Fluctuations and Responses in Stochastic Processes

Joonhyun Yeo

Konkuk University

Pyeong-Chang Summer Institute 2014, 24-30 August, 2014

About PSI

Pyeong-Chang Summer Institute (PSI) is all about learning physics. With ever-increasing diversity of the physics research, both young initiates and mature researchers alike find new physics to learn and old tricks to refresh. PSI strives to teach advanced topics, essential lores, and indispensible tools of trade, and at the same time wish to offer a venue to intermingle, share, and boast.

Setting the stage

- Microscopic description of dynamics (Classical)
  - ➤ $\boxed{\textit{Hamilton}}$

    $$\dot{\mathbf{q}}_i = \frac{\partial H}{\partial \mathbf{p}_i}, \quad \dot{\mathbf{p}}_i = -\frac{\partial H}{\partial \mathbf{q}_i}$$

  - ➤ $\boxed{\textit{Liouville}}$ $\rho(\{\mathbf{q}_i\},\{\mathbf{p}_i\},t)d^N\mathbf{q}d^N\mathbf{p}$: Prob. of finding system at time t inside $d^N\mathbf{q}d^N\mathbf{p}$ in phase space

    $$\begin{aligned}\frac{\partial \rho}{\partial t} &= \left[\frac{\partial H}{\partial \mathbf{q}}\cdot\frac{\partial}{\partial \mathbf{p}} - \frac{\partial H}{\partial \mathbf{p}}\cdot\frac{\partial}{\partial \mathbf{q}}\right]\rho \equiv -\mathcal{L}\rho \\ &= -\frac{\partial}{\partial \mathbf{q}}\cdot\left(\frac{d\mathbf{q}}{dt}\rho\right) - \frac{\partial}{\partial \mathbf{p}}\cdot\left(\frac{d\mathbf{p}}{dt}\rho\right)\end{aligned}$$

    - ★ This follows from Liouville theorem ($d^N\mathbf{q}d^N\mathbf{p}$ is invariant; the Hamiltonian flow is incompressible),
    - ★ And from

      $$0 = \frac{d\rho}{dt} = \frac{\partial \rho}{\partial t} + \frac{\partial \rho}{\partial \mathbf{q}}\cdot\dot{\mathbf{q}} + \frac{\partial \rho}{\partial \mathbf{p}}\cdot\dot{\mathbf{p}}$$

    - ★ Continuity equation (e.g. $\partial_t \rho = -\nabla\cdot\mathbf{j}$, probability conservation)

Mesoscopic Description of Dynamics

- $\boxed{\textbf{Langevin}}$: Effective dynamic equation including stochastic elements
- $\boxed{\textbf{Fokker} - \textbf{Planck}}$: Corresponding probability conservation equation
- Keywords:
  - Fluctuation-Dissipation Theorem (Relation)
  - Fluctuation-Response Relation
  - Linear Response Theory
- References:
  - R. Kubo, Rep. Prog. Phys. **29**, 255 (1966)
  - H. Risken, *The Fokker-Planck Equation*
  - R. Zwanzig, *Nonequilibrium Statistical Mechanics*
  - G. F. Mazenko, *Nonequilibrium Statistical Mechanics*
  - U. C. Täuber, *Critical Dynamics*

1. Langevin Equations

2. Generalized Langevin Equations

3. Fokker-Planck Equation

4. Fluctuation-Response Relations
   - Fokker-Planck equation
   - Liouville Equation

5. FDR and Time-Reversal Symmetry
   - Martin-Siggia-Rose-Janssen-De Dominicis Formalism
   - Time-Reversal Transformations

Langevin equation

Brownian motion

$$m\frac{dv}{dt} = F(t)$$

What to include in $F(t)$?

- frictional force $-\gamma v$: $v(t) = e^{-\gamma t/m} v(0) \to 0$ as $t \to \infty$. Inconsistent with $\langle v^2 \rangle = k_B T/m$ at thermal equilibrium
- Need fluctuating (random) force $\xi(t)$ to keep it alive
  - ➤ Simplest form of random force: Gaussian white noise

$$\langle \xi(t) \rangle = 0, \quad \langle \xi(t)\xi(t') \rangle = 2B\delta(t-t')$$

$$\boxed{m\frac{dv}{dt} = -\gamma v + \xi(t)}$$

- Effect of environment ("heat bath"): systematic part $(-\gamma v)$ + fluctuating part (ξ)
- There is a relationship between the two: Fluctuation-Dissipation Relation

Let $v(t) = e^{-\gamma t/m} w(t)$, then $dw/dt = e^{\gamma t/m}\xi(t)/m$. Therefore

$$v(t) = e^{-\gamma t/m} v(0) + \int_0^t dt' e^{-\gamma(t-t')/m}\xi(t')/m$$

Let us calculate $\langle v(t_1)v(t_2)\rangle$. The cross term is zero. We have to evaluate

$$\begin{aligned}
&\int_0^{t_1} dt' e^{-\gamma(t_1-t')/m} \int_0^{t_2} dt'' e^{-\gamma(t_2-t'')/m} \, \langle\xi(t')\xi(t'')\rangle/m^2 \\
=&e^{-\gamma(t_1+t_2)/m} \int_0^{t_1} dt' \int_0^{t_2} dt'' e^{\gamma(t'+t'')/m} \, 2B\delta(t'-t'')/m^2 \\
=&\frac{B}{\gamma m} e^{-\gamma(t_1+t_2)/m} \left[e^{2\gamma \min(t_1,t_2)/m} - 1\right] = \frac{B}{\gamma m}(e^{-\gamma|t_1-t_2|/m} - e^{-\gamma(t_1+t_2)/m})
\end{aligned}$$

We have

$$\langle v(t_1)v(t_2)\rangle = \left(v^2(0) - \frac{B}{\gamma m}\right) e^{-\gamma(t_1+t_2)/m} + \frac{B}{\gamma m} e^{-\gamma|t_1-t_2|/m}$$

$$\langle v^2(t)\rangle = e^{-2\gamma t/m}\left(v^2(0) - \frac{B}{\gamma m}\right) + \frac{B}{\gamma m} \to \frac{B}{\gamma m} \quad \text{as} \quad t \to \infty$$

Comparing with $\langle v^2\rangle_{\rm eq} = k_B T/m$, we have

$$\boxed{\gamma = \frac{B}{k_B T} = \frac{1}{k_B T}\int_0^\infty dt \langle \xi(t)\xi(0)\rangle} \qquad \texttt{FDR of 2nd kind}$$

Balance between dissipation (driving to "dead" state) and fluctuation (driving to "alive" state) to maintain thermal equilibrium.

Note that

- If $v^2(0) = B/(\gamma m) = k_B T/m$, then $\langle v^2(t)\rangle = \langle v^2\rangle_{\rm eq}$
- If $v^2(0) = B/(\gamma m) = k_B T/m$, then $\langle v(t_1)v(t_2)\rangle = \langle v(t_1 - t_2)v(0)\rangle$

Mean Squared Displacement, $\langle(\Delta x(t))^2\rangle$, where $\Delta x(t) \equiv x(t) - x(0)$.

$$\langle(\Delta x(t))^2\rangle = \int_0^t dt' \int_0^t dt'' \, \langle v(t')v(t'')\rangle.$$

Consider

$$\frac{\partial\langle(\Delta x(t))^2\rangle}{\partial t} = 2\int_0^t dt''\langle v(t)v(t'')\rangle = 2\int_0^t dt''\langle v(t-t'')v(0)\rangle = 2\int_0^t ds\langle v(s)v(0)\rangle$$

We expect $\langle(\Delta x(t))^2\rangle \sim 2Dt$ as $t \to \infty$ with diffusion constant D. We have

$$\boxed{D = \int_0^\infty ds\langle v(s)v(0)\rangle} \qquad \texttt{Green-Kubo formula}$$

Explicit calculation shows that ($*$ Exercise)

$$\begin{aligned}\langle(\Delta x(t))^2\rangle &= \frac{2B}{\gamma^2}\left[t - \frac{m}{\gamma} + \frac{m}{\gamma}e^{-\gamma t/m}\right] + \left(v_0^2 - \frac{B}{\gamma m}\right)\left(\frac{1-e^{-\gamma t/m}}{\gamma/m}\right)^2 \\ &\sim \frac{2B}{\gamma^2}t \qquad \text{as} \quad t \to \infty\end{aligned}$$

We can identify

$$\boxed{D = \frac{B}{\gamma^2} = \frac{k_B T}{\gamma}} \quad \texttt{Einstein relation}$$

We can write for mobility μ as

$$\boxed{\mu \equiv \frac{1}{\gamma} = \frac{1}{k_B T}\int_0^\infty dt \langle v(t) v(0)\rangle} \quad \texttt{FDR of 1st kind}$$

Suppose there is an uniform external driving force f so that

$$m\frac{dv}{dt} = -\frac{v}{\mu} + f + \xi(t)$$

As $t \to \infty$, the average velocity approaches

$$\langle v \rangle \to \mu f$$

Therefore we can regard μ as a response of the velocity to the external driving. So the above FDR is a relationship between the response and the correlation or fluctuation. $\Rightarrow$ $\boxed{\textit{Fluctuation} - \textit{Response Relation}}$

Exercise

Consider for a set of variables $\mathbf{a}(t) = \{a_i(t)\}$, $i = 1, 2, \ldots, N$

$$\frac{da_i}{dt} = \sum_j G_{ij} a_j + \xi_i(t), \quad \text{or} \quad \frac{d\mathbf{a}}{dt} = \mathtt{G} \cdot \mathbf{a} + \boldsymbol{\xi}(t),$$

where

$$\langle \xi_i(t) \rangle = 0, \qquad \langle \xi_i(t) \xi_j(t') \rangle = 2B_{ij} \delta(t - t')$$

The dissipation matrix $\mathtt{G} = \{G_{ij}\}$ is not necessarily a symmetric matrix whose eigenvalues have negative real parts. In the long time limit, we expect $\langle a_i(t) a_j(t) \rangle$ approaches the equilibrium value $\langle a_i a_j \rangle_{\mathrm{eq}} = M_{ij}$. ($\mathtt{B}$ and $\mathtt{M}$ are by definition symmetric matrices.)

Find the relationship among the matrices $\mathtt{G}$, $\mathtt{B}$ and $\mathtt{M}$.
(Hint: Try $\mathbf{a}(t) = e^{\mathtt{G}t} \cdot \mathbf{b}(t)$.)

