0 - \partial_x((dU/dx+\partial_x)c_0) \\ &- v(\partial_x + dU/dx)c_1 + (1-v^2)(dU/dx+\partial_x)((dU/dx+\partial_x)c_0)\Big].\end{aligned} \tag{11}$$

Integrating this equation with respect to v leads to

$$\partial_{t_0}c_1 + \partial_{t_1}c_0 = \partial_x((dU/dx+\partial_x)c_0). \tag{12}$$

Since c_0 is independent of t_0, integrating this equation with respect to t_0 leads to $c_1(x,t) \propto t_0$. To avoid divergence at large t_0, we deduce

$$\partial_{t_1}c_0 = \partial_x((dU/dx+\partial_x)c_0). \tag{13}$$

E. Show that, to leading order in ε, the dynamics of the marginal distribution $Q(x,t) = \int dv P(x,v,t)$ is associated with the following overdamped Langevin equation:

$$\gamma\dot{x} = -dU/dx + \eta, \quad \langle\eta(t)\eta(0)\rangle = 2\gamma T\delta(t). \tag{14}$$

The corresponding Fokker-Planck equation is known as the Smoluchowski equation.

Correction. To leading order in ε, we get $Q(x,t) = c_0(x,\bar{t})$ and $\varepsilon\partial_t Q = \partial_{t_1}c_0$. Substituting back the proper units in the dynamics of c_0, we deduce

$$\partial_t Q = (1/\gamma)\partial_x((dU/dx + T\partial_x)Q). \tag{15}$$

Nonequilibrium soft and active matter: TD4

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1 Escape from a potential barrier: Onsager-Machlup action and instantons

Consider the $1d$ motion of a colloidal particle in a potential $U(x)$ with a local minimum at $x = x_m$, a local maximum at $x = x_M$ and $U(\pm\infty) = \mp\infty$. The dynamics is given by the usual Langevin equation

$$\begin{gathered} \gamma\dot{x}(t) = -U'(x(t)) + \eta(t) \ , \\ \langle\eta(t)\rangle = 0 \ , \quad \langle\eta(t)\eta(t')\rangle = 2\gamma T\delta(t-t') \ , \end{gathered} \tag{1}$$

with the noise $\eta(t)$ interpreted in the Stratonovitch convention.

A. Write the probability $P(x_M, t|x_m, 0)$ of a trajectory starting from the potential minimum and reaching the maximum at time t in terms of an Onsager-Machlup action.

Correction. The probability of the trajectory constrained at startpoint $x(0) = x_m$ and $x(t) = x_M$ is given by Eq. (95) in the Lecture; taking the Stratonovitch convention gives a factor $a = 1/2$, then one has

$$\begin{aligned} P(x_M, t|x_m, 0) &= \int_{x(0)=x_m}^{x(t)=x_M} \mathcal{N} \exp\left\{-\mathcal{S}\left[x(t')\right]\right\} \mathcal{D}x \\ \mathcal{S}\left[x(t')\right] &= \int_0^t \mathrm{d}t' \left\{\frac{1}{4\gamma T}\left[\gamma\dot{x}(t') + U'(x(t'))\right]^2 - \frac{1}{2\gamma}U''(x(t'))\right\} \end{aligned} \tag{2}$$

being $\mathcal{S}[x(t')]$ the Onsager-Machlup action correspondent to the Langevin equation (1).

B. Find the trajectories that minimizes the action integral in the weak noise (low temperature) limit $T \to 0$.

Correction. In the $T \to 0$ limit the term coming from Stratonovitch integration can be neglected. One has then to find the trajectory $\{x(t')\}$ minimizing the action $\mathcal{S}[x(t')]$, *i.e.* satisfying

$$\frac{\delta\mathcal{S}}{\delta x(t')} = 0 \ . \tag{3}$$

One may derive the action and get the solution. A clever approach is to expand the square and note that

$$2\gamma\int_0^t \mathrm{d}t'\dot{x}(t')U'(x(t')) = 2\gamma\left[U(x(t)) - U(x(0))\right] = 2\gamma(U_M - U_m) = 2\gamma\Delta U \ , \tag{4}$$

being $U_M = U(x_M)$, $U_m = U(x_m)$ and exploiting the constraint on the start and end point of the trajectory. Therefore this term does not depend on the trajectory $\{x(t')\}$. The remaining term gives

$$\int_0^t \mathrm{d}t' \left[\gamma^2\dot{x}^2(t') + U'^2(x(t'))\right] \ , \tag{5}$$

which is the sum of two squares, *i.e.* a positive definite term. This is minimized setting the integrand to zero, then

$$\gamma\dot{x}(t') = \pm U'(x(t')) \ . \tag{6}$$

The correct sign is given by boundary conditions; since the particle must ascend the energy landscape from $t' = 0$ to $t' = t$, the + solution must be chosen. Therefore $\gamma \dot{x}(t') = +U'(x(t'))$. This ascending solution is called *instanton* and correspond to the fastest trajectories that can reach the maximum of the potential and lead the particle outside of the valley. Substituting this result in Eq. (5) one has

$$\int_0^t \mathrm{d}t' \left[\gamma^2 \dot{x}^2(t') + U'^2(x(t'))\right] = 2\gamma \Delta U \ . \tag{7}$$

C. Use the solution found to compute the asymptotic behavior of $P(x_M, t|x_m, 0)$ in the $T \to 0$ limit.

Correction. Method of steepest descent: when $\epsilon \approx 0$ one has

$$\int \mathrm{d}x\, e^{-f(x)/\epsilon} \approx e^{-\min_x f(x)/\epsilon} \ , \tag{8}$$

at the lowest order, *i.e.* neglecting prefactors.

Replacing the two contributions and approximating the integral over trajectories, we apply the steepest descent method to the integral over realizations $\mathcal{D}x$ and replace the exponential with the minimal action computed. Therefore

$$P(x_M, t|x_m, 0) \approx e^{-\Delta U/T} \tag{9}$$

which is *independent* on t. The Gaussian fluctuations around this steepest-descent computation yield an estimate for the prefactor.

2 Escape from a potential barrier: Fokker-Planck equation

D. Write the Fokker-Planck equation for the probability distribution $p(x, t|x_0)$ associated to the Langevin Equation (1). Show that it can be written as a continuity equation

$$\frac{\partial}{\partial t} p(x, t|x_0) = -\frac{\partial}{\partial x} J(x, t|x_0) \tag{10}$$

with

$$J(x, t|x_0) = -\frac{T}{\gamma} e^{-U(x)/T} \frac{\partial}{\partial x}\left[e^{U(x)/T} p(x, t|x_0)\right] \tag{11}$$

Correction. The Fokker-Planck equation corresponding to the dynamics in Eq. (1) reads

$$\gamma \frac{\partial}{\partial t} p(x, t|x_0) = \frac{\partial}{\partial x}\left[U'(x) p(x, t|x_0)\right] + T \frac{\partial^2}{\partial x^2} p(x, t|x_0) \ . \tag{12}$$

Dividing by γ and collecting the terms within the spatial derivative in the rhs one obtains

$$J(x, t|x_0) = -\frac{1}{\gamma} U'(x) p(x, t|x_0) - \frac{T}{\gamma}\frac{\partial}{\partial x} p(x, t|x_0) \ , \tag{13}$$

which can be easily transformed into the desired expression.

E. To obtain the escape rate, let's assume that the system is slowly relaxing ($T \ll 1$, $\partial_t p \approx 0$) with constant, uniform small current $J \ll 1$. One can then call $J = qr$, being q the probability of being in the basin around $x = x_m$ and r the escape rate from the basin.

Compute the probability q of being in the well around x_m using the equilibrium approximation $p(x) = p(x_m) e^{-[U(x) - U(x_m)]/T}$ in the small T limit, keeping $p(x_m)$ as a parameter.

Correction. In the small T limit, the probability around the minimum x_m can be approximated again with a Gaussian, giving

$$p(x) \simeq p(x_m) e^{-U''(x_m)(x - x_m)^2/(2T)} \ . \tag{14}$$

Integrating this expression on the real axis gives

$$q = \int_{-\infty}^{+\infty} \mathrm{d}x\, p(x) \simeq p(x_m)\sqrt{\frac{2\pi T}{U''(x_m)}} \tag{15}$$

F. Estimate the current J obtained in Eq. (11) under the assumption $J = \text{const}$ in terms of the properties of the minimum and maximum of the potential $U(x)$. Use the result obtained to compute the escape rate r including its prefactor.

