Active matter – Week 2: Integration and analysis of active systems
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I. SPECTRAL ANALYSIS OF STOCHASTIC PROCESSES

I.A. Correlation function and power spectrum

Considering a linear stochastic differential equation of the following form,

$$\sum_{n=0}^{\infty} a_n \frac{\partial^n x(t)}{\partial t^n} = f(t), \tag{1}$$

where $f(t)$ is a Gaussian stochastic process. Harmonic analysis of the stochastic process $x(t)$ consists, in its *stationary* state, in the study of its Fourier transform

$$\tilde{x}(\omega) = \int_{\mathbb{R}} \mathrm{d}t\, e^{-\mathrm{i}\omega t}\, x(t), \tag{2a}$$

$$x(t) = \frac{1}{2\pi} \int_{\mathbb{R}} \mathrm{d}\omega\, e^{\mathrm{i}\omega t}\, \tilde{x}(\omega). \tag{2b}$$

This analysis comes in handy because (1) may be rewritten in Fourier space,

$$\tilde{x}(\omega) \sum_{n=0}^{\infty} a_n\, (\mathrm{i}\omega)^n = \tilde{f}(\omega), \tag{3}$$

which is now a polynomial equation in ω, with $\tilde{f}(\omega)$ the Fourier transform of f and which is, by linearity, also a Gaussian stochastic process. This formulation is relevant to compute the autocorrelation function of $x(t)$,

$$\begin{aligned} \langle x(t)x(t')\rangle = \langle x(t)x(t')^*\rangle &= \frac{1}{(2\pi)^2} \int_{\mathbb{R}} \mathrm{d}\omega\, e^{\mathrm{i}\omega t} \int_{\mathbb{R}} \mathrm{d}\omega'\, e^{-\mathrm{i}\omega' t'}\, \langle \tilde{x}(\omega)\tilde{x}(\omega')^*\rangle \\ &= \frac{1}{(2\pi)^2} \int_{\mathbb{R}} \mathrm{d}\omega\, e^{\mathrm{i}\omega(t-t')} \int_{\mathbb{R}} \mathrm{d}\omega'\, e^{\mathrm{i}(\omega-\omega')t'}\, \langle \tilde{x}(\omega)\tilde{x}(\omega')^*\rangle\,, \end{aligned} \tag{4}$$

where the first equality is the assumption that $x(t)$ is real-valued. This relation between the correlation function $\langle x(t)x(t')\rangle$ and the power spectrum $\langle \tilde{x}(\omega)\tilde{x}(\omega)^*\rangle$ is a form of the Wiener–Khintchine theorem [1] (§ 1.10 – The Wiener–Khintchine theorem).

I.B. Example: autocorrelation of the Ornstein-Uhlenbeck process

Consider an Ornstein-Uhlenbeck process $x(t)$ described by the following stochastic differential equation,

$$\tau \frac{\partial x(t)}{\partial t} + x(t) = \sqrt{2\tau}\, \eta(t), \tag{5}$$

where $\eta(t)$ is a Gaussian white noise with mean $\langle \eta(t)\rangle = 0$ and variance

$$\langle \eta(t)\eta(t')\rangle = \delta(t-t'), \tag{6}$$

and where we will consider t as the time.

We compute the power spectrum of the stochastic term,

$$\langle \tilde{\eta}(\omega)\tilde{\eta}(\omega')^*\rangle = \int_{\mathbb{R}} \mathrm{d}t \int_{\mathbb{R}} \mathrm{d}t'\, e^{-\mathrm{i}(\omega t - \omega' t')}\, \langle \eta(t)\eta(t')\rangle = \int_{\mathbb{R}} \mathrm{d}t\, e^{-\mathrm{i}(\omega-\omega')t} = 2\pi\, \delta(\omega-\omega'), \tag{7}$$

where the last equality is the definition of the Dirac δ function, and write (5) in Fourier space,

$$\mathrm{i}\omega\tau\tilde{x}(\omega) + \tilde{x}(\omega) = \sqrt{2\tau}\,\eta(t), \tag{8}$$