1 Langevin Equations

2 Generalized Langevin Equations

3 Fokker-Planck Equation

4 Fluctuation-Response Relations
  - Fokker-Planck equation
  - Liouville Equation

5 FDR and Time-Reversal Symmetry
  - Martin-Siggia-Rose-Janssen-De Dominicis Formalism
  - Time-Reversal Transformations

Generalized Langevin equations

Consider generalized friction term including memory effect: (N.B. Formal derivation from Liouville equations using Projection Operators by Mori and Zwanzig)

$$m\frac{dv}{dt} = -\int_0^t dt'\ \gamma(t-t')v(t') + \xi(t)$$

Laplace transform

$$\mathcal{L}\{v\} = \hat{v}(\omega) \equiv \int_0^\infty dt\ e^{i\omega t} v(t), \quad \mathrm{Im}(\omega) > 0,$$

$$\mathcal{L}\{\dot{v}\} = -v(0) - i\omega\hat{v}(\omega), \quad \mathcal{L}\{\int_0^t dt'\gamma(t-t')v(t')\} = \hat{\gamma}(\omega)\hat{v}(\omega)$$

Multiply by $v(0)$ and take the average remembering $\langle\xi(t)v(0)\rangle = 0$ for $t > 0$.

$$\frac{dC(t)}{dt} = -\int_0^t dt'\ \gamma(t-t')C(t') \ \text{ with } \ C(t) \equiv \langle v(t)v(0)\rangle, \quad \text{or}$$

$$\hat{C}(\omega) = \frac{\langle v^2(0)\rangle}{\hat{\gamma}(\omega)/m - i\omega}$$

Suppose adding a time-dependent external driving force $f(t)$. Taking the average and Laplace transform,

$$-i\omega\langle\hat{v}(\omega)\rangle - v(0) = -\frac{1}{m}\hat{\gamma}(\omega)\langle\hat{v}(\omega)\rangle + \frac{1}{m}\hat{f}(\omega),$$

We introduce the response function $\mu(t)$ as

$$\langle v(t)\rangle = \int_0^t dt' \mu(t-t')f(t'), \qquad \hat{\mu}(\omega) = \frac{1}{m}\frac{1}{\hat{\gamma}(\omega)/m - i\omega}$$

We therefore have

$$\hat{\mu}(\omega) = \frac{1}{m\langle v^2(0)\rangle}\hat{C}(\omega), \quad \mu(t) = \frac{1}{m\langle v^2(0)\rangle}\langle v(t)v(0)\rangle$$

If $\langle v^2(0)\rangle = k_B T/m$, then

$$\boxed{\hat{\mu}(\omega) = \frac{1}{k_B T}\int_0^\infty dt\ e^{i\omega t}\langle v(t)v(0)\rangle} \qquad \texttt{FDR of 1st kind}$$

To show FDR of 2nd kind, consider

$$\frac{1}{m^2}\int_0^\infty dt\ e^{i\omega t}\langle\xi(0)\xi(t)\rangle = \int_0^\infty dt\ e^{i\omega t}\left\langle \dot{v}(0)\left[\dot{v}(t)+\frac{1}{m}\int_0^t dt'\ \gamma(t-t')v(t')\right]\right\rangle$$
$$= \int_0^\infty dt\ e^{i\omega t}\langle\dot{v}(0)\dot{v}(t)\rangle + \frac{\hat{\gamma}(\omega)}{m}\int_0^\infty dt\ e^{i\omega t}\langle\dot{v}(0)v(t)\rangle$$

Time-translational invariance:

$$\frac{d}{dt_0}\langle v(t_0)v(t_0+t)\rangle = 0,\quad \langle\dot{v}(t_0)v(t_0+t)\rangle = -\langle v(t_0)\dot{v}(t_0+t)\rangle,\quad \langle\dot{v}(t_0)v(t_0)\rangle = 0$$

Integrating by parts the first term, we have

$$\frac{1}{m^2}\int_0^\infty dt\ e^{i\omega t}\langle\xi(0)\xi(t)\rangle = -i\omega\int_0^\infty dt\ e^{i\omega t}\langle\dot{v}(0)v(t)\rangle + \frac{\hat{\gamma}(\omega)}{m}\int_0^\infty dt\ e^{i\omega t}\langle\dot{v}(0)v(t)\rangle$$
$$= \left(i\omega - \frac{\hat{\gamma}(\omega)}{m}\right)\int_0^\infty dt\ e^{i\omega t}\langle v(0)\dot{v}(t)\rangle$$
$$= \left(i\omega - \frac{\hat{\gamma}(\omega)}{m}\right)\left(-\langle v^2(0)\rangle - i\omega\int_0^\infty dt\ e^{i\omega t}\langle v(0)v(t)\rangle\right)$$
$$= \left(i\omega - \frac{\hat{\gamma}(\omega)}{m}\right)\left(-\langle v^2(0)\rangle - i\omega\frac{\langle v^2(0)\rangle}{\hat{\gamma}(\omega)/m - i\omega}\right)$$

We therefore have

$$\frac{1}{m^2}\int_0^\infty dt\; e^{i\omega t}\langle\xi(0)\xi(t)\rangle = \frac{\langle v^2(0)\rangle}{m}\hat{\gamma}(\omega)$$

or

$$\hat{\gamma}(\omega) = \frac{1}{m\langle v^2(0)\rangle}\int_0^\infty dt\; e^{i\omega t}\langle\xi(0)\xi(t)\rangle$$

If $\langle v^2(0)\rangle = k_B T/m$, then

$$\boxed{\hat{\gamma}(\omega) = \frac{1}{k_B T}\int_0^\infty dt\; e^{i\omega t}\langle\xi(0)\xi(t)\rangle} \qquad \texttt{FDR of 2nd kind}$$

We have a colored noise: non-Markovian dynamics

For $\gamma(t) = \gamma\delta(t)$, we recover the white noise limit.

Detour: Appearance of memory term

Treat a heat bath as a collection of harmonic oscillators: $H = H_S + H_B$

- System

$$H_S = \frac{p^2}{2m} + U(x)$$

- Bath + Coupling

$$H_B = \sum_j \left(\frac{p_j^2}{2} + \frac{\omega_j^2}{2}(q_j - \frac{\gamma_j}{\omega_j^2}x)^2 \right)$$

- Coupling is bilinear: $-\gamma_j q_j x$.
- $\gamma_j^2 x^2/(2\omega_j^2)$ can be absorbed into $U(x)$

Eqs. of motion:

$$\dot{x} = p/m, \qquad \dot{p} = -U'(x) + \sum_j \gamma_j(q_j - \frac{\gamma_j}{\omega_j^2}x)$$

$$\dot{q}_j = p_j, \qquad \dot{p}_j = -\omega_j^2 q_j + \gamma_j x$$

Rewrite the second set as

$$\dot{\mathtt{Q}} = \mathtt{A} \cdot \mathtt{Q} + \mathtt{B}$$

where

$$\mathtt{Q} = \begin{pmatrix} q_j \\ p_j \end{pmatrix}, \quad \mathtt{A} = \begin{pmatrix} 0 & 1 \\ -\omega_j^2 & 0 \end{pmatrix}, \quad \mathtt{B} = \begin{pmatrix} 0 \\ \gamma_j x \end{pmatrix}$$

The solution to this equation is

$$\mathtt{Q}(t) = e^{\mathtt{A}t} \cdot \mathtt{Q}(0) + \int_0^t ds\; e^{\mathtt{A}(t-s)} \cdot \mathtt{B}(s)$$

We can easily show that

$$e^{\mathtt{A}t} = \begin{pmatrix} \cos(\omega_j t) & \frac{1}{\omega_j}\sin(\omega_j t) \\ -\omega_j \sin(\omega_j t) & \cos(\omega_j t) \end{pmatrix}.$$

Integrate by parts the integral in the solution for $q_j(t)$:

$$q_j(t) - \frac{\gamma_j}{\omega_j^2} x(t) = \{q_j(0) - \frac{\gamma_j}{\omega_j^2} x(0)\} \cos(\omega_j t) + \frac{p_j(0)}{\omega_j} \sin(\omega_j t) - \frac{\gamma_j}{\omega_j^2} \int_0^t ds\;\; \cos(\omega_j(t-s)) \frac{p(s)}{m}$$

Inserting this into the first set of equations of motion,

$$\boxed{\dot{p} = -U'(x) - \int_0^t ds\, K(t-s)\frac{p(s)}{m} + \xi(t)},$$

where

$$K(t) = \sum_j \frac{\gamma_j^2}{\omega_j^2}\cos(\omega_j t),$$

and

$$\xi(t) = \sum_j \left[\gamma_j\{q_j(0) - \frac{\gamma_j}{\omega_j^2}x(0)\}\cos(\omega_j t) + \frac{\gamma_j}{\omega_j}p_j(0)\sin(\omega_j t)\right]$$

Suppose we prepare the bath at $t = 0$ following the distribution $\sim \exp(-H_B/(k_B T))$, then

$$\langle p_j(0)\rangle = \langle q_j(0) - \frac{\gamma_j}{\omega_j^2}x(0)\rangle = 0$$

and

$$\left\langle \frac{p_j^2(0)}{2}\right\rangle = \frac{k_B T}{2}, \qquad \frac{\omega_j^2}{2}\left\langle \left(q_j(0) - \frac{\gamma_j}{\omega_j^2}x(0)\right)^2\right\rangle = \frac{k_B T}{2}$$

We finally have

$$\boxed{\langle \xi(t)\xi(t')\rangle = k_B T\sum_j \frac{\gamma_j^2}{\omega_j^2}\cos(\omega(t-t')) = (k_B T)K(t-t')}, \quad \text{FDT of 2nd kind}$$

1 Langevin Equations

2 Generalized Langevin Equations

3 Fokker-Planck Equation

4 Fluctuation-Response Relations
  - Fokker-Planck equation
  - Liouville Equation

5 FDR and Time-Reversal Symmetry
  - Martin-Siggia-Rose-Janssen-De Dominicis Formalism
  - Time-Reversal Transformations

Fokker-Planck Equation

Sometimes we face nonlinear problems like (Brownian particle in a potential)

$$\begin{aligned} \frac{dx}{dt} &= \frac{p}{m} \\ \frac{dp}{dt} &= -\gamma\frac{p}{m} - \nabla U(x) + \xi(t), \qquad \langle \xi(t)\xi(t')\rangle = 2B\delta(t-t') \end{aligned}$$

Consider a general form for $i = 1, 2, \ldots, N$,

$$\boxed{\frac{dx_i}{dt} = f_i(\mathbf{x}(t)) + \xi_i(t)},$$

where $\langle \xi_i(t)\rangle = 0$ and $\langle \xi_i(t)\xi_j(t')\rangle = 2D_{ij}\delta(t-t')$.