Correction. The relation (11) can be rewritten as (neglecting x_0 and t because we are quasi-stationary)

$$\frac{\partial}{\partial x}\left[e^{U(x)/T}p(x)\right] = -\frac{\gamma}{T}e^{U(x)/T}J\ . \tag{16}$$

Integrating this expression between $x = x_m$ and $x = \Lambda \gg x_M$ one has

$$e^{U(x)/T}p(x)\Big|_{x_m}^{\Lambda} = -\frac{\gamma}{T}J\int_{x_m}^{\Lambda} e^{U(x)/T}\ . \tag{17}$$

The lhs can be approximated by the value in x_m noting that the contribution at large $x = \Lambda$ vanishes (small probability outside the well). Conversely, the integrand in the rhs is peaked around the maximum of $U(x)$ at $x = x_M$. In the small T limit, we can approximate it again as a Gaussian (knowing that $U''(x_M) < 0$) and we get

$$-\,e^{U_m/T}p(x_m) \simeq -\frac{\gamma}{T}Je^{U_M/T}\int_{-\infty}^{+\infty}\mathrm{d}x\, e^{U''(x_M)(x-x_M)^2/(2T)} = -\frac{\gamma}{T}Je^{U_M/T}\sqrt{\frac{2\pi T}{|U''(x_M)|}}\ . \tag{18}$$

Therefore we find

$$J = p(x_m)\frac{T}{\gamma}\sqrt{\frac{|U''(x_M)|}{2\pi T}}e^{-\Delta U/T}\ . \tag{19}$$

The escape rate is given by $r = J/q$, which immediately gives

$$r = \frac{1}{2\pi\gamma}\sqrt{U''(x_m)|U''(x_M)|}e^{-\Delta U/T}\ . \tag{20}$$

The time scales associated to the escape from the barrier are given by the curvature of the maximum and minimum of the potential; higher curvature leads to faster escape. Also a low friction coefficient enhances the escape rate, as one would expect as friction corresponds to stronger damping.

Nonequilibrium soft and active matter: TD5

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1 Colloidal cyclic engine

A. Consider the overdamped Langevin dynamics of a colloidal particle confined in a harmonic trap. Give the expression of the average work and heat associated with varying the trap stiffness k.

Correction. The dynamics for a given potential $U(x(t), k(t)) = k(t)x(t)^2/2$ reads

$$\gamma\dot{x} = -kx + \eta, \quad \langle\eta(t)\eta(0)\rangle = 2\gamma T\delta(t). \tag{1}$$

The average work and heat are defined as

$$\begin{aligned} \langle\mathcal{W}\rangle &= \int_0^t dt'\dot{k}\langle\partial_k U(k(t'), x(t'))\rangle = \int_0^t dt'\frac{\dot{k}}{2}\langle x^2(t')\rangle, \\ \langle\mathcal{Q}\rangle &= -\int_0^t dt'\langle\dot{x}(t')\partial_x U(k(t'), x(t'))\rangle = -\int_0^t dt' k(t')\langle\dot{x}(t')x(t')\rangle. \end{aligned} \tag{2}$$

Using the chain rule, we also get

$$\frac{k(t)}{2}\langle x^2(t)\rangle - \frac{k(0)}{2}\langle x^2(0)\rangle = \langle\mathcal{W} - \mathcal{Q}\rangle. \tag{3}$$

B. For a quasistatic protocol from $k(0) = k_0$ to $k(t) = k_1$, derive the average work and heat.

Correction. For a quasistatic protocol, the averages are evaluated in steady state:

$$\begin{aligned} \langle\mathcal{W}\rangle_{qs} &= \int_0^t dt'\frac{\dot{k}}{2}\langle x^2(t')\rangle_s = \frac{1}{2}\int_{k(0)}^{k(t)}\langle x^2\rangle_s dk, \\ \langle\mathcal{Q}\rangle_{qs} &= -\frac{1}{2}\int_0^t dt' k(t')\frac{d}{dt}\langle x(t')^2\rangle_s. \end{aligned} \tag{4}$$

Using the equipartition theorem $\langle x^2\rangle_s = T/k$, we get

$$\langle\mathcal{W}\rangle_{qs} = \frac{T}{2}\int_{k_0}^{k_1}\frac{dk}{k} = \frac{T}{2}\ln\frac{k_1}{k_0}. \tag{5}$$

Besides, since the average potential energy is constant $\langle U\rangle = T/2$, we deduce $\langle\mathcal{Q}\rangle_{qs} = \langle\mathcal{W}\rangle_{qs}$.

C. Consider a cyclic engine which performs the following successive transformations:

$$\begin{aligned} &(1) \quad k: k_0 \to k_1, \quad && T = T_0, \\ &(2) \quad k = k_1, && T: T_0 \to T_1, \\ &(3) \quad k: k_1 \to k_0, && T = T_1, \\ &(4) \quad k = k_0, && T: T_1 \to T_0, \end{aligned} \tag{6}$$

where (1) and (3) are quasistatic. Determine the constraint on the parameters $\{k_0, k_1, T_0, T_1\}$ so that the engine extracts work, namely the average work of the whole cycle $\langle\mathcal{W}_{\text{tot}}\rangle$ is negative. Compute the corresponding efficiency $\mathcal{E} = -\langle\mathcal{W}_{\text{tot}}\rangle/\langle\mathcal{Q}_{\text{hot}}\rangle$, where $\langle\mathcal{Q}_{\text{hot}}\rangle$ is the average heat dissipated while heating and maintaining the system at high temperature.

Correction. There is not any work associated with the transformations (2) and (4), so that the total quasistatic work reads

$$\langle \mathcal{W}_{\rm tot} \rangle = \frac{T_0}{2} \ln \frac{k_1}{k_0} + \frac{T_1}{2} \ln \frac{k_0}{k_1} = \frac{T_0 - T_1}{2} \ln \frac{k_1}{k_0}. \tag{7}$$

To extract work, one must take $(k_1 - k_0)(T_1 - T_0) > 0$. By analogy with the Stirling cycle, where here $\langle x^2 \rangle$ plays the role of the volume, (1) is a compression at low temperature, and (3) is an expansion at high temperature. Taking $T_1 > T_0$, the heat $\mathcal{Q}_{\rm hot}$ is associated with (2) and (3), which can be deduced from the first law as

$$\mathcal{Q}_{\rm hot} = \mathcal{Q}_2 + \mathcal{Q}_3, \quad \langle \mathcal{Q}_2 \rangle = \frac{T_0 - T_1}{2}. \quad \langle \mathcal{Q}_3 \rangle = \frac{T_1}{2} \ln \frac{k_0}{k_1}, \tag{8}$$

The efficiency follows as

$$\mathcal{E} = \mathcal{E}_c \Big[1 + \mathcal{E}_c / \ln(k_1/k_0) \Big]^{-1}, \tag{9}$$

where $\mathcal{E}_c = 1 - T_0/T_1$ is the Carnot efficiency.

D. Find how to modify the cycle to reach the Carnot efficiency $\mathcal{E}_c = 1 - T_0/T_1 < 1$.

Correction. The Carnot cycle consists in replacing (2) and (4) with adiabatic transformations where $\langle \mathcal{Q} \rangle_{qs} = 0$. From (4), it follows that these correspond to $\langle x^2 \rangle_s = T/k$ constant, namely both $k(t)$ and $T(t)$ vary in time at fixed $k(t)/T(t)$. The cycle then consists of the following successive transformations:

$$\begin{aligned}
&(1) \quad k : k_0 \to k_1, \quad T = T_0, \\
&(2) \quad k : k_1 \to k_2, \quad T : T_0 \to T_1, \\
&(3) \quad k : k_2 \to k_3, \quad T = T_1, \\
&(4) \quad k : k_3 \to k_0, \quad T : T_1 \to T_0,
\end{aligned} \tag{10}$$

where $k_2 = k_1 T_1/T_0$ and $k_3 = k_0 T_1/T_0$. Since there is no heat associated with (2) and (4), the corresponding work reads

$$\langle \mathcal{W}_2 + \mathcal{W}_4 \rangle = \frac{T_1 - T_0}{2} + \frac{T_0 - T_1}{2} = 0, \tag{11}$$

so that the total work follows as

$$\langle \mathcal{W}_{\rm tot} \rangle = \frac{T_0}{2} \ln \frac{k_1}{k_0} + \frac{T_1}{2} \ln \frac{k_3}{k_2} = \frac{T_0 - T_1}{2} \ln \frac{k_1}{k_0}. \tag{12}$$

Taking the same definition of efficiency as for the Stirling cycle, and using

$$\mathcal{Q}_{\rm hot} = \mathcal{Q}_2 + \mathcal{Q}_3, \quad \langle \mathcal{Q}_2 \rangle = 0. \quad \langle \mathcal{Q}_3 \rangle = \frac{T_1}{2} \ln \frac{k_3}{k_2} = \frac{T_1}{2} \ln \frac{k_0}{k_1}, \tag{13}$$

we readily deduce $\mathcal{E} = \mathcal{E}_c$.

