Prof. Erwin Frey
B. Nettuno, T. Roth, D. Toffenetti, K. Wharam

Nonequilibrium Field Theories and Stochastic Dynamics
Sheet 7

Exercise 20 – Onsager relations and time-irreversibility

Consider a system which fluctuates around it's equilibrium position. The perturbation from the equilibrium is described by $\boldsymbol{\phi} = (\phi_1, \phi_2, \cdots, \phi_n)$. Assuming that the perturbations are small we can approximate their probability distribution with

$$p(\boldsymbol{\phi}) = \mathcal{N} \exp\left[-\frac{1}{2}\boldsymbol{\phi}^\intercal \boldsymbol{R} \boldsymbol{\phi}\right], \tag{1}$$

where $\boldsymbol{R}^{-1} = \langle \boldsymbol{\phi}\boldsymbol{\phi}^\intercal \rangle$ ($\boldsymbol{R}$ having entries r_{ij}) is the covariance matrix, as shown in the lecture.

a) Motivate briefly from what thermodynamic principle this probability distribution p originates? Why is it gaussian?

We would like to find an equation which describes the dynamics of the perturbations. We take as a candidate a linear Langevin equation in *Itō* interpretation of the following form:

$$\partial_t \boldsymbol{\phi}(t) = -\boldsymbol{\Gamma}\boldsymbol{\phi}(t) + \boldsymbol{\xi}(t), \tag{2}$$

where $\boldsymbol{\xi}(t)$ is a Gaussian white noise with

$$\langle \boldsymbol{\xi}(t) \rangle = 0, \qquad \langle \boldsymbol{\xi}(t)\boldsymbol{\xi}^\intercal(t') \rangle = \boldsymbol{N}\delta(t-t'). \tag{3}$$

The covariance matrix alone is not enough to determine the equation for the dynamics (note that it tells us nothing about the time scales on which the dynamics happen). However, we do not have a full freedom of choice for $\boldsymbol{\Gamma}$ and $\boldsymbol{N}$ either. $\boldsymbol{N}$ has entries N_{ij}. There are theoretical constraints that relate $\boldsymbol{\Gamma}$, $\boldsymbol{N}$ and $\boldsymbol{R}$, and narrow down the set of possible models. These constraints become even stronger, if one assumes that the system approaches thermal equilibrium. In this exercise you will rederive in a different way some of the constraints you already saw in the lecture. Throughout the exercise assume that all the components of $\boldsymbol{\phi}$ have time-reversal parity +1.

b) Show that the formal solution of the Langevin equation can be written as

$$\boldsymbol{\phi}(t) = e^{-\boldsymbol{\Gamma}t}\boldsymbol{\phi}(0) + \int_0^t dt' e^{-\boldsymbol{\Gamma}(t-t')}\boldsymbol{\xi}(t'). \tag{4}$$

You can do it by pretending that $\boldsymbol{\xi}(t')$ is an ordinary function of time and solving the Langevin equation, as you would solve any other non-homogeneous linear ODE. Can you see a simple interpretation of the result, that would allow you to basically write down the solution without performing any calculations?

c) Show that the covariance matrix $\langle \boldsymbol{\phi}(t)\boldsymbol{\phi}^\intercal(t) \rangle$ (equal time correlation function) can be expressed as

$$\langle \boldsymbol{\phi}(t)\boldsymbol{\phi}^\intercal(t) \rangle = e^{-\boldsymbol{\Gamma}t}\boldsymbol{R}^{-1}e^{-\boldsymbol{\Gamma}^\intercal t} + \int_0^t dt' e^{-\boldsymbol{\Gamma}(t-t')}\boldsymbol{N}e^{-\boldsymbol{\Gamma}^\intercal(t-t')}. \tag{5}$$

d) Assuming that the system is at a stationary state, and so $\langle \boldsymbol{\phi}(t)\boldsymbol{\phi}^\intercal(t) \rangle = \boldsymbol{R}^{-1} = \textit{const.}$, show that the matrix describing the amplitudes and correlations of the noise is set by the Onsager coefficients:

$$\boldsymbol{N} = \boldsymbol{L} + \boldsymbol{L}^\intercal, \quad \text{with Onsager coefficients} \quad \boldsymbol{L} = \boldsymbol{\Gamma}\boldsymbol{R}^{-1}. \tag{6}$$

Note that so far we did not assume anything about time reversibility of the dynamics.
Hint: Derivative of a constant is 0.

e) Transform the considered Langevin equation into a Fokker-Planck form and show that the steady-state probability current is given by

$$\boldsymbol{j}(\boldsymbol{\phi}) = \boldsymbol{\Omega}\boldsymbol{\phi}\, p(\boldsymbol{\phi}), \quad \text{with} \quad \boldsymbol{\Omega} = \frac{1}{2}\left(\boldsymbol{L}^\intercal - \boldsymbol{L}\right)\boldsymbol{R}\,. \tag{7}$$

In the expression above $\boldsymbol{\Omega}\boldsymbol{\phi} := \boldsymbol{v}(\boldsymbol{\phi})$ can be interpreted as the mean phase space velocity at point $\boldsymbol{\phi}$. Given this result, what does time-reversibility imply for the Onsager coefficients?

f) Verify that the Gaussian distribution

$$p(\boldsymbol{\phi}) = \exp\left[-\frac{1}{2}\boldsymbol{\phi}^{\intercal}\boldsymbol{R}\boldsymbol{\phi}\right] \tag{8}$$

is indeed the stationary probability distribution. You can do it by showing that the probability current is divergenceless.

g) In the equilibrium case, what is the covariance matrix $\boldsymbol{R}^{-1}$ in terms of $\boldsymbol{\Gamma}$ and $\boldsymbol{N}$?
Imagine now that ϕ describes the displacement from the equilibrium position of a one-dimensional, thermally driven, overdamped harmonic oscillator at temperature T. The Langevin equation in *Itō* interpretation reads

$$\gamma \frac{\mathrm{d}}{\mathrm{d}t}\phi(t) = -k\,\phi(t) + \sqrt{2\gamma\, k_B T}\,\xi(t)\,.$$

k is the spring constant and γ the viscosity. Recall the definition of $\boldsymbol{R}^{-1}$ and identify $\boldsymbol{\Gamma}$ and $\boldsymbol{N}$ to interpret the equilibrium relation $\boldsymbol{R}^{-1} = \boldsymbol{\Gamma}^{-1}\boldsymbol{N}/2$.