Work with the Fokker-Planck equation for the probability density $P(\mathbf{x}, t)$ at time t. Consider

$$P(\mathbf{x}, t+dt) = \int d\mathbf{x}_0 P(\mathbf{x}, t+dt; \mathbf{x}_0, t) = \int d\mathbf{x}_0 P(\mathbf{x}, t+dt|\mathbf{x}_0, t) P(\mathbf{x}_0, t), \qquad (\bigstar)$$

where $P(\mathbf{x}_2, t_2|\mathbf{x}_1, t_1)$ is the conditional probability.

We can write

$$P(\mathbf{x}, t+dt|\mathbf{x}_0, t) = \langle \delta(\mathbf{x} - \mathbf{x}(t+dt)) \rangle_{\mathbf{x}(t)=\mathbf{x}_0} ,$$

where $\langle \cdots \rangle_{\mathbf{x}(t)=\mathbf{x}_0}$ is the average over the noise with the condition that $\mathbf{x}(t) = \mathbf{x}_0$. Note that

$$\Delta x_i \equiv x_i(t+dt) - x_i(t) = f_i(x(t))dt + \int_t^{t+dt} dt' \xi_i(t')$$

and that

$$\int_t^{t+dt} dt' \xi_i(t') = O(\sqrt{dt})$$

We now Taylor expand up to $O(dt)$

$$P(\mathbf{x}, t+dt|\mathbf{x}_0, t) = \langle \delta(\mathbf{x} - \mathbf{x}(t) - \Delta\mathbf{x}) \rangle_{\mathbf{x}(t)=\mathbf{x}_0}$$

Keeping up to $O(dt)$,

$$P(\mathbf{x}, t+dt|\mathbf{x}_0, t) = \delta(\mathbf{x}-\mathbf{x}_0) - \sum_i \left\langle f_i(\mathbf{x}(t))dt + \int_t^{t+dt} dt' \xi_i(t') \right\rangle_{\mathbf{x}(t)=\mathbf{x}_0} \frac{\partial}{\partial x_i}\delta(\mathbf{x}-\mathbf{x}_0)$$

$$+ \sum_{i,j} \left\langle \int_t^{t+dt} dt' \int_t^{t+dt} dt'' \xi_i(t')\xi_j(t'') \right\rangle \frac{1}{2}\frac{\partial^2}{\partial x_i \partial x_j}\delta(\mathbf{x}-\mathbf{x}_0)$$

$$= \delta(\mathbf{x}-\mathbf{x}_0) - (dt)\sum_i f_i(\mathbf{x}_0)\frac{\partial}{\partial x_i}\delta(\mathbf{x}-\mathbf{x}_0) + (dt)\sum_{i,j} D_{ij}\frac{\partial^2}{\partial x_i \partial x_j}\delta(\mathbf{x}-\mathbf{x}_0)$$

Inserting this into (★), we have the F-P equation:

$$\boxed{\frac{\partial}{\partial t}P(\mathbf{x}, t) = -\sum_i \frac{\partial}{\partial x_i}\left(f_i(\mathbf{x})P(\mathbf{x}, t)\right) + \sum_{i,j}\frac{\partial^2}{\partial x_i \partial x_j} D_{ij} P(\mathbf{x}, t)}$$

Detour: Langevin equation with multiplicative noise

Consider the case where $\dot{x}_i = f_i(\mathbf{x}(t)) + \xi_i(\mathbf{x}, t)$ with (summation convention)

$$\xi_i(\mathbf{x}, t) = g_{ia}(\mathbf{x})\eta_a(t), \quad \langle \eta_a(t) \rangle = 0, \quad \langle \eta_a(t)\eta_b(t') \rangle = \delta_{ab}\delta(t - t')$$

The additive noise case corresponds to $g = const.$ and $g_{ia}g_{ja} = 2D_{ij}$.
Then we can write for an arbitrary $\alpha \in [0, 1]$, (with $\Delta\mathbf{x} \equiv \mathbf{x}(t + dt) - \mathbf{x}(t)$)

$$\int_t^{t+dt} dt' \xi_i(t') = g_{ia}(\mathbf{x}(t) + \alpha\Delta\mathbf{x}) \int_t^{t+dt} dt' \eta_a(t'),$$

where the function g is evaluated at some intermediate point.

- $\alpha = 0$: Itô (prepoint)
- $\alpha = \frac{1}{2}$: Stratonovich (midpoint)

Unlike the ordinary calculus, α-dependent term makes the difference as

$$\begin{aligned}\left\langle \int_t^{t+dt} dt'\xi_i(\mathbf{x},t') \right\rangle =& \alpha \left\langle (\partial_j g_{ia}(\mathbf{x}(t)))(\Delta x)_j \int_t^{t+dt} dt'\eta_a(t') \right\rangle \\ =& \alpha \left\langle (\partial_j g_{ia}(\mathbf{x}(t))) \int_t^{t+dt} dt''\xi_j(t'') \int_t^{t+dt} dt'\eta_a(t') \right\rangle \\ =& \alpha(dt) g_{ja}(\mathbf{x})(\partial_j g_{ia}(\mathbf{x}))\end{aligned}$$

Following the same steps as above, we obtain

$$\begin{aligned}\frac{\partial}{\partial t}P(\mathbf{x},t) =& -\sum_i \frac{\partial}{\partial x_i}\left([f_i(\mathbf{x}) + \alpha g_{ja}(\mathbf{x})\partial_j g_{ia}(\mathbf{x})]\, P(\mathbf{x},t)\right) \\ &+ \frac{1}{2}\sum_{i,j}\frac{\partial^2}{\partial x_i \partial x_j} g_{ia}(\mathbf{x}) g_{ja}(\mathbf{x}) P(\mathbf{x},t)\end{aligned}$$

The Langevin equation with multiplicative noise must be supplemented by the prescription parameter α which tells us how to interpret the mupltiplicative noise.

- The F-P equation is of the form

$$\partial_t P(\mathbf{x},t) = -\mathtt{L}(\mathbf{x})P = -\boldsymbol{\nabla}\cdot\mathbf{J},$$

where

$$\boxed{\mathtt{L}(\mathbf{x}) = \sum_i \frac{\partial}{\partial x_i} f_i(\mathbf{x}) - \sum_{i,j}\frac{\partial^2}{\partial x_i \partial x_j} D_{ij}}$$

is the F-P differential operator and

$$\boxed{J_i = f_i P - \sum_j \partial_j D_{ij} P}$$

is the probability current.

- Stationary solution: $P^{\mathrm{s}}(x)$ satisfies $\partial_t P^{\mathrm{s}} = \mathtt{L}P^{\mathrm{s}} = 0$ or $\boldsymbol{\nabla}\cdot\mathbf{J}^{\mathrm{s}} = 0$.

▷ Examples

- Brownian motion

$$\boxed{\partial_t P(p,t) = \partial_p(\frac{\gamma}{m}p + B\partial_p)P(p,t)}$$

Maxwell-Boltzmann dist.

$$P_{\rm eq} \sim \exp(-p^2/(2mk_B T))$$

becomes the stationary solution if $\gamma = B/(k_B T)$. [FDR of 2nd kind] In this case $J^{\rm s} = 0$.

- Brownian particle in a potential (Kramer's equation)

$$\frac{dx}{dt} = \frac{p}{m}$$
$$\frac{dp}{dt} = -\gamma\frac{p}{m} - \nabla U(x) + \xi(t), \qquad \langle \xi(t)\xi(t')\rangle = 2B\delta(t-t')$$

$$\boxed{\partial_t P(x,p,t) = -\partial_x \frac{p}{m} P(x,p,t) - \partial_p(-\frac{\gamma}{m}p - (\partial_x U(x)) - B\partial_p)P(x,p,t)}$$

Again equilibrium dist.

$$P_{\rm eq} \sim \exp\left[-\frac{p^2}{2mk_BT} - \frac{U(x)}{k_BT}\right]$$

becomes the stationary solution $P^{\rm s}$ if $\gamma = B/(k_BT)$.

In this case, stationary currents

$$J_x^{\rm s}(x,p) = \frac{p}{m} P^{\rm s}(x,p), \quad J_p^{\rm s}(x,p) = (-\frac{\gamma}{m} p - (\partial_x U(x)) - B\partial_p) P^{\rm s}(x,p)$$

do <u>not</u> vanish. But the "irreversible" part

$$J_p^{\rm s,ir}(x,p) \equiv (-\frac{\gamma}{m} p - B\partial_p) P^{\rm s}(x,p) = 0$$

does vanish. The "reversible" part $J_p^{\rm s,rev}(x,p) \equiv -(\partial_x U(x)) P^{\rm s}(x,p)$ satisfies

$$\partial_x J_x^{\rm s} + \partial_p J_p^{\rm s,rev} = 0$$

- Driven colloidal particle in a periodic potential

  - Overdamped limit: Friction is so large that inertia term can be negelcted. In 1d,

$$\dot{x} = \gamma^{-1} f(x) + \eta(t), \quad \langle \eta(t)\eta(t')\rangle = 2D\delta(t - t'),$$

where $D = B\gamma^{-2}$. In equilibrium Einstein relation holds; $B = \gamma(k_B T)$ or $D = (k_B T)/\gamma$.