Nonequilibrium soft and active matter: TD6

Department of Physics and Materials Science, University of Luxembourg

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1 Optimal control of Brownian particle

A. Consider the overdamped Langevin dynamics of a colloidal particle confined in a potential with control parameter α. Give the expression of the average work associated with varying α.

Correction. The dynamics for a given potential $U(x(t), \alpha(t))$ reads

$$\gamma \dot{x} = -\partial_x U + \eta, \quad \langle \eta(t)\eta(0)\rangle = 2\gamma T \delta(t). \tag{1}$$

The average work is defined as

$$\langle \mathcal{W} \rangle = \int_0^t dt' \dot{\alpha}(t') \langle \partial_\alpha U(x(t'), \alpha(t')\rangle. \tag{2}$$

B. Consider the response function associated with measuring the effect on $\langle \partial_\alpha U \rangle$ of perturbing the dynamics by increasing $\alpha(t)$ by a small amount $\Delta\alpha$. Give the expression of the response in terms of an appropriate correlation function.

Correction. The response function R is defined by

$$\langle \partial_\alpha U(x(t), \alpha(t))\rangle - \langle \partial_\alpha U \rangle_s = \int_{-\infty}^t dt' \Big[\alpha(t') - \alpha(t)\Big] R(t - t'), \tag{3}$$

where $\langle \partial_\alpha U \rangle_s$ is the steady state average. The perturbation $\alpha \to \alpha - \Delta\alpha$ amounts to changing the potential as $U \to U - \Delta\alpha \partial_\alpha U$. It follows that $\partial_\alpha U$ is both the observable which perturbs the energy, and the observable with respect to which the perturbation is measured. The fluctuation-dissipation theorem then reads:

$$R(t - t') = -\frac{1}{T}\frac{d}{dt}\Big\langle \Big[\partial_\alpha U(x(t), \alpha(t)) - \langle \partial_\alpha U \rangle_s\Big] \partial_\alpha U(x(t'), \alpha(t'))\Big\rangle, \tag{4}$$

which can also be written as

$$R(t - t') = \frac{1}{T}\frac{d}{dt'} \langle \partial_\alpha U(x(t), \alpha(t)) \partial_\alpha U(x(t'), \alpha(t'))\rangle_c, \tag{5}$$

where we have introduced the connected correlation $\langle A(t)B(t')\rangle_c = \langle A(t)B(t')\rangle - \langle A\rangle_s \langle B\rangle_s$.

C. Assuming that the control parameter varies slowly in time, show that the average work reads

$$\langle \mathcal{W} \rangle = \langle \mathcal{W} \rangle_{qs} + \int_0^t \dot{\alpha}(t')^2 \zeta(\alpha(t'))dt', \tag{6}$$

where $\langle \mathcal{W} \rangle_{qs}$ is the average quasistatic work, and $\zeta(\alpha)$ can be written in terms of an appropriate correlation function.

Correction. Substituting the definition of the response (3) into that of work (2), we get

$$\langle \mathcal{W} \rangle = \langle \mathcal{W} \rangle_{qs} + \int_0^t dt' \dot{\alpha}(t') \int_{-\infty}^{t'} dt'' \Big[\alpha(t'') - \alpha(t')\Big] R(t' - t''), \quad \langle \mathcal{W} \rangle_{qs} = \int_{\alpha(0)}^{\alpha(t)} \langle \partial_\alpha U \rangle_s d\alpha. \tag{7}$$

Expanding the control parameter to leading order as $\alpha(t'') = \alpha(t') + (t'' - t')\dot{\alpha}(t')$, we deduce

$$\langle \mathcal{W} \rangle = \langle \mathcal{W} \rangle_{qs} + \int_0^t dt' \dot{\alpha}(t')^2 \int_{-\infty}^{t'} dt''(t'' - t')R(t' - t''). \tag{8}$$

Finally, using the fluctuation-dissipation theorem (5), the work can be written as in (6), where

$$\zeta(\alpha) = \frac{1}{T} \int_{-\infty}^{t'} dt''(t'' - t') \frac{d}{dt''} \langle \partial_\alpha U(x(t'), \alpha(t')) \partial_\alpha U(x(t''), \alpha(t'')) \rangle_c, \tag{9}$$

and, with the change of variable $t'' \to t' - t''$, the term $\zeta(\alpha)$ reads

$$\zeta(\alpha) = -\frac{1}{T} \int_0^{\infty} dt'' t'' \frac{d}{dt''} \langle \partial_\alpha U(x(t''), \alpha(t'')) \partial_\alpha U(x(0), \alpha(0)) \rangle_c, \tag{10}$$

where we have used the invariance of correlations under time reversal and time translation.

D. Deduce that, for the optimal protocol, the correction to the average quasistatic work scales like the inverse of the protocol time.

Correction. The optimal protocol follows from minimizing $\int_0^t \mathcal{L}(\alpha, \dot{\alpha}) dt'$ with Lagrangian $\mathcal{L}(\alpha, \dot{\alpha}) = \dot{\alpha}^2 \zeta(\alpha)$. The associated Euler-Lagrange equation $\partial_\alpha \mathcal{L} = (d/dt)\partial_{\dot{\alpha}} \mathcal{L}$ corresponds here to

$$\dot{\alpha}^2 \zeta(\alpha) = \mathcal{E}, \tag{11}$$

where $\mathcal{E}$ is constant throughout the protocol. Using separation of variable, and integrating over the whole protocol, we get

$$\int_{\alpha(0)}^{\alpha(t)} \sqrt{\zeta(\alpha)} d\alpha = \sqrt{\mathcal{E}} \int_0^t dt', \tag{12}$$

yielding $\mathcal{E} \sim 1/t^2$. We then deduce the following scaling

$$\langle \mathcal{W} \rangle - \langle \mathcal{W} \rangle_{qs} = \mathcal{E} \int_0^t dt' \sim 1/t. \tag{13}$$

Nonequilibrium soft and active matter: TD7

Department of Physics and Materials Science, University of Luxembourg

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1 Active particle in a harmonic trap

Consider the $1d$ dynamics of an Active Ornstein-Uhlenbeck Particle (AOUP) in a harmonic potential $U(x) = \frac{1}{2}kx^2$

$$\begin{aligned} \gamma\dot{x}(t) &= -kx(t) + f(t) + \xi(t) \ , \quad \langle\xi(t)\xi(0)\rangle = 2\gamma T\delta(t) \ , \\ \dot{f}(t) &= -\frac{1}{\tau}f(t) + \eta(t) \ , \quad \langle\eta(t)\eta(0)\rangle = \frac{2v_0^2}{\tau}\delta(t) \ , \\ \langle\xi(t)\eta(0)\rangle &= \langle\xi(0)\eta(t)\rangle = 0 \ . \end{aligned} \tag{1}$$

A. Give an explicit solution for $x(t)$ in function of $f(t)$ and $\xi(t)$, assuming $x(0) = 0$.

Correction. The solution can be found noting that the homogeneous equation associated to Eq. (1) reads $\gamma\dot{x}(t) = -kx(t)$, which admits solutions $x(t) = Ae^{-kt/\gamma}$. With the method of undetermined coefficients, we can find a solution assuming $x(t) = A(t)e^{-kt/\gamma}$; plugging this into Eq. (1) one has

$$\begin{aligned} \gamma\dot{A}(t)e^{-kt/\gamma} &= f(t) + \xi(t) \\ A(0) = x(0) &= 0 \ . \end{aligned} \tag{2}$$

Bringing the exponential and $1/\gamma$ to the rhs, $A(t)$ is determined by integrating the two sides

$$A(t) = A(t) - A(0) = \frac{1}{\gamma}\int_0^t ds\, e^{ks/\gamma}\left[f(s) + \xi(s)\right] \ , \tag{3}$$

which finally gives for $x(t)$

$$x(t) = \frac{1}{\gamma}\int_0^t ds\, e^{-k(t-s)/\gamma}\left[f(s) + \xi(s)\right] \ . \tag{4}$$

B. Compute the average $\langle x^2(t)\rangle$ using the explicit solution from point **A** and the correlation function $\langle f(t)f(t')\rangle$.