such that the power spectrum of $x(t)$ can be written as

$$\langle\tilde{x}(\omega)\tilde{x}(\omega')^*\rangle = \frac{\langle\tilde{\eta}(\omega)\tilde{\eta}(\omega')^*\rangle}{(\mathrm{i}\omega\tau+1)(-\mathrm{i}\omega'\tau+1)} = \frac{4\pi\tau\,\delta(\omega-\omega')}{1+\omega^2\tau^2}, \tag{9}$$

where we have used $\omega = \omega'$ in the last equality for ease of computation and justified by the presence of $\delta(\omega-\omega')$. We finally compute the autocorrelation function of $x(t)$ using (4),

$$\langle x(t)x(t')\rangle = \frac{1}{(2\pi)^2}\int_{\mathbb{R}}\mathrm{d}\omega\,e^{\mathrm{i}\omega(t-t')}\int_{\mathbb{R}}\mathrm{d}\omega'\,e^{\mathrm{i}(\omega-\omega')t'}\,\frac{4\pi\tau\,\delta(\omega-\omega')}{1+\omega^2\tau^2} = \frac{1}{2\pi}\int_{\mathbb{R}}\mathrm{d}\omega\,e^{\mathrm{i}\omega(t-t')}\,\frac{2\tau}{1+\omega^2\tau^2} = e^{-|t-t'|/\tau}, \tag{10}$$

where the last Fourier relation, between the exponential function

$$t \mapsto e^{-[t|/\tau} \tag{11a}$$

and the Lorentzian function

$$\omega \mapsto 2\tau/(1+\omega^2\tau^2), \tag{11b}$$

is a useful general result.[1] It is noteworthy that for $\omega\tau \gg 1$, *i.e.* for time scales $1/\omega$ much smaller than τ, then $1/(1+\omega^2\tau^2) \sim 1/(\omega^2\tau^2) \ll 1$, therefore fluctuations are damped. On the contrary for $\omega\tau \ll 1$, *i.e.* for time scales $1/\omega$ much larger than τ, then $1/(1+\omega^2\tau^2) \sim 1$, therefore fluctuations are the largest. This highlights that τ is the characteristic time scale of variations of $x(t)$, which loses its autocorrelation at times $t \gg \tau$.

I.C. Example: velocity fluctuations in a chain of active Ornstein-Uhlenbeck particles

This section is an adaptation of some of the derivations of [2, 3] to the case of discrete one-dimensional active Ornstein-Uhlenbeck particles (AOUPs). We consider an ensemble of N AOUPs on a periodic ring, with positions

$$r_i = r_i^0 + u_i, \tag{13a}$$

$$r_i^0 = i\sigma, \tag{13b}$$

$$r_{i+N} = r_i, \tag{13c}$$

where σ is an effective diameter, and we consider the following overdamped equation of motion, where each particle interacts harmonically with its neighbours,

$$\zeta\dot{r}_i = -k(r_i - r_{i-1} - \sigma) + k(r_{i+1} - r_i - \sigma) + \lambda_i, \tag{14a}$$

or equivalently using the displacements u_i from the reference positions r_i^0,

$$\zeta\dot{u}_i = -k(2u_i - u_{i-1} - u_{i+1}) + \lambda_i, \tag{14b}$$

where ζ is a drag coefficient, k is a spring constant, and the λ_i are fluctuation-inducing terms. We choose the λ_i to follow Ornstein-Uhlenbeck processes,

$$\tau_p\dot{\lambda}_i = -\lambda_i + \sqrt{2\zeta^2 v_0^2 \tau_p}\eta_i, \tag{15}$$

where the $\eta_i(t)$ are Gaussian white noises with means $\langle\eta_i(t)\rangle = 0$ and variances

$$\langle\eta_i(t)\eta_j(t')\rangle = \delta_{ij}\,\delta(t-t'). \tag{16}$$

[1] It is easier to compute the direct Fourier transform,

$$\int_{\mathbb{R}}\mathrm{d}t\,e^{-\mathrm{i}\omega\tau}e^{-|t|/\tau} = \int_{-\infty}^{0}\mathrm{d}t\,e^{(-\mathrm{i}\omega+1/\tau)t} + \int_{0}^{\infty}\mathrm{d}t\,e^{(-\mathrm{i}\omega-1/\tau)t} = \frac{1}{-\mathrm{i}\omega+1/\tau} - \frac{1}{-\mathrm{i}\omega-1/\tau} = \frac{2\tau}{1+\omega^2\tau^2}. \tag{12}$$