Stationary state satisfies

$$\frac{d}{dx}\left(-\gamma^{-1} f(x) + D\frac{d}{dx}\right) P^{\mathrm{s}}(x) = 0$$

If $f(x) = -V'(x) + F$ where $V(x)$ is a periodic potential and F is a uniform drive, one can have nonzero stationary current

$$J^{\mathrm{s}} = \gamma^{-1} f(x) P^{\mathrm{s}}(x) - DP^{\mathrm{s}\prime}(x) \neq 0.$$

  - Nonequilibrium steady state (NESS): Detailed Balance is broken

Detailed Balance

The Fokker-Planck equation can be written as

$$\frac{\partial}{\partial t} P(\mathbf{x}, t) = \int d\mathbf{x}' \; \left[W_{\mathbf{x},\mathbf{x}'} \; P(\mathbf{x}', t) - W_{\mathbf{x}',\mathbf{x}} P(\mathbf{x}, t) \right],$$

where $W_{\mathbf{x},\mathbf{x}'}$ is the transition rate from $\mathbf{x}'$ to $\mathbf{x}$ given by

$$W_{\mathbf{x},\mathbf{x}'} = -\mathtt{L}(\mathbf{x})\delta(\mathbf{x} - \mathbf{x}') = \left[-\sum_i \partial_i f_i(\mathbf{x}) + \sum_{i,j} D_{ij} \partial_i \partial_j \right] \delta(\mathbf{x} - \mathbf{x}')$$

The Detailed Balance condition for the stationary state distribution is defined by

$$\boxed{W_{\mathbf{x},\mathbf{x}'} P^{\mathrm{s}}(\mathbf{x}') = W_{\mathbf{x}',\mathbf{x}} P^{\mathrm{s}}(\mathbf{x})}$$

$$
\begin{aligned}
\text{(l.h.s.)} &= -\,\mathtt{L}(\mathbf{x})\delta(\mathbf{x}-\mathbf{x}')P^{\mathrm{s}}(\mathbf{x}') = -\mathtt{L}(\mathbf{x})P^{\mathrm{s}}(\mathbf{x})\delta(\mathbf{x}-\mathbf{x}') \\
&= -\left(\mathtt{L}(\mathbf{x})P^{\mathrm{s}}(\mathbf{x})\right)\delta(\mathbf{x}-\mathbf{x}') + \sum_i \left(-f_i(\mathbf{x})P^{\mathrm{s}}(\mathbf{x}) + 2\sum_j D_{ij}(\partial_j P^{\mathrm{s}}(\mathbf{x}))\right)\partial_i\delta(\mathbf{x}-\mathbf{x}') \\
&\quad + \sum_{i,j} D_{ij}\partial_i\partial_j\delta(\mathbf{x}-\mathbf{x}')
\end{aligned}
$$

$$
\begin{aligned}
\text{(r.h.s.)} &= \left[-\sum_i \partial'_i f_i(\mathbf{x}') + \sum_{i,j} D_{ij}\partial'_i\partial'_j\right]\delta(\mathbf{x}'-\mathbf{x})P^{\mathrm{s}}(\mathbf{x}) \\
&= P^{\mathrm{s}}(\mathbf{x})\left[-\sum_i \partial'_i f_i(\mathbf{x}') + \sum_{i,j} D_{ij}\partial'_i\partial'_j\right]\delta(\mathbf{x}'-\mathbf{x}) \\
&= P^{\mathrm{s}}(\mathbf{x})\left[\sum_i f_i(\mathbf{x})\partial_i + \sum_{i,j} D_{ij}\partial_i\partial_j\right]\delta(\mathbf{x}-\mathbf{x}') \equiv -P^{\mathrm{s}}(\mathbf{x})\mathtt{L}^{\dagger}(\mathbf{x})\delta(\mathbf{x}-\mathbf{x}')
\end{aligned}
$$

- Coefficient of $\delta(\mathbf{x}-\mathbf{x}')$: $\boxed{\mathrm{L}(\mathbf{x})P^{\mathrm{s}}(\mathbf{x})=0}$
- Coefficient of $\partial_i\delta(\mathbf{x}-\mathbf{x}')$:

$$-f_i(\mathbf{x})P^{\mathrm{s}}(\mathbf{x})+2\sum_j D_{ij}(\partial_j P^{\mathrm{s}}(\mathbf{x}))=f_i(\mathbf{x})P^{\mathrm{s}}(\mathbf{x}),\quad \text{or}\quad \boxed{J_i^{\mathrm{s}}=0}$$

- Coefficient of $\partial_i\partial_j\delta(\mathbf{x}-\mathbf{x}')$: automatically satisfied

In the presence of odd-parity variables like momentum (which changes sign under time reversal), we introduce $\epsilon_i = +1$ if x_i is even (e.g. position) and $\epsilon_i = -1$ if x_i is odd (e.g. momentum).

The DB condition in this case is

$$\boxed{W_{\mathbf{x},\mathbf{x}'} P^{\mathrm{s}}(\mathbf{x}') = W_{\boldsymbol{\epsilon}\mathbf{x}',\boldsymbol{\epsilon}\mathbf{x}} P^{\mathrm{s}}(\boldsymbol{\epsilon}\mathbf{x})}$$

$$\begin{aligned}
(\text{r.h.s.}) &= \left[-\sum_i \epsilon_i \partial_i' f_i(\boldsymbol{\epsilon}\mathbf{x}') + \sum_{i,j} \epsilon_i \epsilon_j D_{ij} \partial_i' \partial_j'\right] \delta(\mathbf{x}' - \mathbf{x}) P^{\mathrm{s}}(\boldsymbol{\epsilon}\mathbf{x}) \\
&= P^{\mathrm{s}}(\boldsymbol{\epsilon}\mathbf{x}) \left[-\sum_i \epsilon_i \partial_i' f_i(\boldsymbol{\epsilon}\mathbf{x}') + \sum_{i,j} \epsilon_i \epsilon_j D_{ij} \partial_i' \partial_j'\right] \delta(\mathbf{x}' - \mathbf{x}) \\
&= P^{\mathrm{s}}(\boldsymbol{\epsilon}\mathbf{x}) \left[\sum_i \epsilon_i f_i(\boldsymbol{\epsilon}\mathbf{x}) \partial_i + \sum_{i,j} \epsilon_i \epsilon_j D_{ij} \partial_i \partial_j\right] \delta(\mathbf{x} - \mathbf{x}') \equiv -P^{\mathrm{s}}(\boldsymbol{\epsilon}\mathbf{x}) \mathrm{L}^{\dagger}(\boldsymbol{\epsilon}\mathbf{x}) \delta(\mathbf{x} - \mathbf{x}')
\end{aligned}$$

- Coefficient of $\delta(\mathbf{x}-\mathbf{x}')$: $\boxed{\mathtt{L}(\mathbf{x})P^{\mathrm{s}}(\mathbf{x}) = 0}$
- Coefficient of $\partial_i\delta(\mathbf{x}-\mathbf{x}')$:

$$-f_i(\mathbf{x})P^{\mathrm{s}}(\mathbf{x}) + 2\sum_j D_{ij}(\partial_j P^{\mathrm{s}}(\mathbf{x})) = \epsilon_i f_i(\boldsymbol{\epsilon}\mathbf{x})P^{\mathrm{s}}(\boldsymbol{\epsilon}\mathbf{x})$$

- Coefficient of $\partial_i\partial_j\delta(\mathbf{x}-\mathbf{x}')$: $\boxed{D_{ij}P^{\mathrm{s}}(\mathbf{x}) = \epsilon_i\epsilon_j D_{ij}P^{\mathrm{s}}(\boldsymbol{\epsilon}\mathbf{x})} \rightarrow \boxed{P^{\mathrm{s}}(\mathbf{x}) = P^{\mathrm{s}}(\boldsymbol{\epsilon}\mathbf{x})}$

Define $\mathbf{f} \equiv \mathbf{f}^{\rm rev} + \mathbf{f}^{\rm ir}$:

$$f_i^{\rm rev}(\mathbf{x}) \equiv \frac{1}{2}[f_i(\mathbf{x}) - \epsilon_i f_i(\boldsymbol{\epsilon}\mathbf{x})], \quad f_i^{\rm ir}(\mathbf{x}) \equiv \frac{1}{2}[f_i(\mathbf{x}) + \epsilon_i f_i(\boldsymbol{\epsilon}\mathbf{x})]$$

such that $f_i^{\rm rev}(\boldsymbol{\epsilon}\mathbf{x}) = -\epsilon_i f_i^{\rm rev}(\mathbf{x})$ behaves like $\dot{x}_i$ and $f_i^{\rm ir}(\boldsymbol{\epsilon}\mathbf{x}) = \epsilon_i f_i^{\rm ir}(\mathbf{x})$ behaves opposite to $\dot{x}_i$ under time reversal.

For example,

$$\dot{x} = \underbrace{p/m}_{f_x^{rev}}, \qquad \dot{p} = \underbrace{-(\gamma/m)p}_{f_p^{ir}} \underbrace{-U'(x)}_{f_p^{rev}} + \xi$$

The second condition for DB becomes

$$\boxed{f_i^{\mathrm{ir}}(\mathbf{x})P^{\mathrm{s}}(\mathbf{x}) - \sum_j D_{ij}\partial_j P^{\mathrm{s}}(\mathbf{x}) \equiv J_i^{\mathrm{s,ir}}(\mathbf{x}) = 0}$$

or

$$f_i^{\mathrm{ir}}(\mathbf{x}) = -\sum_j D_{ij}\partial_j \phi(\mathbf{x}), \quad \text{where} \quad P^{\mathrm{s}}(\mathbf{x}) = e^{-\phi(\mathbf{x})}$$

The total stationary current $J_i^{\mathrm{s}} = J_i^{\mathrm{s,rev}} + J_i^{\mathrm{s,ir}}$: The first condition becomes

$$\boxed{\sum_i \partial_i J_i^{\mathrm{s,rev}}(\mathbf{x}) = \sum_i \partial_i (f_i^{\mathrm{rev}}(\mathbf{x})P^{\mathrm{s}}(\mathbf{x})) = 0}$$

1 Langevin Equations

2 Generalized Langevin Equations

3 Fokker-Planck Equation

4 Fluctuation-Response Relations
- Fokker-Planck equation
- Liouville Equation

5 FDR and Time-Reversal Symmetry
- Martin-Siggia-Rose-Janssen-De Dominicis Formalism
- Time-Reversal Transformations

Fluctuation-Response Relations / Fokker-Planck Equations

For the F-P eq. $\partial_t P = -\mathtt{L} P$, consider the case where we apply a small time-dependent perturbation such that

$$\mathtt{L}(\mathbf{x}, t) = \mathtt{L}_0(\mathbf{x}) + \mathtt{L}_1(\mathbf{x}, t) = \mathtt{L}_0(\mathbf{x}) + \lambda(t)\mathtt{L}_1(\mathbf{x}), \quad \lambda \text{ small}$$

Let P^{s} be the stationary solution of $\mathtt{L}_0$: $\mathtt{L}_0(\mathbf{x})P^{\mathrm{s}}(\mathbf{x}) = 0$.
Write $P = P^{\mathrm{s}} + P_1$ then the F-P eq. becomes for small λ

$$\partial_t(P^{\mathrm{s}} + P_1) = -(\mathtt{L}_0 + \mathtt{L}_1)(P^{\mathrm{s}} + P_1), \quad \text{or} \quad \partial_t P_1 = -\mathtt{L}_0 P_1 - \mathtt{L}_1 P^{\mathrm{s}} + O(\lambda^2)$$

The solution with initial condition $P_1(\mathbf{x}, -\infty) = 0$, $P(\mathbf{x}, -\infty) = P^{\mathrm{s}}(\mathbf{x})$ is

$$P_1(\mathbf{x}, t) = -\int_{-\infty}^{t} dt' \; e^{-\mathtt{L}_0(\mathbf{x})(t-t')}\mathtt{L}_1(\mathbf{x}, t')P^{\mathrm{s}}(\mathbf{x})$$