Correction. Squaring and averaging the solution found above one has

$$\langle x^2(t)\rangle = \frac{1}{\gamma^2}\int_0^t\int_0^t dt_1dt_2e^{-k(2t-t_1-t_2)/\gamma}\langle f(t_1)f(t_2) + f(t_1)\xi(t_2) + f(t_2)\xi(t_1) + \xi(t_1)\xi(t_2)\rangle \ . \tag{5}$$

The correlations can be computed in this way from right to left

- $\langle\xi(t_1)\xi(t_2)\rangle = 2\gamma T\delta(t_1 - t_2)$ is the thermal white noise
- $\langle f(t_1)\xi(t_2)\rangle = \langle\xi(t_1)f(t_2)\rangle = 0$ because $f(t)$ depends only on $\eta(t)$ which is independent from $\xi(t)$, therefore the correlations factorize as $\langle\xi(t_1)f(t_2)\rangle = \langle\xi(t_1)\rangle\langle f(t_2)\rangle = 0$.
- $\langle f(t_1)f(t_2)\rangle = v_0^2e^{-|t_1-t_2|/\tau}$ as it has been shown from Eq. (1) during the lecture.

So

$$x^2(t) = \frac{1}{\gamma^2}\int_0^t\int_0^t dt_1dt_2e^{-k(2t-t_1-t_2)/\gamma}\left[v_0^2e^{-|t_1-t_2|/\tau} + 2\gamma T\delta(t_1 - t_2)\right] \ . \tag{6}$$

The delta function contribution can be integrated over t_2 by replacing $t_2 = t_1$ in the integrand and gives

$$\begin{aligned}\frac{1}{\gamma^2}\int_0^t\int_0^t dt_1 dt_2 e^{-k(2t-t_1-t_2)/\gamma} 2\gamma T\delta(t_1-t_2) = \frac{2T}{\gamma}\int_0^t dt_1 e^{-2k(t-t_1)/\gamma} = \frac{2T}{\gamma}\frac{\gamma}{2k}\left(1-e^{-2kt/\gamma}\right) \\ = \frac{T}{k}\left(1-e^{-2kt/\gamma}\right) \ .\end{aligned} \tag{7}$$

The contribution from the exponential is symmetric by exchanging $t_1 \leftrightarrow t_2$ in the integral. It can be therefore integrated in the triangle $0 < t_1 < t$, $0 < t_2 < t_1$ where $|t_1 - t_2| = t_1 - t_2$ and then doubled. So one has

$$\begin{aligned}&\frac{1}{\gamma^2}\int_0^t\int_0^t dt_1 dt_2 e^{-k(2t-t_1-t_2)/\gamma} v_0^2 e^{-|t_1-t_2|/\tau} \\ &\quad = \frac{2v_0^2}{\gamma^2}\int_0^t\int_0^{t_1} dt_1 dt_2 e^{-k(2t-t_1-t_2)/\gamma} v_0^2 e^{-(t_1-t_2)/\tau} \\ &\quad = \frac{2v_0^2}{\gamma^2} e^{-2kt/\gamma}\int_0^t dt_1 e^{(k/\gamma-1/\tau)t_1}\int_0^{t_1} dt_2 e^{(k/\gamma+1/\tau)t_2} \\ &\quad = \frac{2v_0^2}{\gamma^2} e^{-2kt/\gamma}\int_0^t dt_1 e^{(k/\gamma-1/\tau)t_1}\frac{\gamma\tau}{\gamma+k\tau}\left(e^{(k/\gamma+1/\tau)t_1}-1\right) \\ &\quad = \frac{2v_0^2}{\gamma^2} e^{-2kt/\gamma}\frac{\gamma\tau}{\gamma+k\tau}\int_0^t dt_1\left(e^{2kt_1/\gamma}-e^{(k/\gamma-1/\tau)t_1}\right) \\ &\quad = \frac{2v_0^2\tau}{\gamma(\gamma+k\tau)} e^{-2kt/\gamma}\left[\frac{\gamma}{2k}\left(e^{2kt/\gamma}-1\right)-\frac{\gamma\tau}{\gamma-k\tau}\left(e^{(k/\gamma-1/\tau)t}-1\right)\right] \\ &\quad = \frac{2v_0^2\tau}{\gamma+k\tau}\left[\frac{1}{2k}\left(1-e^{-2kt/\gamma}\right)-\frac{\tau}{\gamma-k\tau}\left(e^{-(k/\gamma+1/\tau)t}-e^{-2kt/\gamma}\right)\right] \ .\end{aligned} \tag{8}$$

The sum of the two contributions then gives

$$\left\langle x^2(t)\right\rangle = \left(\frac{T}{k}+\frac{\tau}{\gamma+k\tau}\frac{v_0^2}{k}\right)\left(1-e^{-2kt/\gamma}\right)+\frac{2v_0^2\tau^2}{k^2\tau^2-\gamma^2}\left(e^{-(k/\gamma+1/\tau)t}-e^{-2kt/\gamma}\right) \tag{9}$$

C. Prove that in the steady state one has

$$\lim_{t\to\infty}\left\langle x^2(t)\right\rangle = \left\langle x^2\right\rangle_s = \frac{T}{k}+\frac{\tau}{\gamma+k\tau}\frac{v_0^2}{k} \ . \tag{10}$$

Use the result to compute $\langle U(x)\rangle_s$ and discuss the change of energy equipartition induced by the activity.

Correction. Taking the limit $t \to \infty$ in Eq. (9), all the exponentials have negative coefficients in front of t and so they vanish in that limit. The only surviving term is then

$$\lim_{t\to\infty}\left\langle x^2(t)\right\rangle = \left\langle x^2\right\rangle_s = \frac{T}{k}+\frac{\tau}{\gamma+k\tau}\frac{v_0^2}{k} \ , \tag{11}$$

which proves the relation.

It is straightforward that, with $U(x) = \frac{1}{2}kx^2$, one has

$$\langle U(x)\rangle_s = \frac{1}{2}k\left\langle x^2\right\rangle_s = \frac{T}{2}+\frac{\tau}{\gamma+k\tau}\frac{v_0^2}{2} \ . \tag{12}$$

The equipartition relation $\langle U(x)\rangle_s = T/2$ is broken by the activity that introduces an additional contribution to the internal energy.

2 Monothermal engine with active particles

Using active particles it is possible to extract work from a quasistatic protocol with a constant temperature T. Consider an AOUP dynamics as described in Eq. (1).

The control parameters for this system are the potential stiffness k, the persistence time τ, the self-propulsion speed v_0 and the friction γ. Indicating a generic couple of control parameters with α and β, the extracted work in a protocol on the (α, β) plane is given by

$$\begin{aligned}\langle \mathcal{W} \rangle_{\text{qs}} &= \int_0^t \left[\dot{\alpha}(t) \langle \partial_\alpha U \rangle_s + \dot{\beta}(t) \langle \partial_\beta U \rangle_s \right] dt \\ &= \oint_{\partial\Sigma} \left[\langle \partial_\alpha U \rangle_s d\alpha + \langle \partial_\beta U \rangle_s d\beta \right] \\ &= \pm \iint_\Sigma \left[-\partial_\beta \langle \partial_\alpha U \rangle_s + \partial_\alpha \langle \partial_\beta U \rangle_s \right] d\alpha d\beta \end{aligned} \tag{13}$$

where Σ denotes the surface enclosed by the protocol contour $\partial\Sigma$ in the plane, and the $\pm$ sign in the last line depends on the protocol orientation (+ for counterclockwise, $-$ for clockwise).

D. Which control parameter must be necessarily varied along a protocol to extract work from the AOUP dynamics at constant T?

Correction. The work along a quasistatic protocol over the control parameters α_i reads

$$\langle \mathcal{W} \rangle_s = \sum_i \int_0^t dt\, \dot{\alpha}_i(t) \langle \partial_{\alpha_i} U(x) \rangle_s \tag{14}$$

Since $U(x) = \frac{1}{2} k x^2$, it is necessary to vary the potential stiffness k to extract work from a monothermal protocol.

E. Give the extracted work from a quasistatic rectangular protocol in the stiffness-persistence plane, taking $k \in [k_1 : k_2]$ and $\tau \in [\tau_1 : \tau_2]$.