We identify equations (5) and (15) and use the result (10) to compute the autocorrelation function of the η_i,

$$\langle \lambda_i(t)\lambda_j(t')\rangle = \zeta^2 v_0^2\, \delta_{ij}\, e^{-|t-t'|/\tau_p}, \tag{17}$$

where we identify v_0 to a self-propulsion velocity and τ_p to a persistence time. Comparing (14) and (17) we see that fluctuations are induced by *coloured* (time-correlated) noises λ_i and that dissipation is provided by a *white* (instantaneous) drag $-\zeta\dot{r}_i$. This system thus breaks the second fluctuation-dissipation relation introduced in the previous lecture[2]: the energy provided by fluctuations is not dissipated at the same rate, therefore the system is driven out of thermodynamic equilibrium. Since energy is provided to individual particles via the terms λ_i, the system is *active*.

AOUPs are a model of *self-propelled* particles[3]: the active force λ_i tends to "push" particle i in a given direction for a time of order τ_p. This model has been used to characterise crawling MDCK cells [4] or colloidal particles in a bath of persistently moving bacteria [5].

There are spatial and temporal dimensions to (14) and we thus need to consider fluctuations in both space and time. We will in particular be interested in the spatial fluctuations of the velocities $v_i = \dot{u}_i$. Since this is a discrete and periodic system, we introduce the ensemble of wavenumbers

$$q_n = \frac{2\pi}{N\sigma} n, \tag{20a}$$

with $n \in [\![0, N-1]\!]$, and the discrete Fourier transform

$$\tilde{u}_{q_n}(t) = \sum_{i=1}^{N} e^{-\mathrm{i} q_n r_i^0}\, u_i(t), \tag{20b}$$

$$u_i(t) = \frac{1}{N} \sum_{n=0}^{N-1} e^{\mathrm{i} q_n r_i^0}\, \tilde{u}_{q_n}(t), \tag{20c}$$

with the following orthogonality relation

$$\sum_{i=1}^{N} e^{\mathrm{i}(q_n - q_m) r_i^0} = N\, \delta_{q_n, q_m} = N\, \delta_{m,n}. \tag{20d}$$

We introduce the continuous-time Fourier transform of these discrete-space Fourier transform,

$$\tilde{U}_{q_n}(\omega) = \int_{\mathbb{R}} \mathrm{d}t\, e^{-\mathrm{i}\omega t}\, \tilde{u}_{q_n}(t), \tag{21a}$$

$$\tilde{u}_{q_n}(t) = \frac{1}{2\pi} \int_{\mathbb{R}} \mathrm{d}\omega\, e^{\mathrm{i}\omega t}\, \tilde{U}_{q_n}(\omega). \tag{21b}$$

We can then write (14) in Fourier space,[4]

$$\mathrm{i}\omega\zeta \tilde{U}_{q_n}(\omega) = -k\tilde{U}_{q_n}(\omega)\left(2 - e^{\mathrm{i}q_n\sigma} - e^{-\mathrm{i}q_n\sigma}\right) + \tilde{\Lambda}_{q_n}(\omega) = -2k\tilde{U}_{q_n}(\omega)(1 - \cos(q_n\sigma)) + \tilde{\Lambda}_{q_n}(\omega). \tag{23}$$

With $\tilde{V}_{q_n}(\omega) = \mathrm{i}\omega\tilde{U}_{q_n}(\omega)$ the Fourier transform of the velocity, we compute its spectrum

$$\left\langle \tilde{V}_{q_n}(\omega)\tilde{V}^*_{q_m}(\omega')\right\rangle = \frac{\omega\omega' \left\langle \tilde{\Lambda}_{q_n}(\omega)\tilde{\Lambda}^*_{q_m}(\omega')\right\rangle}{[\mathrm{i}\omega\zeta + 2k(1-\cos(q_n\sigma))]\,[-\mathrm{i}\omega'\zeta + 2k(1-\cos(q_m\sigma))]}, \tag{24}$$

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[2] We can rewrite (14) as a generalised Langevin equation,

$$\int_0^t \mathrm{d}s\, \zeta(t-s)\, \dot{r}(s) = -\frac{\partial}{\partial r} U + F(t), \tag{18}$$

where $\zeta(t-t') = \zeta\,\delta(t-t')$ and $\langle F(t)F(t')\rangle = \zeta^2 v_0^2 e^{-|t-t'|/\tau_p}$ according to (17). At thermodynamic equilibrium, the fluctuation-dissipation theorem would impose

$$\left\langle F(t)\cdot F(t')\right\rangle = k_B T\, \zeta(t-t'), \tag{19}$$

which would imply here $v_0^2\tau = k_B T/\zeta = D$ (where the second equality is the Einstein relation) and $\tau_p \to 0$.