The average of an observable $A(\mathbf{x})$ is given by

$$\langle A \rangle_t \equiv \int d\mathbf{x} \; P(\mathbf{x}, t)A(\mathbf{x}).$$

The response to the perturbation is studied using the response function

$$\begin{aligned} R_A(t, t') &\equiv \left.\frac{\delta \langle A \rangle_t}{\delta \lambda(t')}\right|_{\lambda=0} \\ &= -\int d\mathbf{x} \; A(\mathbf{x})e^{-\mathtt{L}_0(\mathbf{x})(t-t')}\mathtt{L}_1(\mathbf{x})P^{\mathrm{s}}(\mathbf{x}), \quad t > t' \end{aligned}$$

We define the correlation function $C^0_{AB}(t,t') = \langle A(t)B(t')\rangle_0$ of two observables $A(\mathbf{x})$ and $B(\mathbf{x})$ at two different times $t > t'$ in the stationary state as

$$C^0_{AB}(t,t') = \int d\mathbf{x} \int d\mathbf{x}' A(\mathbf{x}) P(\mathbf{x},t|\mathbf{x}',t') P^{\mathrm{s}}(\mathbf{x}') B(\mathbf{x}')$$

The symbolic solution to the F-P eq. is $P(\mathbf{x},t) = \exp[-\mathrm{L}_0(\mathbf{x})(t-t_0)]P(\mathbf{x},t_0)$, so the conditional probability is $P(\mathbf{x},t|\mathbf{x}',t') = \exp[-\mathrm{L}_0(\mathbf{x})(t-t')]\delta(\mathbf{x}-\mathbf{x}')$

$$C^0_{AB}(t,t') = \int d\mathbf{x} A(\mathbf{x}) e^{-\mathrm{L}_0(\mathbf{x})(t-t')} B(\mathbf{x}) P^{\mathrm{s}}(\mathbf{x}), \qquad t > t'$$

For $t' > t$,

$$C^0_{AB}(t,t') = \int d\mathbf{x} B(\mathbf{x}) e^{-\mathrm{L}_0(\mathbf{x})(t'-t)} A(\mathbf{x}) P^{\mathrm{s}}(\mathbf{x}), \qquad t' > t$$

We have the Fluctuation-Response Relation

$$\boxed{R_A(t,t') = \begin{cases} C^0_{AB}(t,t'), & t > t' \\ 0, & t < t' \end{cases}}$$

where

$$\boxed{B(\mathbf{x}) \equiv -\frac{1}{P^{\mathrm{s}}(\mathbf{x})} \mathrm{L}_1(\mathbf{x}) P^{\mathrm{s}}(\mathbf{x})}$$

☐ Example 1: Perturbation of the stationary state satisfying DB

Consider for some i

$$\dot{x}_i = f_i(\mathbf{x}) + \underbrace{\lambda(t)}_{perturbation} + \xi_i(t)$$

$$\mathtt{L}_1^{\mathtt{i}}(\mathbf{x}, t) = \lambda(t)\partial_i, \qquad \mathtt{L}_1^{\mathtt{i}}(\mathbf{x}) = \partial_i$$

$$B_i(\mathbf{x}) = -\frac{1}{P^{\mathrm{s}}(\mathbf{x})}\partial_i P^{\mathrm{s}}(\mathbf{x}) = -\sum_j [D^{-1}]_{ij} f_j^{\mathrm{ir}}(\mathbf{x}),$$

where we have used the DB condition, $J_i^{\mathrm{s,ir}} = f_i^{\mathrm{ir}} P^{\mathrm{s}} - \sum_j D_{ij}\partial_j P^{\mathrm{s}} = 0$.

$$\boxed{R_A^i(t, t') = -\sum_j [D^{-1}]_{ij} \langle A(t) f_j^{\mathrm{ir}}(t')\rangle_0}, \qquad t > t'$$

△ Special case: $\boxed{f = f^{\mathrm{ir}}}$: Consider (summation convention)

$$\begin{aligned} \mathrm{L}_0(x_i P^{\mathrm{s}}(\mathbf{x})) =& \partial_k(f_k x_i P^{\mathrm{s}}) - \partial_k\partial_l(D_{kl} x_i P^{\mathrm{s}}) \\ =& f_i P^{\mathrm{s}} + \underbrace{x_i\partial_k(f_k P^{\mathrm{s}}) - x_i D_{kl}\partial_k\partial_l P^{\mathrm{s}}}_{x_i \mathrm{L}_0 P^{\mathrm{s}} = 0} - 2D_{ik}\partial_k P^{\mathrm{s}} = -f_i P^{\mathrm{s}} \end{aligned}$$

For $t > t'$

$$\begin{aligned} R^i_A(t,t') =& -[D^{-1}]_{ij} \int d\mathbf{x} A(\mathbf{x}) e^{-\mathrm{L}_0(\mathbf{x})(t-t')} f_j(\mathbf{x}) P^{\mathrm{s}}(\mathbf{x}) \\ =& [D^{-1}]_{ij} \int d\mathbf{x} A(\mathbf{x}) e^{-\mathrm{L}_0(\mathbf{x})(t-t')} \mathrm{L}_0(x_j P^{\mathrm{s}}(\mathbf{x})) \\ =& [D^{-1}]_{ij} \frac{d}{dt'} \langle A(t) x_j(t') \rangle_0 \end{aligned}$$

- Overdamped system

$$\dot{x} = \gamma^{-1} f(x) + \xi(t), \quad \langle \xi(t)\xi(t') \rangle = 2D\delta(t-t'), \qquad D = k_B T/\gamma$$

Note that $f = f^{\rm ir}$. Therefore, we have

$$R_A(t,t') = -D^{-1}\gamma^{-1}\langle A(t) f(t') \rangle_0 = -\frac{1}{k_B T}\langle A(t) f(t') \rangle_0, \qquad t > t'$$

and

$$\boxed{R_A(t,t') = \frac{1}{D}\langle A(t)\dot{x}(t') \rangle_0}, \quad t > t'$$

- Brownian motion with momentum dependent irreversible force

$$\dot{p} = -\frac{\gamma}{m}p + f(x) + g(p) + \xi(t), \quad \langle \xi(t)\xi(t')\rangle = 2B\delta(t-t'), \quad B = \gamma k_B T$$

$g(p)$ is irreversible: $g(-p) = -g(p)$. Total irreversible force: $-\gamma p/m + g(p)$. Therefore we have

$$\begin{aligned} R_A(t,t') &= -B^{-1}\langle A(t')(-\gamma p(t')/m + g(p(t'))\rangle_0 \\ &= \frac{1}{k_B T}\langle A(t)\frac{p(t')}{m}\rangle_0 - \frac{1}{B}\langle A(t)g(p(t'))\rangle_0 \end{aligned}$$

☐ Example 2: Perturbation of stationary state without DB Consider again for some i (We also assume that $f = f^{\mathrm{ir}}$.)

$$\dot{x}_i = f_i(\mathbf{x}) + \lambda(t) + \xi_i(t), \quad \mathrm{L}_1^{\mathrm{i}}(\mathbf{x}, t) = \lambda(t)\partial_i,$$

Without assuming DB, we have for $P^{\mathrm{s}} = e^{-\phi}$,

$$\frac{J_i^{\mathrm{s}}}{P^{\mathrm{s}}} = f_i(\mathbf{x}) + \sum_j D_{ij}\partial_j\phi(\mathbf{x}) \equiv \nu_i \neq 0$$

$$B_i(\mathbf{x}) = -\frac{1}{P^{\mathrm{s}}(\mathbf{x})}\partial_i P^{\mathrm{s}}(\mathbf{x}) = \partial_i\phi(\mathbf{x}) = \sum_j [D^{-1}]_{ij}(\nu_j - f_j)$$

Therefore,

$$\boxed{R_A^i(t,t') = \langle A(t)\partial_i\phi(t')\rangle = \sum_j [D^{-1}]_{ij}\langle A(t)(\nu_j(t') - f_j(t'))\rangle}, \qquad t > t'$$

We again have

$$\mathrm{L}_0(x_i P^{\mathrm{s}}(\mathbf{x})) = \partial_k(f_k x_i P^{\mathrm{s}}) - \partial_k\partial_l(D_{kl}x_i P^{\mathrm{s}}) = f_i P^{\mathrm{s}} - 2D_{ik}\partial_k P^{\mathrm{s}} = (2\nu_i - f_i)P^{\mathrm{s}}$$

or $\mathrm{L}_0(x_i P^{\mathrm{s}}) - \nu_i P^{\mathrm{s}} = (\nu_i - f_i)P^{\mathrm{s}}$. Therefore, we can also write

$$\boxed{R_A^i(t,t') = \sum_j [D^{-1}]_{ij}\langle A(t)(\dot{x}_j(t') - \nu_j(t'))\rangle}, \qquad t > t'$$

1 Langevin Equations

2 Generalized Langevin Equations

3 Fokker-Planck Equation

4 Fluctuation-Response Relations
- Fokker-Planck equation
- Liouville Equation

5 FDR and Time-Reversal Symmetry
- Martin-Siggia-Rose-Janssen-De Dominicis Formalism
- Time-Reversal Transformations

Fluctuation-Response Relations / Liouville equations

The Liouville eq. (with $\mathbf{x} \equiv (\{\mathbf{q}_i, \mathbf{p}_i\})$)

$$\partial_t \rho(\mathbf{x}, t) = \left[\frac{\partial H}{\partial \mathbf{q}} \cdot \frac{\partial}{\partial \mathbf{p}} - \frac{\partial H}{\partial \mathbf{p}} \cdot \frac{\partial}{\partial \mathbf{q}}\right] \rho = \{H, \rho\}_{\mathrm{PB}} \equiv -\mathcal{L}_0 \rho(\mathbf{x}, t)$$

Apply a small time-dependent perturbation to Hamiltonian as $H - \lambda(t) M(\mathbf{x})$.

$$\mathcal{L}(\mathbf{x}, t) = \mathcal{L}_0(\mathbf{x}) + \lambda(t) \mathcal{L}_1(\mathbf{x}),$$

where $\mathcal{L}_1 \rho = \{M, \rho\}_{\mathrm{PB}}$. Equilibrium dist. $\rho_{\mathrm{eq}} = (1/Z) \exp(-\beta H)$ is the stationary solution of $\mathcal{L}_0$: $\mathcal{L}_0(\mathbf{x}) \rho_{\mathrm{eq}}(\mathbf{x}) = 0$.
Write $\rho = \rho_{\mathrm{eq}} + \rho_1$ then the Liouville eq. becomes for small λ

$$\partial_t \rho_1 = -\mathcal{L}_0 \rho_1 - \mathcal{L}_1 \rho_{\mathrm{eq}} + O(\lambda^2)$$