Correction. The extracted work in a $2d$ protocol is given by

$$\langle \mathcal{W} \rangle_{\text{qs}} = \int_0^t \dot{k}(t) \langle \partial_k U \rangle_s = \oint_{\partial\Sigma} \langle \partial_k U \rangle_s dk. \tag{15}$$

For an harmonic potential, one immediately has $\partial_k U = \frac{1}{2} x^2$ and $\partial_\tau U = \langle \partial_\tau U \rangle = 0$.
Using the stationary position fluctuations for AOUPs, one has

$$\langle x^2 \rangle_s = \frac{T}{k} + \frac{\tau}{\gamma + k\tau} v_0^2 , \quad \langle \partial_k U \rangle_s = \frac{1}{2} \langle x^2 \rangle_s . \tag{16}$$

The integral over the rectangular contour in the (k, τ) plane reads

$$\begin{aligned}\langle \mathcal{W} \rangle_{\text{qs}} &= \int_{k_1}^{k_2} \int_{\tau_1}^{\tau_2} dk d\tau\, \partial_\tau \langle \partial_k U \rangle_s \\ &= \int_{k_1}^{k_2} dk \left[\langle \partial_k U \rangle_s (\tau_2) - \langle \partial_k U \rangle_s (\tau_1) \right] \\ &= \int_{k_1}^{k_2} dk \left(\frac{\tau_2}{\gamma + k\tau_2} - \frac{\tau_1}{\gamma + k\tau_1} \right) \frac{v_0^2}{k} \\ &= \frac{v_0^2}{\gamma} \left[\tau_1 \ln \frac{k_2(\gamma + k_1\tau_2)}{k_1(\gamma + k_2\tau_2)} - \tau_2 \ln \frac{k_2(\gamma + k_1\tau_1)}{k_1(\gamma + k_2\tau_1)} \right] \end{aligned} \tag{17}$$

The last expression is non-vanishing if $k_1 \neq k_2$ and $\tau_1 \neq \tau_2$, proving that we can extract work from the the motion of an active particle even at constant temperature.

F. Give the extracted work from a quasistatic rectangular protocol in the stiffness-speed plane, taking $k \in [k_1 : k_2]$ and $v_0 \in [v_1 : v_2]$.

Correction. The computation above can be repeated in the (k, v_0) plane, obtaining

$$\langle \mathcal{W} \rangle_{\mathrm{qs}} = \frac{v_2^2 - v_1^2}{2\gamma} \tau \ln \frac{k_2(\gamma + k_1 \tau)}{k_1(\gamma + k_2 \tau)} \ . \tag{18}$$

Nonequilibrium soft and active matter: TD8

Department of Physics and Materials Science, University of Luxembourg

1 Active Matter in a confining potential

A. Consider a colloidal Run-and-Tumble Particle (RTP) moving along a 1-dimensional axis x, subject to a potential $U(x)$ and to a thermal bath with mobility μ and vanishing temperature $T = 0$. The particle in $1d$ can only have two orientations $\sigma(t) = \pm 1$, corresponding to self-propulsion $f(t) = v_0\sigma(t)$, and the orientation changes following a Poissonian process with tumble rate $\lambda/2$.

At zero temperature the dynamics is given by

$$\dot{x} = -\mu U'(x) + v_0\sigma(t) \ . \tag{1}$$

and the Master Equation reads

$$\begin{aligned} \partial_t P_+ &= \partial_x \left(\mu U'(x) - v_0\right) P_+ - \frac{\lambda}{2}(P_+ - P_-) \ , \\ \partial_t P_- &= \partial_x \left(\mu U'(x) + v_0\right) P_- + \frac{\lambda}{2}(P_+ - P_-) \ , \end{aligned} \tag{2}$$

being $P_\pm(x,t)$ the density of $\pm$ particles in x at time t.

A. Write the evolution equations for the global density $\rho(x,t) = P_+(x,t) + P_-(x,t)$ and the magnetisation $m(x,t) = P_+(x,t) - P_-(x,t)$. Decouple the equations and prove that the steady state solution for $\rho(x)$ reads

$$\rho(x) \propto \left[1 - \left(\frac{\mu U'(x)}{v_0}\right)^2\right]^{-1} \exp\left[-\int_0^x \frac{\lambda\mu U'(y)}{v_0^2 - (\mu U'(y))^2} dy\right] \Theta(x^* - |x|) \ , \tag{3}$$

assuming a generic even potential $U(x)$ and being x^* determined by the condition $U'(x^*) = v_0/\mu$.

Correction. Adding and substracting Eq. (2) one finds

$$\begin{aligned} \partial_t \rho &= \partial_x \left(\mu U'(x)\rho - v_0 m\right) \ , \\ \partial_t m &= \partial_x \left(\mu U'(x) m - v_0\rho\right) - \lambda m \ . \end{aligned} \tag{4}$$

The first equation defines a density current $J(x,t) = \mu U'(x)\rho - v_0 m$ which must be constant and vanish at boundaries in the steady state, therefore one has $J = 0$ therein and the magnetisation reads $m(x) = (\mu U'(x)/v_0)\rho(x)$. Substituting in the second equation one has

$$\frac{d}{dx}\left\{\left[1 - \left(\frac{\mu U'(x)}{v_0}\right)^2\right]\rho(x)\right\} + \frac{\lambda\mu U'(x)}{v_0^2}\rho(x) = 0 \ . \tag{5}$$

This equation can be solved defining the auxiliary field $\bar{\rho}(x) = \left[1 - \left(\frac{\mu U'(x)}{v_0}\right)^2\right]\rho(x)$, for which one has

$$\frac{d}{dx}\bar{\rho}(x) + \frac{\lambda\mu}{v_0^2}\frac{U'(x)}{1 - \left(\frac{\mu U'(x)}{v_0}\right)^2}\bar{\rho}(x) = 0 \ . \tag{6}$$

The last equation can now be integrated by separation of variables; bringing $\bar{\rho}(x)$ in the lhs and the other terms in the rhs, one has

$$\frac{1}{\bar{\rho}(x)}\frac{d}{dx}\bar{\rho}(x) = \frac{d}{dx}\ln\bar{\rho}(x) = -\frac{\lambda\mu}{v_0^2}\frac{U'(x)}{1 - \left(\frac{\mu U'(x)}{v_0}\right)^2} \quad \Rightarrow \quad \ln\bar{\rho}(x) = -\frac{\lambda\mu}{v_0^2}\int_0^x \frac{U'(y)}{1 - \left(\frac{\mu U'(y)}{v_0}\right)^2} dy + \ln\bar{\rho}_0 \tag{7}$$

Assuming an even, confining potential $U(x)$, the integral above can be performed for all $|x| < x^*$, where $U'(x^*) = v_0/\mu$.

At this position the conservative force balances the outward active self-propulsion, and the particle cannot climb the potential any further.
Coming back to the original density field $\rho(x)$ we finally find

$$\rho(x) = \rho_0 \left[1 - \left(\frac{\mu U'(x)}{v_0}\right)^2\right]^{-1} \exp\left[-\int_0^x \frac{\lambda\mu U'(y)}{v_0^2 - (\mu U'(y))^2} dy\right] \Theta(x^* - |x|) \,, \tag{8}$$

being ρ_0 determined by normalisation. The magnetisation follows accordingly.

B. Find the stationary solution for the density and magnetisation field in an harmonic potential $U(x) = \frac{1}{2}kx^2$. Identify the distribution width x^* and the exponent governing the adhesion/repulsion of the RTPs to the barrier at $x = \pm x^*$.

Correction. Substituting $U(x) = \frac{1}{2}kx^2$ in Eq. (3) one has

$$\begin{aligned}\rho(x) &= \tilde{\rho}_0 \left[1 - \left(\frac{\mu k}{v_0} x\right)^2\right]^{-1+\frac{\lambda}{2\mu k}} \Theta(v_0/\mu k - |x|) \\ &= \tilde{\rho}_0 \left[1 - (x/x^*)^2\right]^\alpha \Theta(x^* - |x|) \,,\end{aligned} \tag{9}$$

being then $x^* = v_0/\mu k$, and $\alpha = -1 + \lambda/(2\mu k)$ and $\tilde{\rho}_0$ a new normalisation factor. The magnetisation reads

$$m(x) = \frac{\mu U'(x)}{v_0}\rho(x) = \frac{x}{x^*}\rho(x) \,. \tag{10}$$

The exponent α controls the adhesion to the boundaries at $x = \pm x^*$. Indeed $\alpha > -1$, therefore the global density is finite. If $\alpha < 0$ (high self-propulsion speed v_0, high persistence time $\tau = 1/\lambda$), the density diverges close to the boundaries, *i.e.* the RTPs tend to accumulate close to them.
If $\alpha = 0$ ($\lambda = 2\mu k$), the density is uniform between $-x^*$ and x^*.
Finally, if $\alpha > 0$ (low self-propulsion, low persistence), the barrier is repulsive and $\rho(\pm x^*) = 0$.