[3] Active Brownian particles (see (43) and (47)) are also a form of self-propelled particles.

[4] We used

$$\sum_{i=1}^{N} e^{-\mathrm{i}q_n r_i^0}\, u_{i+j}(t) = \sum_{i=1}^{N} e^{q_n j\sigma}\, e^{-\mathrm{i}q_n(r_i^0 + j\sigma)}\, u_{i+j}(t) = e^{q_n j\sigma} \sum_{i=1}^{N} e^{-\mathrm{i}q_n r_{i+j}^0}\, u_{i+j}(t) = e^{q_n j\sigma}\, \tilde{u}_{q_n}(t), \tag{22}$$

which itself uses (13) and periodic boundary conditions, to derive (23).

and where the spectrum of the driving noise is

$$\begin{aligned}\left\langle \tilde{\Lambda}^*_{q_n}(\omega)\tilde{\Lambda}^*_{q_m}(\omega')\right\rangle &= \int_{\mathbb{R}} \mathrm{d}t\, e^{-\mathrm{i}\omega t} \int_{\mathbb{R}} \mathrm{d}t'\, e^{\mathrm{i}\omega' t'} \sum_{i=1}^{N} e^{-\mathrm{i}q_n r_i^0} \sum_{j=1}^{N} e^{\mathrm{i}q_m r_j^0} \, \langle \lambda_i(t)\lambda_j(t')\rangle \\ &= \int_{\mathbb{R}} \mathrm{d}t\, e^{-\mathrm{i}\omega t} \int_{\mathbb{R}} \mathrm{d}t'\, e^{\mathrm{i}\omega' t'} \, \zeta^2 v_0^2 \, e^{-|t-t'|/\tau_p} \sum_{i=1}^{N} e^{-\mathrm{i}(q_n-q_m) r_i^0} \\ &= \frac{4\pi\tau_p\zeta^2 v_0^2 \, \delta(\omega-\omega')\, N\, \delta_{q_n,q_m}}{1+\omega^2\tau_p^2},\end{aligned} \tag{25}$$

where we have used (17) between the first and the second lines, and (9) and (20d) between the second and third lines. We inject (25) in (24),

$$\left\langle \tilde{V}_{q_n}(\omega)\tilde{V}_{q_m}(\omega')\right\rangle = \frac{4\pi\tau_p\zeta^2 v_0^2\, \omega^2\, \delta(\omega-\omega')\, N\, \delta_{q_n,q_m}}{[\omega^2\zeta^2 + 4k^2(1-\cos(q_m\sigma))^2]\left[1+\omega^2\tau_p^2\right]}, \tag{26}$$

where we have used $\omega = \omega'$ and $q_n = q_m$ due to the presence of $\delta(\omega-\omega')$ and δ_{q_n,q_m}. In order to evaluate the equal-time spatial fluctuations of the velocities, we need to take the inverse Fourier transform in time of (26). We will first evaluate this inverse Fourier transform with simpler notations and then identify the terms in (26). We compute