The solution with initial condition $\rho_1(\mathbf{x}, -\infty) = 0, \rho(\mathbf{x}, -\infty) = \rho_{\mathrm{eq}}(\mathbf{x})$ is

$$\rho_1(\mathbf{x}, t) = -\int_{-\infty}^{t} dt' \; e^{-\mathcal{L}_0(\mathbf{x})(t - t')} \lambda(t') \mathcal{L}_1(\mathbf{x}) \rho_{\mathrm{eq}}(\mathbf{x})$$

The average of an observable $A(\mathbf{x})$ is given by

$$\langle A \rangle_t \equiv \int d\mathbf{x}\ \rho(\mathbf{x}, t) A(\mathbf{x}).$$

The response to the perturbation is studied using the response function

$$R_A(t, t') \equiv \left. \frac{\delta \langle A \rangle_t}{\delta \lambda(t')} \right|_{\lambda=0} = -\int d\mathbf{x}\ A(\mathbf{x}) e^{-\mathcal{L}_0(\mathbf{x})(t-t')} \mathcal{L}_1(\mathbf{x}) \rho_{\rm eq}(\mathbf{x}), \qquad t > t'$$

Now

$$\mathcal{L}_1(\mathbf{x}) \rho_{\rm eq}(\mathbf{x}) = \{M, \rho_{\rm eq}\}_{\rm PB} = -\beta \rho_{\rm eq} \{M, H\}_{\rm PB}$$

Note that

$$\begin{aligned} \dot{M}(\mathbf{x}) &= \frac{\partial M}{\partial \mathbf{q}} \cdot \dot{\mathbf{q}} + \frac{\partial M}{\partial \mathbf{p}} \cdot \dot{\mathbf{p}} = \frac{\partial M}{\partial \mathbf{q}} \cdot \frac{\partial H}{\partial \mathbf{p}} - \frac{\partial M}{\partial \mathbf{p}} \cdot \frac{\partial H}{\partial \mathbf{q}} \\ &= -\{H, M\}_{\rm PB} = \mathcal{L}_0 M(\mathbf{x}) \end{aligned}$$

The formal solution to this is $M(t) = \exp[\mathcal{L}_0 t] M(0)$ ("Heisenberg" picture). Therefore

$$R_A(t, t') = \beta \int d\mathbf{x}\ A(\mathbf{x}) e^{-\mathcal{L}_0(\mathbf{x})(t-t')} \dot{M}(\mathbf{x}) \rho_{\rm eq}(\mathbf{x}), \qquad t > t'$$

In general, define (equilibrium) time-correlation function of two observables A and B as

$$\begin{aligned}\langle A(t)B(t')\rangle &= \int d\mathbf{x}\ \left(e^{\mathcal{L}_0 t}A(\mathbf{x})\right)\left(e^{\mathcal{L}_0 t'}B(\mathbf{x})\right)\rho_{\rm eq}(\mathbf{x}) \\ &= \int d\mathbf{x}\ \left(e^{\mathcal{L}_0 t}A(\mathbf{x})\right)e^{\mathcal{L}_0 t'}B(\mathbf{x})\rho_{\rm eq}(\mathbf{x}) \\ &= \int d\mathbf{x}\ A(\mathbf{x})e^{-\mathcal{L}_0(t-t')}B(\mathbf{x})\rho_{\rm eq}(\mathbf{x}),\end{aligned}$$

where we have used two properties of $\mathcal{L}_0$ (Show these!)

$$\int d\mathbf{x}\ A(\mathbf{x})\mathcal{L}_0 B(\mathbf{x}) = -\int d\mathbf{x}\left(\mathcal{L}_0 A(\mathbf{x})\right)B(\mathbf{x}),$$

$$e^{\mathcal{L}_0 t}A(\mathbf{x})B(\mathbf{x}) = \left(e^{\mathcal{L}_0 t}A(\mathbf{x})\right)\left(e^{\mathcal{L}_0 t}B(\mathbf{x})\right)$$

We therefore have

$$\boxed{R_A(t,t') = \beta\langle A(t)\dot{M}(t')\rangle}, \qquad t > t'$$

- Example: Electrical Conductivity (Very Rough; Classical)
  - Consider a set of N particles of charge q_i located at $\mathbf{x}_i$.
  - Apply a uniform time-varying electric field $\mathbf{E}(t)$.
  - Interaction Hamiltonian is

$$H_I = \sum_i q_i \Phi(\mathbf{x}_i),$$

where $\Phi(\mathbf{x})$ is the elctrostatic potential for $\mathbf{E}(t) = -\boldsymbol{\nabla}\Phi(\mathbf{x})$. We can easily see that $\Phi(\mathbf{x}) = -\mathbf{x} \cdot \mathbf{E}(t)$. We have

$$H_I = -\sum_i q_i \mathbf{x}_i \cdot \mathbf{E}(t) = -\mathbf{P} \cdot \mathbf{E}(t),$$

where $\mathbf{P} \equiv \sum_i q_i \mathbf{x}_i$ is the total dipole moment.

- For the conductivity we have correspondences:

$$A \Leftrightarrow \mathbf{J}, \quad \lambda(t) \Leftrightarrow \mathbf{E}(t), \quad M \Leftrightarrow \mathbf{P}$$

Without perturbing **E**, we expect $\langle J_\alpha \rangle = 0$. In the presence of **E**, we expect

$$\langle J_\alpha(t)\rangle = \int_{-\infty}^{\infty} dt'\ R_{\alpha\beta}(t-t')E_\beta(t').$$

We can identify that the response function is the conductivity

$$R_{\alpha\beta}(t-t') = \sigma_{\alpha\beta}(t-t')$$

Using the fact that $\dot{\mathbf{P}} = \sum_i q_i \dot{\mathbf{x}}_i = V\mathbf{J}$ in the FDR, we have

$$\boxed{\sigma_{\alpha\beta}(t) = \theta(t)\beta\langle J_\alpha(t)\dot{P}_\beta(0)\rangle = \theta(t)\beta V\langle J_\alpha(t)J_\beta(0)\rangle \equiv \theta(t)\beta V C_{\alpha\beta}(t)}$$

The Fourier-Laplace transform

$$\tilde{\sigma}_{\alpha\beta}(\omega) = \int_{-\infty}^{\infty} dt\ e^{i\omega t}\sigma_{\alpha\beta}(t) = \int_0^{\infty} dt\ e^{i\omega t}\sigma_{\alpha\beta}(t)$$

Using the integral representation of the theta function,

$$\theta(t) = i\int_{-\infty}^{\infty} \frac{d\omega'}{2\pi}\,\frac{e^{-i\omega' t}}{\omega' + i\epsilon}, \quad \epsilon = 0^+$$

we have

$$\begin{aligned}
\tilde{\sigma}_{\alpha\beta}(\omega) =& i\beta V \int_{-\infty}^{\infty} dt\; e^{i\omega t} \int_{-\infty}^{\infty} \frac{d\omega'}{2\pi}\,\frac{e^{-i\omega' t}}{\omega' + i\epsilon} \int_{-\infty}^{\infty} \frac{d\bar{\omega}}{2\pi} e^{-i\bar{\omega} t}\tilde{C}_{\alpha\beta}(\bar{\omega}) \\
=& i\beta V \int_{-\infty}^{\infty} \frac{d\omega'}{2\pi} \int_{-\infty}^{\infty} \frac{d\bar{\omega}}{2\pi}\,\frac{\tilde{C}_{\alpha\beta}(\bar{\omega})}{\omega' + i\epsilon}(2\pi)\delta(\omega - \omega' - \bar{\omega}) \\
=& -i\beta V \int_{-\infty}^{\infty} \frac{d\bar{\omega}}{2\pi}\,\frac{\tilde{C}_{\alpha\beta}(\bar{\omega})}{\bar{\omega} - \omega - i\epsilon} \\
=& -i\beta V \mathcal{P} \int_{-\infty}^{\infty} \frac{d\bar{\omega}}{2\pi}\,\frac{\tilde{C}_{\alpha\beta}(\bar{\omega})}{\bar{\omega} - \omega} + \frac{1}{2}\beta V \tilde{C}_{\alpha\beta}(\omega)
\end{aligned}$$

Longitudinal DC conductivity

$$\begin{aligned}\sigma_L \equiv& \frac{1}{3}\sum_\alpha \tilde{\sigma}_{\alpha\alpha}(0)\\ =& \frac{1}{3}\sum_\alpha \left[-i\beta V\mathcal{P}\int_{-\infty}^{\infty}\frac{d\bar{\omega}}{2\pi}\frac{\tilde{C}_{\alpha\alpha}(\bar{\omega})}{\bar{\omega}} + \frac{1}{2}\beta V\tilde{C}_{\alpha\alpha}(0)\right]\\ =& \frac{\beta V}{6}\sum_\alpha \tilde{C}_{\alpha\alpha}(0),\end{aligned}$$

where we have used the fact that $C_{\alpha\alpha}(t) = C_{\alpha\alpha}(-t)$, and $\tilde{C}_{\alpha\alpha}(\omega) = \tilde{C}_{\alpha\alpha}(-\omega)$. We finally obtain the Green-Kubo formula as

$$\boxed{\sigma_L = \frac{\beta V}{3}\sum_\alpha \int_0^\infty dt\,\langle J_\alpha(t)J_\alpha(0)\rangle}$$

1 Langevin Equations

2 Generalized Langevin Equations

3 Fokker-Planck Equation

4 Fluctuation-Response Relations
  - Fokker-Planck equation
  - Liouville Equation

5 FDR and Time-Reversal Symmetry
  - Martin-Siggia-Rose-Janssen-De Dominicis Formalism
  - Time-Reversal Transformations

FDR and Time-Reversal Symmetry

Martin-Siggia-Rose-Janssen-De Dominicis Functional-Integral Formalism

Consider again

$$\frac{dx_i}{dt} = f_i(x(t)) + \xi_i(t), \qquad\qquad (\star)$$

where $\langle \xi_i(t) \rangle = 0$ and $\langle \xi_i(t)\xi_j(t') \rangle = 2D_{ij}\delta(t-t')$.