C. Prove that in the equilibrium limit $\lambda = 1/\tau \to +\infty$ and $v_0^2 = \lambda\mu T$ the density profile $\rho(x)$ from Eq. (3) converges to the equilibrium distribution $\rho(x) \propto e^{-U(x)/T}$. Discuss how the departure from equilibrium (finite tumble rate *i.e.* persistence) affects the equilibrium solution.

Correction. Substituting $v_0^2 = \lambda\mu T$ in Eq. (3), one has

$$\rho(x) = \rho_0 \left[1 - \frac{\mu U'(x)^2}{\lambda T}\right]^{-1} \exp\left[-\int_0^x \frac{\lambda\mu U'(y)}{\lambda\mu T - (\mu U'(y))^2} dy\right] \Theta(x^* - |x|) \,, \tag{11}$$

The barrier at x^* diverges as $x^* = \sqrt{\lambda T/\mu k^2}$, therefore the particles are not confined in the equilibrium limit. Taking the limit $\lambda \to \infty$ in Eq. (3), the second term goes to 1 and the second reduces to $\exp(-U(x)/T)$, therefore

$$\lim_{\substack{\lambda\to\infty \\ v_0^2=\lambda\mu T}} \rho(x) = \frac{e^{-U(x)/T}}{Z} \tag{12}$$

Nonequilibrium soft and active matter: TD9

Department of Physics and Materials Science, University of Luxembourg

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1 The pressure of active particles

Consider a $2d$ system of particles in the plane (x, y), with bulk density ρ_0 and temperature T. The particles do not interact with each other, but interact with a wall parallel to the y axis, represented by the wall potential $V(x)$. The walls start at $x = \pm x_w$, so $V(x) = 0$ for $|x| < x_w$, and confines the particles, namely $V(x \to \pm\infty) = +\infty$.

The pressure on the wall at $x = x_w$ can be then computed as the force per unit length exerted by the particles on it, i.e. $-F_w(x) = \partial_x V(x)$ using Newton's third law. One then has

$$P = -\int_0^{+\infty} dx \rho(x) F_w(x) = \int_0^{+\infty} dx \rho(x) \partial_x V(x) \ , \tag{1}$$

being $\rho(x) = \left\langle \sum_{i=1}^N \delta(x - x_i) \right\rangle$ the single-particle density function along the x-axis. The system is translationally invariant along y, therefore $\rho(\mathbf{r}) = \rho(x)$.

A. Show that at equilibrium the pressure P exerted by non-interacting particles corresponds to the ideal gas law.

Correction. At equilibrium, the density reads $\rho(x) = \rho_0 e^{-V(x)/T}$. Then

$$P = \int_0^{+\infty} dx \rho_0 e^{-V(x)/T} \partial_x V(x) = -\rho_0 T \int_0^{+\infty} dx \frac{d}{dx} e^{-V(x)/T} = \rho_0 T \tag{2}$$

having exploited that $V(+\infty) = +\infty$. This gives the ideal gas law in natural units where $k_B = 1$.

B. Consider a system of non-interacting Run-and-Tumble Particles (RTP) in $2d$ with self-propulsion speed v_0 and tumble rate α, confined by a wall $V(x)$ as in the previous part. Assuming that there the system is uniform over the y axis, the dynamics of the single-particle position and angle distribution $\mathcal{P}(x, \theta, t)$ is described by the Master Equation

$$\partial_t \mathcal{P} = -\partial_x \left[\left(v_0 \cos\theta - \mu_t \partial_x V(x) \right) \mathcal{P} - D_t \partial_x \mathcal{P} \right] - \alpha \mathcal{P} + \frac{\alpha}{2\pi} \int_0^{2\pi} d\theta' \, \mathcal{P}(x, \theta', t) \ . \tag{3}$$

The n-th angular moment of the stationary distribution is defined as $m_n(x) = \int_0^{2\pi} d\theta \, \cos(n\theta) \, \mathcal{P}(x, \theta)$. Derive from Eq. (3) the equations for $m_0(x) = \rho(x)$ and $m_1(x)$ and use this result to compute the pressure from Eq. (1).

Correction. Integrating Eq. (3) over $0 < \theta < 2\pi$ and setting $\partial_t = 0$ (steady state) one has the equation for $\rho(x)$:

$$0 = -\partial_x \left[v_0 m_1(x) - \mu_t (\partial_x V(x)) \rho(x) - D_t \partial_x \rho(x) \right] \ . \tag{4}$$

Multiplying both sides by $\cos\theta$ and repeating the integration one finds for $m_1(x)$:

$$0 = -\partial_x \left[v_0 \frac{\rho(x) + m_2(x)}{2} - \mu_t (\partial_x V(x)) m_1(x) - D_t \partial_x m_1(x) \right] - \alpha m_1(x) \ . \tag{5}$$

The first result defines a density current $\partial_x J = 0$, which must vanish in any confined system. Then

$$(\partial_x V(x)) \rho(x) = \frac{1}{\mu_t} \left[v_0 m_1(x) - D_t \partial_x \rho(x) \right] \quad \Rightarrow \quad P = \frac{1}{\mu_t} \int_0^{+\infty} dx \left[v_0 m_1(x) - D_t \partial_x \rho(x) \right] \ . \tag{6}$$

The second equation gives $m_1(x)$ in terms of a current derivative. Bringing $m_1(x)$ from Eq. (5) in the lhs and substituting it in the rhs of Eq. (6) we find

$$\begin{aligned} P &= \frac{1}{\mu_t}\int_0^{+\infty} dx\, \partial_x \left\{ \frac{v_0}{\alpha}\left[-v_0 \frac{\rho(x)+m_2(x)}{2} + \mu_t(\partial_x V(x)) m_1(x) + D_t \partial_x m_1(x)\right] - D_t\rho(x)\right\} \\ &= \frac{1}{\mu_t}\left(\frac{v_0^2}{2\alpha} + D_t\right)\rho_0 \ , \end{aligned} \tag{7}$$

having exploited the isotropy of the system, which gives $m_n(0) = 0$ for $n > 0$, and $\rho(0) = \rho_0$ (bulk pressure). Conversely, $m_n(\infty) = 0$ for all n because of the confining wall. The non-interacting RTPs then follow an equation of state. Remarkably, if one defines $D_t = \mu_t T_p$ (passive temperature) and $v_0^2 = 2\mu_t\alpha T_a$ (active temperature), one finally has $P = (T_p + T_a)\rho_0$. Thus the activity corresponds in a temperature shift in the ideal gas law for non-interacting particles.

C. A common feature of active particles is their tendency to align with walls after a collision. This behavior is induced by an effective torque, *i.e.* an aligning term $\mu_r\Gamma(x,\theta)$ acting on the evolution of θ when particles collide with the wall. Add this term to the motion of non-interacting particles described in Eq. (3) and derive the pressure. What can you say about the equation of state?

Correction. The torque acts over $\dot{\theta}$ and the Master Equation then reads

$$\partial_t \mathcal{P} = -\partial_x\left[(v_0\cos\theta - \mu_t\partial_x V(x))\,\mathcal{P} - D_t\partial_x\mathcal{P}\right] - \alpha\mathcal{P} + \frac{\alpha}{2\pi}\int_0^{2\pi} d\theta'\, \mathcal{P}(x,\theta',t) - \mu_r\partial_\theta\left[\Gamma(x,\theta)\mathcal{P}\right] \ . \tag{8}$$

Its inclusion does not modify Eq. (4) but affects Eq. (5), which now reads

$$\begin{aligned} 0 &= -\partial_x\left[v_0\frac{\rho(x)+m_2(x)}{2} - \mu_t(\partial_x V(x))m_1(x) - D_t\partial_x m_1(x)\right] - \alpha m_1(x) - \mu_r\int_0^{2\pi} d\theta\cos\theta\,\partial_\theta\left[\Gamma(x,\theta)\mathcal{P}\right] \\ &= -\partial_x\left[v_0\frac{\rho(x)+m_2(x)}{2} - \mu_t(\partial_x V(x))m_1(x) - D_t\partial_x m_1(x)\right] - \alpha m_1(x) - \mu_r\int_0^{2\pi} d\theta\sin\theta\,\Gamma(x,\theta)\mathcal{P}(x,\theta) \ , \end{aligned} \tag{9}$$

giving the pressure

$$\begin{aligned} P =& \frac{1}{\mu_t}\int_0^{+\infty} dx\, \partial_x \left\{ \frac{v_0}{\alpha}\left[-v_0 \frac{\rho(x)+m_2(x)}{2} + \mu_t(\partial_x V(x)) m_1(x) + D_t \partial_x m_1(x)\right] - D_t\rho(x)\right\} \\ & - \frac{v_0\mu_r}{\alpha\mu_t}\int_0^{+\infty} dx \int_0^{2\pi} d\theta\, \sin\theta\,\Gamma(x,\theta)\mathcal{P}(x,\theta) \\ =& \frac{1}{\mu_t}\left(\frac{v_0^2}{2\alpha} + D_t\right)\rho_0 - \frac{v_0\mu_r}{\alpha\mu_t}\int_0^{+\infty} dx \int_0^{2\pi} d\theta\, \sin\theta\,\Gamma(x,\theta)\mathcal{P}(x,\theta) \ . \end{aligned} \tag{10}$$

The last term depends on the specific form of the wall torque $\Gamma(x,\theta)$, and on the specific distribution $\mathcal{P}(x,\theta)$ which depends as well on $\Gamma(x,\theta)$ and $V(x)$. Therefore there is no equation of state when the particles undergo a torque when interacting with the wall.