$$\begin{aligned}\frac{1}{(2\pi)^2}\int_{\mathbb{R}}\mathrm{d}\omega\int_{\mathbb{R}}\mathrm{d}\omega'\, e^{\mathrm{i}(\omega-\omega')t}\,\frac{\omega^2\,\delta(\omega-\omega')}{[a^2+\omega^2b^2]\,[c^2+\omega^2d^2]} &= \frac{1}{(2\pi)^2}\int_{\mathbb{R}}\mathrm{d}\omega\,\frac{1}{d^2/c^2-b^2/a^2}\left[\frac{1/c^2}{a^2+\omega^2b^2}-\frac{1/a^2}{c^2+\omega^2d^2}\right] \\ &= \frac{1}{(2\pi)^2}\int_{\mathbb{R}}\mathrm{d}\omega\,\left[\frac{a^2}{a^2+\omega^2b^2}-\frac{c^2}{c^2+\omega^2d^2}\right]\frac{1}{a^2d^2-b^2c^2} \\ &= \frac{1}{(2\pi)^2}\pi\left[\frac{a^2}{ab}-\frac{c^2}{cd}\right]\frac{1}{a^2d^2-b^2c^2} \\ &= \frac{1}{4\pi}\left[\frac{ad}{bd}-\frac{bc}{bd}\right]\frac{1}{a^2d^2-b^2c^2} \\ &= \frac{1}{4\pi\, bd(ad+bc)},\end{aligned} \tag{27a}$$

where we have used the following identity

$$\int_{\mathbb{R}}\mathrm{d}\omega\,\frac{1}{a^2+\omega^2b^2} = \frac{\pi}{ab}, \tag{27b}$$

and finally identify (27a) and the inverse Fourier transform in time of (26)

$$\begin{aligned}\langle \tilde{v}_{q_n}(\omega)\tilde{v}_{q_m}(\omega')^*\rangle &= \frac{1}{(2\pi)^2}\int_{\mathbb{R}}\mathrm{d}\omega\int_{\mathbb{R}}\mathrm{d}\omega'\, e^{\mathrm{i}(\omega-\omega')t}\,\left\langle \tilde{V}_{q_n}(\omega)\tilde{V}_{q_m}(\omega')\right\rangle \\ &= \frac{4\pi\tau_p\zeta^2v_0^2N\delta_{q_n,q_m}}{4\pi\zeta\tau_p\left[\zeta+2k\tau_p(1-\cos(q_n\sigma))\right]} \\ &= \frac{v_0^2\,N\,\delta_{q_n,q_m}}{1+2\frac{k\tau_p}{\zeta}(1-\cos(q_n\sigma))}.\end{aligned} \tag{28}$$

We introduce the following length scale,

$$\xi = \sigma\sqrt{k\tau_p/\zeta}, \tag{29}$$

such that in the limit $q_n\sigma \ll 1$ we can write,

$$\langle \tilde{v}_{q_n}(\omega)\tilde{v}_{q_m}(\omega')^*\rangle \underset{q_n\sigma\ll 1}{=} \frac{v_0^2\,N\,\delta_{q_n,q_m}}{1+q_n^2\xi^2}. \tag{30}$$

Therefore on length scales $1/q_n$ larger than particle-particle distance σ, the fluctuation spectrum of the velocities is a Lorentzian (11b) with a typical lengthscale ξ. We conclude that velocities in the system are correlated over a length scale ξ which grows with the persistence time τ_p of the driving forces: correlations in time of the driving lead to correlations in space of the dynamics. This should be contrasted with systems at thermodynamic equilibrium which are described by the Maxwell-Boltzmann distribution in which positions and velocities are indenpendent and are thus devoid of velocity correlations.

II. INTEGRATION OF STOCHASTIC PROCESSES

II.A. Deterministic differential equations: Euler method

Given an ordinary first-order differential equation,

$$\frac{\partial y(t)}{\partial t} = f(y(t), t), \tag{31}$$

we can solve it numerically using a Taylor-expansion of the source function f. We write

$$f(y(t), t) = f(y(0), 0) + \sum_{n=1}^{\infty} \frac{1}{n!} \left. \frac{\partial^n f(y(t), t)}{\partial y(t)^n} \right|_{y(t)=y(0)} (y(t) - y(0))^n + \sum_{n=1}^{\infty} \frac{1}{n!} \left. \frac{\partial^n f(y(t), t)}{\partial t^n} \right|_{t=0} t^n, \tag{32a}$$

$$y(t) - y(0) = \sum_{n=1}^{\infty} \frac{1}{n!} \left. \frac{\partial^n y(t)}{\partial t^n} \right|_{t=0} t^n = \sum_{n=1}^{\infty} \frac{1}{n!} \left. \frac{\partial^{n-1} f(y(t), t)}{\partial t^{n-1}} \right|_{t=0} t^n, \tag{32b}$$