Let us use the distribution function $P_\xi[\boldsymbol{\xi}]$ for the Gaussian white noise, which satisfies

$$\int \mathcal{D}\boldsymbol{\xi} P_\xi[\boldsymbol{\xi}]\xi_i(t) = 0, \qquad \int \mathcal{D}\boldsymbol{\xi} P_\xi[\boldsymbol{\xi}]\xi_i(t)\xi_j(t') = 2D_{ij}\delta(t-t')$$

It is given by (summation convention)

$$\begin{aligned} P_\xi[\xi] =& \mathcal{Z}^{-1}\exp(-\frac{1}{4}\int dt\ \xi_i(t)D^{-1}_{ij}\xi_j(t)) \\ =& \mathcal{Z}^{-1}\exp(-\frac{1}{4}\int dt \int dt'\ \xi_i(t)D^{-1}_{ij}\delta(t-t')\xi_j(t')), \end{aligned}$$

where

$$\mathcal{Z} = \int \mathcal{D}\xi\ \exp(-\frac{1}{4}\int dt\ \xi_i(t)D^{-1}_{ij}\xi_j(t)).$$

Gaussian Integrals

Consider (summation convention)

$$P_0(\mathbf{x}) = \frac{1}{Z_0}\exp(-\frac{1}{2}x_i A_{ij} x_j),$$

where

$$Z_0 = \int \prod_i dx_i \exp[-\frac{1}{2}x_i A_{ij} x_j] = (2\pi)^{n/2}(\det \mathtt{A})^{-1/2}.$$

From

$$Z_0(b) = \int \prod_i dx_i \exp[-\frac{1}{2}x_i A_{ij} x_j + b_i x_i] = Z_0 \exp[b_i A^{-1}_{ij} b_j]$$

we have

$$\langle x_i x_j \rangle_0 = \int \prod_i dx_i \; x_i x_j P_0(\mathbf{x}) = \frac{1}{Z_0}\,\frac{\partial^2}{\partial b_i \partial b_j} Z_0(b)\Big|_{\mathbf{b}=0} = A^{-1}_{ij}$$

$\langle x_i x_j \cdots x_n \rangle_0$ can be expressed in terms of $\langle x_i x_j \rangle_0$.

Perturbation Expansion (0-dim. field theory)

Consider for example

$$P(\mathbf{x}) = \frac{1}{Z}\exp(-\frac{1}{2}x_i A_{ij} x_j + \lambda \sum_i x_i^4),$$

where

$$Z = \int \prod_i dx_i \exp[-\frac{1}{2}x_i A_{ij} x_j + \lambda \sum_i x_i^4)].$$

Expand

$$\exp[\lambda \sum_i x_i^4] = 1 + \lambda \sum_i x_i^4 + \frac{1}{2}\lambda^2 \sum_i x_i^4 \sum_j x_j^4 + O(\lambda^3)$$

Express

$$\langle x_i x_j \rangle = \int \prod_i dx_i \; x_i x_j P(\mathbf{x})$$

in terms of $\langle x_i x_j \rangle_0$.

The transition probability is

$$P(\mathbf{x}_\tau, \tau|\mathbf{x}_0, 0) = \int \mathcal{D}\boldsymbol{\xi}\ P_\xi[\boldsymbol{\xi}]\ \delta(\mathbf{x}(\tau) - \mathbf{x}_\tau), \qquad (*)$$

where $\mathbf{x}(t)$ is the solution to $(\star)$ with the initial condition $\mathbf{x}(0) = \mathbf{x}_0$.
Now we use the identity

$$1 = \int \mathcal{D}\mathbf{x}\ \delta(\dot{\mathbf{x}}(t) - f(\mathbf{x}(t)) - \boldsymbol{\xi}(t))\ J[\mathbf{x}],$$

where

$$J[\mathbf{x}] = \det\left[\frac{\delta\xi_i(t)}{\delta x_j(t')}\right]$$

is the Jacobian. Using the integral representation of the delta-function,

$$1 = \int \mathcal{D}\mathbf{x} \int \mathcal{D}\hat{\mathbf{x}}\ J[\mathbf{x}] \exp\left[-i\sum_j \int_0^\tau dt\ \hat{x}_j(t)\{\dot{x}_j(t) - f_j(x(t)) - \xi_j(t)\}\right]$$

Inserting this into $(*)$,

$$
\begin{aligned}
P(\mathbf{x}_\tau, \tau | \mathbf{x}_0, 0) &= \int \mathcal{D}\xi P_\xi[\xi] \int_{\mathbf{x}(0)=\mathbf{x}_0}^{\mathbf{x}(\tau)=\mathbf{x}_\tau} \mathcal{D}\mathbf{x} \int \mathcal{D}\hat{\mathbf{x}}\ J[\mathbf{x}]\ e^{-i\sum_i \int_0^\tau dt\ \hat{x}_i(t)\{\dot{x}_i(t)-f_i(\mathbf{x}(t))-\xi_i(t)\}} \\
&= \int_{\mathbf{x}(0)=\mathbf{x}_0}^{\mathbf{x}(\tau)=\mathbf{x}_\tau} \mathcal{D}\mathbf{x} \int \mathcal{D}\hat{\mathbf{x}}\ J[\mathbf{x}] \\
&\qquad \times \exp\left[-\int_0^\tau dt\ \left\{\sum_{i,j} \hat{x}_i(t) D_{ij} \hat{x}_j(t) + i \sum_i \hat{x}_i(t)\{\dot{x}_i(t) - f_i(\mathbf{x}(t))\}\right\}\right]
\end{aligned}
$$

Define

$$
S_0[\mathbf{x}, \hat{\mathbf{x}}] \equiv \int_0^\tau dt\ \left\{\sum_{i,j} \hat{x}_i(t) D_{ij} \hat{x}_j(t) + i \sum_i \hat{x}_i(t)\{\dot{x}_i(t) - f_i(\mathbf{x}(t))\}\right\}
$$

The average of an observable $A[\mathbf{x}(t)]$ which depends on the $\mathbf{x}(t)$, $0 \le t \le \tau$ is given by

$$\langle A[\mathbf{x}(t)]\rangle = \int d\mathbf{x}_\tau \int d\mathbf{x}_0 \; P_i(\mathbf{x}_0) \int_{\mathbf{x}(0)=\mathbf{x}_0}^{\mathbf{x}(\tau)=\mathbf{x}_\tau} \mathcal{D}\mathbf{x} \int \mathcal{D}\hat{\mathbf{x}} \; J[\mathbf{x}] A[\mathbf{x}(t)] e^{-S_0[\mathbf{x},\hat{\mathbf{x}}]}$$
$$= \int \mathcal{D}\mathbf{x} \int \mathcal{D}\hat{\mathbf{x}} \; J[\mathbf{x}] A[\mathbf{x}(t)] e^{-S_0[\mathbf{x},\hat{\mathbf{x}}]} P_i(\mathbf{x}_0),$$

where $P_i(\mathbf{x}_0)$ is the initial distribution.
This can be understood from

$$P(\mathbf{x}_k, t_k) = \int d\mathbf{x}_{\mathbf{k-1}} P(\mathbf{x}_k, t_k | \mathbf{x}_{k-1}, t_{k-1}) P(\mathbf{x}_{k-1}, t_{k-1})$$

For a finite time interval $[0, \tau]$, we divide it into M infinitesimal intervals such that $t_0 = 0$ and $t_M = \tau$, $\mathbf{x}_M = \mathbf{x}_\tau$ and $dt = \tau/M$.

$$P(\mathbf{x}_\tau, \tau | \mathbf{x}_0, 0) = \int d\mathbf{x}_1 \cdots d\mathbf{x}_{M-1} \prod_{k=1}^{M} P(\mathbf{x}_k, t_k | \mathbf{x}_{k-1}, t_{k-1})$$

Onsager-Machlup

Integrating away $\hat{\mathbf{x}}$, we have

$$\langle A[\mathbf{x}]\rangle \sim \int \mathcal{D}\mathbf{x} J[\mathbf{x}] A[\mathbf{x}] \exp[-S_{\mathrm{OM}}[\mathbf{x}]] P_i(\mathbf{x}_0),$$

where

$$S_{\mathrm{OM}}[\mathbf{x}] = \frac{1}{4}\int_0^\tau dt \sum_{i,j}\{\dot{x}_i(t) - f_i(\mathbf{x}(t))\} D_{ij}^{-1}\{\dot{x}_j(t) - f_j(\mathbf{x}(t))\}$$

□ Evaluation of Jacobian

$$J[\mathbf{x}] = \det\left[\frac{\delta \xi_i(t)}{\delta x_j(t')}\right] \equiv \det \mathbb{M}_{ij}(t,t') = \det\left[\delta_{ij}\frac{d}{dt}\delta(t-t') - \frac{\partial f_i}{\partial x_j}\delta(t-t')\right]$$

We can write

$$\mathbb{M}_{ij}(t,t') = \sum_k \int dt'' \mathbb{M}^{(0)}_{ik}(t,t'')\mathbb{M}^{(1)}_{kj}(t'',t'),$$

where

$$\mathbb{M}^{(0)}_{ik}(t,t'') = \delta_{ik}\frac{d}{dt}\delta(t-t'')$$

and

$$\mathbb{M}^{(1)}_{kj}(t'',t') = \delta_{kj}\delta(t''-t') - \theta(t''-t')\frac{\partial f_k}{\partial x_j}$$

Note that $\det \mathbb{M} = \det \mathbb{M}^{(0)} \det \mathbb{M}^{(1)}$ and that $\det \mathbb{M}^{(0)}$ is a constant which can be absorbed into the functional integral measure.