Nonequilibrium soft and active matter: TD10

Department of Physics and Materials Science, University of Luxembourg

1 Tracer dynamics: Perturbation at large density

A. Consider the overdamped Langevin dynamics of $N+1$ passive colloidal particles, interacting with the pair-wise potential $U = (1/2)\sum_{i,j=0}^{N} V(x_i - x_j)$, where $V(0) = 0$. Write down the coupled dynamics for i/ a given tracer particle with position x_0, and ii/ the stochastic density field $\rho(x,t) = \sum_{i=1}^{N} \delta[x - x_i(t)]$ of other particles.

Correction. The dynamics for the position of tracer and other particles reads

$$\begin{aligned} \gamma \dot{x}_0 &= -\sum_{j=0}^{N} \partial_{x_0} V(x_0 - x_j) + \eta_0, \quad \langle \eta_0(t)\eta_0(0)\rangle = 2\gamma T \delta(t), \\ \gamma \dot{x}_i &= -\sum_{j=0}^{N} \partial_{x_i} V(x_i - x_j) + \eta_i, \quad \langle \eta_i(t)\eta_j(0)\rangle = 2\gamma T \delta_{ij}\delta(t). \end{aligned} \tag{1}$$

Applying Itô's lemma, the dynamics of the stochastic density follows as

$$\begin{aligned} &\partial_t \rho(x,t) = \frac{1}{\gamma}\partial_x \left[T\partial_x \rho(x,t) + \rho(x,t)\left(\int dx' \rho(x',t)\partial_x V(x-x') + \partial_x V(x - x_0(t)) \right) \right] + \partial_x \Lambda(x,t), \\ &\langle \Lambda(x,t)\Lambda(x',t)\rangle = (2T\rho(x,t)/\gamma)\delta(x-x')\delta(t-t'), \end{aligned} \tag{2}$$

where we have used that, for $i \neq 0$, we can write

$$\sum_{j=0}^{N} \partial_{x_i} V(x_i - x_j) = \int \rho(x',t)\partial_{x_i} V(x_i - x')dx' + \partial_{x_i} V(x_i - x_0). \tag{3}$$

B. For large values of the total density $\rho_0 = \int dx \rho(x,t)$, consider the scaled density ϕ, defined by $\rho(x,t) = \rho_0(1 + \phi(x,t)/\sqrt{\rho_0})$, and the scaled the interaction potential $v(x) = \rho_0 V(x)$. Derive the linear dynamics of ϕ. Give the solution for the Fourier modes $\phi_q(t) = (1/L)\int e^{iqx}\phi(x,t)dx$, where L is the system size.

Correction. From the dynamics (2), we get

$$\begin{aligned} \partial_t \phi(x,t) = &\frac{1}{\gamma}\left[T(\partial_x)^2\phi(x,t) + \int dx' \phi(x',t)(\partial_x)^2 v(x-x') + (\partial_x)^2 \frac{v(x-x_0(t))}{\sqrt{\rho_0}} \right] + \partial_x \frac{\Lambda(x,t)}{\sqrt{\rho_0}} \\ &+ \frac{1}{\gamma}\partial_x \left[\frac{1}{\rho_0}\phi(x,t)\partial_x v(x-x_0(t)) + \frac{1}{\sqrt{\rho_0}}\phi(x,t)\int dx' \phi(x',t)\partial_x v(x-x') \right], \\ \langle \Lambda(x,t)\Lambda(x',t)\rangle = &(2T\rho_0/\gamma)(1 + \phi(x,t)/\sqrt{\rho_0})\delta(x-x')\delta(t-t'). \end{aligned} \tag{4}$$

To leading order, it reads

$$\begin{aligned} &\partial_t \phi(x,t) = \frac{1}{\gamma}\left[T(\partial_x)^2\phi(x,t) + \int dx' \phi(x',t)(\partial_x)^2 v(x-x') + (\partial_x)^2 \frac{v(x-x_0(t))}{\sqrt{\rho_0}} \right] + \partial_x \frac{\Lambda(x,t)}{\sqrt{\rho_0}}, \\ &\langle \Lambda(x,t)\Lambda(x',t)\rangle = (2T\rho_0/\gamma)\delta(x-x')\delta(t-t'). \end{aligned} \tag{5}$$

and, in the Fourier domain, it yields

$$\begin{aligned} &\dot{\phi}_q(t) = -\lambda(q)\phi_q(t) + (1/\sqrt{\rho_0})\Big[-(q^2/\gamma)v_q e^{iqx_0(t)} + iq\Lambda_q(t) \Big], \quad \lambda(q) = (q^2/\gamma)(T + v_q), \\ &\langle \Lambda_q(t)\Lambda_q(t')\rangle = \frac{2\rho_0 T}{L\gamma}\delta_{q+q'}\delta(t-t'). \end{aligned} \tag{6}$$

where we have used that, for arbitrary functions $f(x)$ and $g(x)$, one has

$$\int dx f(x-x_0)e^{iqx} = f_q e^{iqx_0}, \qquad \int dx dx' f(x-x')g(x')e^{iqx} = f_q\, g_q. \tag{7}$$

The solution for ρ_q follows readily as

$$\phi_q(t) = \frac{1}{\sqrt{\rho_0}} \int_{-\infty}^{t} dt' e^{-(t-t')\lambda(q)} \Big[-(q^2/\gamma)v_q e^{iqx_0(t')} + iq\Lambda_q(t) \Big], \tag{8}$$

where we have set the lower bound of the integral to $-\infty$ to discard the contribution of the initial condition.

C. Show that the tracer dynamics can then be written in a closed form satisfying the fluctuation-dissipation theorem.

Correction. Given that

$$\sum_{j=0}^{N} \partial_{x_0} V(x_j - x_0) = -\frac{1}{\sqrt{\rho_0}} \int dx \phi(x,t)\partial_x v(x-x_0) = \frac{L}{\sqrt{\rho_0}} \sum_q iq\phi_q(t)v_q e^{-iqx_0}, \tag{9}$$

where we have used $V(0) = 0$, substituting the solution for ρ_q in the tracer dynamics, we get

$$\gamma\dot{x}_0 = \frac{1}{\rho_0}\sum_q iq \int_{-\infty}^{t} dt' e^{-(t-t')\lambda(q)} \Big[-(q^2/\gamma)v_q^2 e^{iq(x_0(t')-x_0(t))} + iqv_q e^{iqx_0(t')}\Lambda_q(t') \Big] + \eta_0. \tag{10}$$

Integrating by parts the first term in the integrand, the dynamics can be written as

$$\begin{aligned}
&\gamma\dot{x}_0 + \int_{-\infty}^{t} dt' \zeta(t-t')\dot{x}_0(t') = \eta_0 + \xi, \\
&\zeta(t-t') = \frac{L}{\gamma\rho_0}\sum_q \frac{q^4}{\lambda(q)} v_q^2 e^{-(t-t')\lambda(q)} e^{iq(x_0(t')-x_0(t))}, \\
&\xi(t) = -\frac{L}{\rho_0}\sum_q q^2 v_q \int_{-\infty}^{t} dt' e^{-(t-t')\lambda(q)} e^{iqx_0(t')}\Lambda_q(t').
\end{aligned} \tag{11}$$