and considering $t = o(1)$ we integrate (31),

$$y(t) = y(0) + \int_0^t \mathrm{d}s \left. \frac{\mathrm{d}y(t)}{\mathrm{d}t} \right|_{t=s} = y(0) + \int_0^t \mathrm{d}s \, [f(y(0), 0) + \mathcal{O}(s)] = y(0) + f(y(0), 0)t + \mathcal{O}(t^2), \tag{33}$$

which outlines the Euler method. Using a discrete ensemble of coordinates t we may use the following integration method with a step Δt,

$$t_0, \ldots, t_n, \; t_{i+1} - t_i = \Delta t, \tag{34a}$$

$$y(t_i) \approx y_i = y_{i-1} + f(y_{i-1}, t_{i-1}) \, \Delta t. \tag{34b}$$

which makes an error of order Δt^2 at each step according to (33). We may reduce this error by decreasing Δt or using methods which use more derivatives of f such as Runge-Kutta methods [6] (§ 17 – Integration of ordinary differential equations). It is also noteworthy that the error increases with the first derivative of f, thus larger values of the latter should be dealt with smaller values of the step Δt. Both decreasing the step Δt or increasing the error order in Δt of the integration method increase computational time to solve a differential equation on a given length interval, therefore these should be chosen wisely.

II.B. Stochastic differential equations: Euler-Maruyama method

This section is largely based on [7]. We consider the integration of stochastic differential equation by adding an additional stochastic term to (31),

$$\frac{\mathrm{d}y(t)}{\mathrm{d}t} = f(y(t), t) + g(y(t), t)\eta(t), \tag{35}$$

where g is a deterministic function, and $\eta(t)$ is a Gaussian white noise with mean $\langle \eta(t) \rangle = 0$ and variance

$$\langle \eta(t)\eta(t') \rangle = \delta(t - t'). \tag{36}$$

With the same procedure as (32), we Taylor-expand our stochastic term as

$$g(y(t), t)\eta(t) = \sum_{n=0}^{\infty} g_n \, t^n \, \eta(t), \tag{37}$$

where $g_0 = g(y(0), 0)$ and the higher-order terms depend on the derivatives of g with respect to $y(t)$ and t. We solve (35) with

$$y(t) = y(0) + f(y(0), 0)t + \mathcal{O}(t^2) + \sum_{n=0}^{\infty} \int_0^t \mathrm{d}s \, g_n \, t^n \, \eta(s), \tag{38}$$

where the first three terms on the right-hand side derive from (33), and the last term is a linear combination of random Gaussian variables and is thus also a random Gaussian variable. We single out the following variables,

$$G_n = \int_0^t \mathrm{d}s\, g_n\, t^n\, \eta(s), \tag{39}$$

which are also Gaussian and are thus uniquely determined by their mean and variance,

$$\langle G_n \rangle = \left\langle \int_0^t \mathrm{d}s\, g_n\, t^n\, \eta(s) \right\rangle = 0, \tag{40a}$$

$$\left\langle G_n^2 \right\rangle = \left\langle \left(\int_0^t \mathrm{d}s\, g_n\, t^n\, \eta(s) \right)^2 \right\rangle = g_n^2 \int_0^t \mathrm{d}s \int_0^t \mathrm{d}s'\, t^{2n}\, \langle \eta(s)\eta(s') \rangle = g_n^2 \int_0^t \mathrm{d}s\, t^{2n} = \frac{1}{2n+1}\, g_n^2\, t^{2n+1}, \tag{40b}$$

and thus write, considering $t = o(1)$,

$$y(t) = y(0) + f(y(0), 0)t + G_0 + \mathcal{O}(t^{3/2}), \tag{41}$$

where $\langle G_0 \rangle = 0$ and $\left\langle G_0^2 \right\rangle = g_0^2\, t = g(y(0), 0)^2\, t$, which outlines the Euler-Maruyama method. Using a discrete ensemble of coordinates t we may use the following integration method,

$$t_0, \ldots, t_n \text{ with } t_{i+1} - t_i = \Delta t, \tag{42a}$$

$$y(0) = y_0 \text{ and } y(t_i) \approx y_i = y_{i-1} + f(y_{i-1}, t_{i-1})\, \Delta t + g(y_{i-1}, t_{i-1}) \sqrt{\Delta t}\, \lambda_{i-1} + \mathcal{O}(\Delta t^{3/2}) \tag{42b}$$

where the λ_i are random numbers taken from a Gaussian distribution with zero mean and unit variance, and where λ_i and λ_j are independent for $i \neq j$, such that the last term in (42b) has the same statistics as G_0 (39).