Exercise 21 – Onsager relations for model A and B

In this problem we will recapitulate calculations from the lecture and fill some gaps. In the following we aim at quantifying the relation between the noise amplitude N_{ij} characterizing the noise in the Langevin equation for the order parameter field ϕ_i and the Onsager coefficients L_{ij} for both model A and model B dynamics. To this end consider the free energy functional in Gaussian approximation (in Fourier space)

$$\mathcal{F}_{\text{harm.}}[\boldsymbol{\phi}(\mathbf{q},t)] = \frac{1}{2}\sum_{\mathbf{q}} r_{ij}(\mathbf{q})\phi_i(\mathbf{q})\phi_j(-\mathbf{q}) \tag{9}$$

a) Show that the covariance matrix in Fourier space (equilibrium correlation function) $C_{ij}(\mathbf{q},\mathbf{q}') := \langle\phi_i(\mathbf{q})\phi_j(\mathbf{q}')\rangle$ is given by

$$C_{ij}(\mathbf{q},\mathbf{q}') = C_{ij}(\mathbf{q})\delta_{\mathbf{q},-\mathbf{q}'} = \beta^{-1}\,(r^{-1})_{ij}(\mathbf{q})\,. \tag{10}$$

Where $\beta = 1/(k_{\mathrm{B}}T)$

b) In the lecture we discussed model A and derived the phenomenological equation

$$\partial_t\phi_i(\mathbf{q},t) = -L_{ij}\frac{\delta\mathcal{F}[\boldsymbol{\phi}]}{\delta\phi_j(-\mathbf{q},t)} + \zeta_i(\mathbf{q},t)\,, \tag{11}$$

describing the dynamics of a non-conserved field (in Fourier space) subject to white noise. The main idea behind this was to impose gradient dynamics, i. e. that the fields deterministically tend to relax back to their equilibrium values, following the gradient in $\mathcal{F}[\boldsymbol{\phi}]$ for the steepest-descent path towards the free-energy minimum. The noise terms for each field add random fluctuations to this relaxation process and, even if we have reached the minimum after some time, may drive us away from it again.
Apply the same reasoning for a system where the fields must obey a conservation law, for instance when $\boldsymbol{\phi}$ describes chemical concentrations or some other kind of *density* and argue that the corresponding phenomenological equation reads

$$\partial_t\phi_i(\mathbf{q},t) = -L_{ij}q^2\frac{\delta F[\boldsymbol{\phi}]}{\delta\phi_j(-\mathbf{q},t)} + \zeta_i(\mathbf{q},t)\,. \tag{12}$$

What is the origin of the q^2 term?

c) Consider the Langevin equation for the order parameter field $\boldsymbol{\phi}$

$$\partial_t\phi_i(\mathbf{q},t) = -L_{ij}q^a\frac{\delta F[\boldsymbol{\phi}]}{\delta\phi_j(-\mathbf{q},t)} + \zeta_i(\mathbf{q},t) \tag{13}$$

in the Gaussian approximation. Here $a = 0, 2$ corresponds to model A and B, respectively, and

$$\langle\zeta_i(\mathbf{q},t)\rangle = 0, \tag{14}$$

$$\langle\zeta_i(\mathbf{q},t)\zeta_j(\mathbf{q}',t')\rangle = N_{ij}(q)\delta_{\mathbf{q},-\mathbf{q}'}\delta(t-t')\,. \tag{15}$$

Derive the equation of motion for $\bar{\phi}_i(\mathbf{q}, t) \equiv \langle \phi_i(\mathbf{q}) \rangle (t)$. The average is taken with respect to the conditional probability density of the Fokker-Planck equation corresponding to the above Langevin equation. Use this result to derive an equation of motion for $C_{ij}(\mathbf{q}, t)$. Explain the major idea behind the calculation. Your result should read

$$\partial_t C_{ij}(\mathbf{q}, t) = -\Gamma_{ik}(\mathbf{q}) C_{kj}(\mathbf{q}, t) \quad \text{with } \Gamma_{ik}(\mathbf{q}) = q^a L_{ij} r_{jk}(\mathbf{q}) \,. \tag{16}$$

Fourier transform Eq. (16) and follow the calculations in the lecture notes to find a solution for $C_{ij}(\mathbf{q}, \omega)$.

Hint: Define the right half-sided Fourier transform as

$$C^+_{ij}(\mathbf{q}, \mathbf{q}', \omega) = \int_0^\infty \mathrm{d}t \exp(i\omega t) C_{ij}(\mathbf{q}, \mathbf{q}', t) \,, \tag{17}$$

and proceed analogously for the left half-sided Fourier transform.

d) Solve the Langevin equation, Eq. (13), using the noise correlations and derive an expression for $C_{ij}(\mathbf{q}, \omega)$.

e) Use your results from part c) and d) to show that

$$N_{ij} = \beta^{-1}(L_{ij} + L_{ji}) q^a \,. \tag{18}$$

Your solutions should be handed in by uploading them to Moodle by **Wednesday,** 18^{th} **June 2025, 10:00 am**.