The correlations of the noise ξ read

$$\begin{aligned}
&\langle \xi(t_1)\xi(t_2)\rangle \\
&= \frac{L^2}{\rho_0^2}\sum_{q_1,q_2} (q_1q_2)^2 v_{q_1}v_{q_2} e^{i(q_1x_0(t_1)+q_2x_0(t_2))} \int_{-\infty}^{t_1} dt_1' \int_{-\infty}^{t_2} dt_2' \langle \Lambda_{q_1}(t_1')\Lambda_{q_2}(t_2')\rangle e^{-(t_1-t_1')\lambda(q_1)-(t_2-t_2')\lambda(q_2)} \\
&= \frac{2TL}{\gamma\rho_0}\sum_{q_1} q_1^4 v_{q_1}^2 e^{iq_1(x_0(t_1)-x_0(t_2))} \int_{-\infty}^{t_1} dt_1' e^{-(t_2+t_1-2t_1')\lambda(q_1)} \\
&= \frac{TL}{\gamma\rho_0}\sum_{q_1} \frac{q_1^4}{\lambda(q_1)} v_{q_1}^2 e^{iq_1(x_0(t_1)-x_0(t_2))} e^{-(t_2-t_1)\lambda(q_1)},
\end{aligned} \tag{12}$$

where we have used the correlations of $\Lambda_q(t)$ in (6), $\lambda(-q) = \lambda(q)$, and $v_q = v_{-q}$ assuming that $v(x) = v(-x)$. It follows that $\langle \xi(t_1)\xi(t_2)\rangle = T\zeta(t_1-t_2)$, as expected from the fluctuation-dissipation theorem.

Nonequilibrium soft and active matter: TD11

Department of Physics and Materials Science, University of Luxembourg

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1 Collective dynamics with multiple temperatures

A. Consider the overdamped dynamics of two sets of particles with positions x_i with pair-wise potential of the form $U(\{x_i\}) = (1/2)\sum_{i,j=1}^{N} V(x_i - x_j)$ at two different temperatures T: particles 1 to n are subject to $T = T_a$, and particles $n+1$ to N are subject to temperature $T = T_b$. Give the corresponding overdamped Langevin dynamics for these particles.

Correction. The dynamics reads

$$\begin{aligned}
&\text{for } i \in [1,n]: \; \gamma \dot{x}_i = -\partial_{x_i} \sum_{j=1}^{N} V(x_i - x_j) + \eta_{a,i}, \quad \langle \eta_{a,i}(t)\eta_{a,j}(0)\rangle = 2\gamma T_a \delta_{ij}\delta(t-t'), \\
&\text{for } i \in [n+1,N]: \; \gamma \dot{x}_i = -\partial_{x_i} \sum_{j=1}^{N} V(x_i - x_j) + \eta_{b,i}, \quad \langle \eta_{b,i}(t)\eta_{b,j}(0)\rangle = 2\gamma T_b \delta_{ij}\delta(t-t'),
\end{aligned} \tag{1}$$

where the noise terms $\eta_{a,i}$ and $\eta_{b,i}$ are uncorrelated.

B. Show that the coupled dynamics for the density fields $\rho_a(x,t) = \sum_{i=1}^{n} \delta[x - x_i(t)]$ and $\rho_b(x,t) = \sum_{i=n+1}^{N} \delta[x - x_i(t)]$ reads

$$\begin{aligned}
\partial_t \rho_a(x,t) &= \frac{1}{\gamma}\partial_x \Big[T_a \partial_x \rho_a(x,t) + \rho_a(x,t) \int dx' \rho(x,t) \partial_x V(x-x') \Big] + \partial_x \Lambda_a(x,t), \\
\partial_t \rho_b(x,t) &= \frac{1}{\gamma}\partial_x \Big[T_b \partial_x \rho_b(x,t) + \rho_b(x,t) \int dx' \rho(x,t) \partial_x V(x-x') \Big] + \partial_x \Lambda_b(x,t),
\end{aligned} \tag{2}$$

where $\rho = \rho_a + \rho_b$, and $\{\Lambda_a, \Lambda_b\}$ are some noise terms.

Correction. Applying Itô's lemma, we get

$$\begin{aligned}
\partial_t \rho_a(x,t) &= \sum_{i=1}^{n} \Big[-\dot{x}_i(t)\partial_x + (T_a/\gamma)(\partial_x)^2 \Big] \delta[x - x_i(t)], \\
\partial_t \rho_b(x,t) &= \sum_{i=n+1}^{N} \Big[-\dot{x}_i(t)\partial_x + (T_b/\gamma)(\partial_x)^2 \Big] \delta[x - x_i(t)],
\end{aligned} \tag{3}$$

and, substituting the particle-based dynamics, we deduce

$$\begin{aligned}
\partial_t \rho_a(x,t) &= \frac{T_a}{\gamma}(\partial_x)^2 \rho_a(x,t) - \frac{1}{\gamma}\partial_x \sum_{i=1}^{n} \Big[\eta_{a,i}(t) - \sum_{j=1}^{N} \partial_x V(x - x_j) \Big] \delta[x - x_i(t)], \\
\partial_t \rho_b(x,t) &= \frac{T_b}{\gamma}(\partial_x)^2 \rho_b(x,t) - \frac{1}{\gamma}\partial_x \sum_{i=n+1}^{N} \Big[\eta_{b,i}(t) - \sum_{j=1}^{N} \partial_x V(x - x_j) \Big] \delta[x - x_i(t)],
\end{aligned} \tag{4}$$

from which the dynamics (2) follows readily by identifying the noise terms as

$$\Lambda_a(x,t) = \frac{1}{\gamma}\sum_{i=1}^{n} \eta_{a,i}(t)\delta[x - x_i(t)], \qquad \Lambda_b(x,t) = \frac{1}{\gamma}\sum_{i=n+1}^{N} \eta_{b,i}(t)\delta[x - x_i(t)]. \tag{5}$$

C. Give the statistics of $\{\Lambda_a, \Lambda_b\}$ in terms of the density fields.

Correction. The noise terms are linear combination of zero-mean Gaussian white noises $\{\eta_{a,i}, \eta_{b,i}\}$, hence they also have Gaussian with zero-mean. The correlations are then given by

$$\begin{aligned}
\langle \Lambda_a(x,t)\Lambda_a(x',t')\rangle &= (2T_a/\gamma)\delta(x-x')\delta(t-t')\rho_a(x,t), \\
\langle \Lambda_b(x,t)\Lambda_b(x',t')\rangle &= (2T_b/\gamma)\delta(x-x')\delta(t-t')\rho_b(x,t), \\
\langle \Lambda_a(x,t)\Lambda_b(x',t')\rangle &= 0.
\end{aligned} \tag{6}$$

D. Consider the case where the many-body potential now reads:

$$U(\{x_i\}) = \frac{1}{2}\left[\sum_{i,j=1}^{n} V_{aa}(x_i - x_j) + \sum_{i,j=n+1}^{N} V_{bb}(x_i - x_j) + 2\sum_{i=1}^{n}\sum_{j=n+1}^{N} V_{ab}(x_i - x_j)\right]. \tag{7}$$

Show that the system relaxes to the Boltzmann distribution in terms of a well-defined free energy when $T_a = T_b = T$.

Correction. Following the same procedure as above, one gets

$$\begin{aligned}
\partial_t \rho_a(x,t) &= \partial_x\left[\frac{\rho_a(x,t)}{\gamma}\partial_x \frac{\delta \mathcal{F}}{\delta \rho_a(x,t)} + \Lambda_a(x,t)\right], \\
\partial_t \rho_b(x,t) &= \partial_x\left[\frac{\rho_b(x,t)}{\gamma}\partial_x \frac{\delta \mathcal{F}}{\delta \rho_b(x,t)} + \Lambda_b(x,t)\right],
\end{aligned} \tag{8}$$

where

$$\begin{aligned}
\mathcal{F} = T\int dx\Big[\rho_a(x)(\ln\rho_a(x) - 1) + \rho_b(x)(\ln\rho_b(x) - 1)\Big] \\
+ \frac{1}{2}\iint dx dx'\Big[\rho_a(x)\rho_a(x')V_{aa}(x-x') + \rho_b(x)\rho_b(x')V_{bb}(x-x') + 2\rho_a(x)\rho_b(x')V_{ab}(x-x')\Big].
\end{aligned} \tag{9}$$

The statistics of the noise terms $\{\Lambda_a, \Lambda_b\}$ is unchanged by setting now $T_a = T_b = T$. It follows that the dynamics of the density field is now at equilibrium, with steady state given by $P_s[\rho_a, \rho_b] \sim e^{-\mathcal{F}/T}$.