III. PROBLEMS

III.A. Mean squared displacement of an isolated active Brownian particle

We consider an isolated active Brownian particle (ABP) [8], with position r and orientation θ, which follows the following overdamped equation of motion

$$\boldsymbol{v} = \dot{\boldsymbol{r}} = v_0 \begin{pmatrix} \cos\theta \\ \sin\theta \end{pmatrix}, \tag{43a}$$

$$\dot{\theta} = \sqrt{2/\tau_p}\, \eta, \tag{43b}$$

where v_0 is a self-propulsion velocity, τ_p is a persistence time, and η is Gaussian white noise with mean $\langle \eta(t) \rangle = 0$ and variance $\langle \eta(t)\eta(t') \rangle = \delta(t - t')$.

1. Show that

$$\langle \boldsymbol{v}(t) \cdot \boldsymbol{v}(t') \rangle = v_0^2 \operatorname{Re}\left(\left\langle e^{\mathrm{i}(\theta(t)-\theta(t'))} \right\rangle \right) \tag{44}$$

and

$$\left\langle (\theta(t) - \theta(t'))^2 \right\rangle = 2|t - t'|/\tau. \tag{45}$$

2. Considering a random Gaussian variable X, with mean $\langle X \rangle = \mu$ and variance $\left\langle (X - \langle X \rangle)^2 \right\rangle = \sigma^2$, its characteristic function satisfies [9]

$$\left\langle e^{\mathrm{i}zX} \right\rangle = e^{\mathrm{i}\mu z - \sigma^2 z^2/2}. \tag{46}$$

Using this relation, compute the velocity autocorrelation function $\langle \boldsymbol{v}(t) \cdot \boldsymbol{v}(t') \rangle$ as a function of v_0 and τ_p.

3. Compute the mean squared displacement $\left\langle |\boldsymbol{r}(t) - \boldsymbol{r}(0)|^2 \right\rangle$.

4. Use the script `demoABP2D.py` (or write your own!) to simulate trajectories of an ABP and check its mean squared displacement.

III.B. Velocity fluctuations in a chain of active Ornstein-Uhlenbeck particles

Use the script `quickAOUP1D.py` which integrates (14) to check the velocity spectrum $\left\langle |\tilde{v}_{q_n}(\omega)|^2 \right\rangle$ (30).

III.C. Density fluctuations in two-dimensional active Brownian particles

Consider an ensemble of N active Brownian particles (ABPs), interacting through a repulsive harmonic potential, which follow the following overdamped equation of motion

$$\zeta \dot{\boldsymbol{r}}_i = -\frac{\partial U}{\partial \boldsymbol{r}_i} + v_0 \begin{pmatrix} \cos\theta_i \\ \sin\theta_i \end{pmatrix}, \tag{47a}$$

$$U = \sum_{i \neq j} \frac{1}{2} k(\sigma - |\boldsymbol{r}_j - \boldsymbol{r}_i|)^2\, \Theta(\sigma - |\boldsymbol{r}_j - \boldsymbol{r}_i|), \tag{47b}$$

$$\dot{\theta}_i = \sqrt{2/\tau_p}\, \eta_i, \tag{47c}$$

where $\boldsymbol{r}_i$ and θ_i are their positions and orientations, ζ their drag coefficient, v_0 and τ_p their self-propulsion velocity and persistence time, η_i are Gaussian white noises with mean $\langle \eta_i(t) \rangle = 0$ and variance $\langle \eta_i(t)\eta_j(t') \rangle = \delta_{ij}\delta(t - t')$, σ their diameter, k is a spring constant, and Θ is the Heaviside function.[5]

Using the script `quickABP2D.py`, observe how the behaviour of the system changes as you increase the persistence time τ_p. In particular, pay attention to density fluctuations at large τ_p.

[5] We define the Heaviside function as $\Theta(x < 0) = 0$ and $\Theta(x \geq 0) = 1$.

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IV. SOLUTIONS

IV.A. Mean squared displacement of an isolated active Brownian particle

1. We compute

$$\begin{aligned}\langle \boldsymbol{v}(t)\cdot\boldsymbol{v}(t')\rangle &= v_0^2\,\langle \cos(\theta(t))\cos(\theta(t')) + \sin(\theta(t))\sin(\theta(t'))\rangle \\ &= v_0^2\,\langle \cos(\theta(t)-\theta(t'))\rangle \\ &= v_0^2\,\mathrm{Re}\left(\left\langle e^{\mathrm{i}(\theta(t)-\theta(t'))}\right\rangle\right),\end{aligned} \tag{48}$$

consistently with (44), and

$$\begin{aligned}\left\langle(\theta(t)-\theta(t'))^2\right\rangle &= \left\langle\left(\int_{t'}^{t}\mathrm{d}s\,\dot\theta(s)\right)^2\right\rangle \\ &= \int_{t'}^{t}\mathrm{d}s\int_{t'}^{t}\mathrm{d}s'\,\left\langle\dot\theta(s)\dot\theta(s')\right\rangle \\ &= 2/\tau\int_{t'}^{t}\mathrm{d}s\int_{t'}^{t}\mathrm{d}s'\,\langle\eta(s)\eta(s')\rangle \\ &= 2/\tau\int_{t'}^{t}\mathrm{d}s\,\mathrm{sign}(t-t') \\ &= 2|t-t'|/\tau,\end{aligned} \tag{49}$$

where we have introduced $\mathrm{sign}(t-t')$ to take into account the direction of the integration[6], and consistently with (45).

2. We first note that

$$\langle\theta(t)-\theta(t')\rangle = \left\langle\int_{t'}^{t}\mathrm{d}s\,\dot\theta(s)\right\rangle = \sqrt{2/\tau}\int_{t'}^{t}\mathrm{d}s\,\langle\eta(s)\rangle = 0, \tag{51}$$

thus with $\mu = 0$ and $\sigma^2 = 2|t-t'|/\tau$ (49) we use (46) and (48) to write

$$\langle\boldsymbol{v}(t)\cdot\boldsymbol{v}(t')\rangle = v_0^2\,e^{-\frac{1}{2}2|t-t'|/\tau_p} = v_0^2\,e^{-|t-t'|/\tau_p}. \tag{52}$$

3. It is noteworthy that the velocity autocorrelations of the overdamped (52) have the same functional form as the velocity autocorrelation of a diffusing inertial Brownian particle studied in the previous lecture. We follow the same route and write,

$$\begin{aligned}\left\langle|\boldsymbol{r}(t)-\boldsymbol{r}(0)|^2\right\rangle = \left\langle\left(\int_0^t\mathrm{d}s\,\boldsymbol{v}(s)\right)^2\right\rangle &= \int_0^t\mathrm{d}s\int_0^t\mathrm{d}s'\,\langle\boldsymbol{v}(s)\cdot\boldsymbol{v}(s')\rangle \\ &= v_0^2\int_0^t\mathrm{d}s\int_0^t\mathrm{d}s'\,e^{-|s-s'|/\tau_p} \\ &= v_0^2\int_0^t\mathrm{d}s\int_0^t\left[\int_0^s\mathrm{d}s'\,e^{-(s-s')/\tau_p} + \int_s^t\mathrm{d}s'\,e^{-(s'-s)/\tau_p}\right] \\ &= v_0^2\int_0^t\mathrm{d}s\,\tau_p\left[1-e^{-s/\tau_p} - (e^{-(t-s)/\tau_p}-1)\right] \\ &= v_0^2\tau_p\left[2t-\tau_p\left(1-e^{-t/\tau_p}+1-e^{-t/\tau_p}\right)\right] \\ &= 2v_0^2\tau_p\left[t+\tau_p(e^{-t/\tau_p}-1)\right],\end{aligned} \tag{53}$$

where we have used (52) between the first and second lines.

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[6] We define the sign function,

$$\mathrm{sign}(t-t') = \begin{cases}-1 & \text{if } t<t', \\ 0 & \text{if } t=t', \\ 1 & \text{if } t>t'.\end{cases} \tag{50}$$