We therefore have

$$\begin{aligned}J[\mathbf{x}] =& \mathcal{N} \det \mathbb{M}^{(1)} = \mathcal{N} \exp[\mathrm{tr} \ln \mathbb{M}^{(1)}] \\ =& \mathcal{N} \exp \Big[- \theta(0) \int dt \sum_i \frac{\partial f_i(\mathbf{x}(t))}{\partial x_i} \\ & - \frac{1}{2} \int dt_1 \int dt_2\, \theta(t_1 - t_2)\theta(t_2 - t_1) \sum_{i,j} \frac{\partial f_i(\mathbf{x}(t_1))}{\partial x_j} \frac{\partial f_j(\mathbf{x}(t_2))}{\partial x_i} - \cdots \Big]\end{aligned}$$

All but the first term vanish due to the properties of the theta function. We have

$$\boxed{J[\mathbf{x}] = \mathcal{N} \exp \left[-\theta(0) \int dt \sum_i \frac{\partial f_i(\mathbf{x}(t))}{\partial x_i} \right] \equiv \mathcal{N} \exp[-S_J[\mathbf{x}]]}$$

The appearance of $\theta(0)$ is intimately related to the discretization scheme for the stochastic differential equation. (e.g. $\theta(0) = 0 \Leftrightarrow$ Itô, $\theta(0) = 1/2 \Leftrightarrow$ Stratonovich)

☐ More general average

$$\langle \mathcal{O}[\mathbf{x}, \hat{\mathbf{x}}] \rangle = \int \mathcal{D}\mathbf{x} \int \mathcal{D}\hat{\mathbf{x}}\, \mathcal{O}[\mathbf{x}, \hat{\mathbf{x}}] e^{-S_0[\mathbf{x},\hat{\mathbf{x}}] - S_J[\mathbf{x}]} P_i(\mathbf{x}(0))$$

Alternative Derivation

Recall that

$$P(\mathbf{x}', t+dt) = \int d\mathbf{x}\; P(\mathbf{x}', t+dt|\mathbf{x}, t)P(\mathbf{x}, t)$$

From the Fokker-Planck equation, $\partial_t P = -\mathtt{L}P$, we have

$$P(\mathbf{x}', t+dt) = e^{-(dt)\mathtt{L}(\mathbf{x}')}P(\mathbf{x}', t),$$

where

$$\mathtt{L}(\mathbf{x}) = \sum_i \frac{\partial}{\partial x_i} f_i(\mathbf{x}) - \sum_{i,j} \frac{\partial^2}{\partial x_i \partial x_j} D_{ij}$$

We can therefore write the short-time transition probability as (summation convention)

$$\begin{aligned} P(\mathbf{x}', t+dt|\mathbf{x}, t) =& e^{-(dt)\mathtt{L}(\mathbf{x}')}\delta(\mathbf{x}'-\mathbf{x}) = \left(1-(dt)\mathtt{L}(\mathbf{x}')\right)\delta(\mathbf{x}'-\mathbf{x}) \\ =& \delta(\mathbf{x}'-\mathbf{x}) - (dt)\partial_i'[f_i(\mathbf{x}')\delta(\mathbf{x}'-\mathbf{x})] + (dt)D_{ij}\partial_i'\partial_j'\delta(\mathbf{x}'-\mathbf{x}) \\ =& \delta(\mathbf{x}'-\mathbf{x}) - (dt)f_i(\mathbf{x})\partial_i'\delta(\mathbf{x}'-\mathbf{x}) + (dt)D_{ij}\partial_i'\partial_j'\delta(\mathbf{x}'-\mathbf{x}) \end{aligned}$$

Introduce new variables for some constant a

$$\mathbf{u} = \mathbf{u}(\mathbf{x}', \mathbf{x}) \equiv \mathbf{x}' - \mathbf{x}, \qquad \mathbf{v} = \mathbf{v}(\mathbf{x}', \mathbf{x}) \equiv a\mathbf{x}' + (1-a)\mathbf{x}$$

Inverse:

$$\mathbf{x}' = \mathbf{x}'(\mathbf{u}, \mathbf{v}) \equiv (1-a)\mathbf{u} + \mathbf{v}, \qquad \mathbf{x} = \mathbf{x}(\mathbf{u}, \mathbf{v}) \equiv -a\mathbf{u} + \mathbf{v}$$

Now note that

$$\begin{aligned} -f_i(\mathbf{x})\partial_i'\delta(\mathbf{x}'-\mathbf{x}) &= -\, f_i(\mathbf{x}(\mathbf{u},\mathbf{v}))\frac{\partial}{\partial u_i}\delta(\mathbf{u}) \\ &= -\,\frac{\partial}{\partial u_i}\left(f_i(\mathbf{x}(\mathbf{0},\mathbf{v}))\delta(\mathbf{u})\right) + \left.\frac{\partial f_i(\mathbf{x}(\mathbf{u},\mathbf{v}))}{\partial u_i}\right|_{\mathbf{u}=0}\delta(\mathbf{u}) \\ &= -\, f_i(\mathbf{x}(\mathbf{0},\mathbf{v}))\frac{\partial}{\partial u_i}\delta(\mathbf{u}) + \left.\frac{\partial f_i(\mathbf{x}(\mathbf{u},\mathbf{v}))}{\partial x_i}\frac{\partial x_i}{\partial u_i}\right|_{\mathbf{u}=0}\delta(\mathbf{u}) \end{aligned}$$

Let us call

$$\bar{\mathbf{x}} \equiv \mathbf{x}(\mathbf{0},\mathbf{v}) = a\mathbf{x}' + (1-a)\mathbf{x}$$

We therefore have

$$\boxed{-f_i(\mathbf{x})\partial_i'\delta(\mathbf{x}'-\mathbf{x}) = -f_i(\bar{\mathbf{x}})\partial_i'\delta(\mathbf{x}'-\mathbf{x}) - a\frac{\partial f_i(\bar{\mathbf{x}})}{\partial \bar{x}_i}\delta(\mathbf{x}'-\mathbf{x})}$$

We have an intrinsic ambiguity in this kind of expression.

This looks weird!
But in QM, we have $\hat{p} \Leftrightarrow -i(\partial/\partial x)$ and

$$\langle x'|\hat{p}|x\rangle = -i\frac{\partial}{\partial x'}\delta(x'-x), \qquad \langle x'|\hat{p}f(\hat{x})|x\rangle = -if(x)\frac{\partial}{\partial x'}\delta(x'-x).$$

We know that

$$[\hat{p}, f(\hat{x})] = -if'(x),$$

or

$$\hat{p}f(\hat{x}) = (1-a)\hat{p}f(\hat{x}) + a\left(f(\hat{x})\hat{p} - if'(x)\right)$$

Using

$$\langle x'|f(\hat{x})\hat{p}|x\rangle = -if(x')\frac{\partial}{\partial x'}\delta(x'-x),$$

we have

$$-if(x)\frac{\partial}{\partial x'}\delta(x'-x) = -i\left\{(1-a)f(x) + af(x')\right\}\frac{\partial}{\partial x'}\delta(x'-x) - if'(x)\delta(x'-x),$$

This is exactly the same as above if we identify

$$(1-a)f(x) + af(x') \simeq f(\bar{x})$$

for the two points x and x' separated by dt.

Using the integral representation of the delta function

$$\delta(\mathbf{x}' - \mathbf{x}) = \int \frac{d\mathbf{y}}{(2\pi)^N} \exp[-i\mathbf{y} \cdot (\mathbf{x}' - \mathbf{x})],$$

we have

$$\begin{aligned} P(\mathbf{x}', t + dt|\mathbf{x}, t) &= \int \frac{d\mathbf{y}}{(2\pi)^N}\, e^{-i\mathbf{y}\cdot(\mathbf{x}'-\mathbf{x})} \left[1 + (dt) i y_i f_i(\bar{\mathbf{x}}) - (dt) a \frac{\partial f_i(\bar{\mathbf{x}})}{\partial \bar{x}_i} - (dt) D_{ij} y_i y_j\right] \\ &= \int \frac{d\mathbf{y}}{(2\pi)^N} \exp\left[-i\mathbf{y} \cdot (\mathbf{x}' - \mathbf{x}) + (dt) i y_i f_i(\bar{\mathbf{x}}) - (dt) a \frac{\partial f_i(\bar{\mathbf{x}})}{\partial \bar{x}_i} - (dt) D_{ij} y_i y_j\right] \\ &= \int \frac{d\mathbf{y}}{(2\pi)^N} \exp\left\{-(dt)\left[y_i D_{ij} y_j + i y_i \left(\frac{x_i' - x_i}{dt} - f_i(\bar{\mathbf{x}})\right) + a \frac{\partial f_i(\bar{\mathbf{x}})}{\partial \bar{x}_i}\right]\right\} \end{aligned}$$

For a finite time interval $[0,\tau]$, we divide it into M infinitesimal intervals such that $t_0 = 0$ and $t_M = \tau$ and $dt = \tau/M$. Then we can easily see that

$$P(\mathbf{x},\tau) = \int d\mathbf{x}_0 \cdots d\mathbf{x}_{M-1} \prod_{k=1}^{M} P(\mathbf{x}_k, t_k | \mathbf{x}_{k-1}, t_{k-1}) P(\mathbf{x}_0, 0)$$

We need integration variables $\mathbf{y}_0, \cdots, \mathbf{y}_{M-1}$ to express the conditional probabilities.

In the limit $dt \to 0$, this gives exactly the same path-integral representation as before if we identify $\mathbf{y} = \hat{\mathbf{x}}$.

We identify $\theta(0)$ obtained earlier can be identified with the discretization scheme parameter a.

Detour: Fokker-Planck equation for multiplicative noises

The most general form for the Fokker-Planck operator (including the possiblilty of multiplicative noise) is

$$\mathtt{L}(\mathbf{x}) = \sum_i \frac{\partial}{\partial x_i} A_i(\mathbf{x}) - \sum_{i,j} \frac{\partial^2}{\partial x_i \partial x_j} D_{ij}(\mathbf{x})$$

We have to evaluate

$$\begin{aligned}
D_{ij}(\mathbf{x})\partial_i'\partial_j'\delta(\mathbf{x}'-\mathbf{x}) =& D_{ij}(\mathbf{x}(\mathbf{u},\mathbf{v}))\frac{\partial^2}{\partial u_i \partial u_j}\delta(\mathbf{u}) \\
=& \frac{\partial}{\partial u_i}\left(D_{ij}(\mathbf{x}(\mathbf{u},\mathbf{v}))\frac{\partial}{\partial u_j}\delta(\mathbf{u})\right) - \frac{\partial D_{ij}(\mathbf{x}(\mathbf{u},\mathbf{v}))}{\partial u_i}\frac{\partial}{\partial u_j}\delta(\mathbf{u}) \\
=& \frac{\partial^2}{\partial u_i \partial u_j}\left(D_{ij}(\mathbf{x}(\mathbf{0},\mathbf{v}))\delta(\mathbf{u})\right) - \frac{\partial}{\partial u_i}\left(\left(\frac{\partial}{\partial u_j}D_{ij}(\mathbf{x}(\mathbf{0},\mathbf{v}))\right)\delta(\mathbf{u})\right) \\
& - \frac{\partial}{\partial u_j}\left(\left(\frac{\partial}{\partial u_i}D_{ij}(\mathbf{x}(\mathbf{0},\mathbf{v}))\right)\delta(\mathbf{u})\right) + \left(\frac{\partial^2}{\partial u_i \partial u_j}D_{ij}(\mathbf{x}(\mathbf{0},\mathbf{v}))\right)\delta(\mathbf{u})
\end{aligned}$$

$$
\begin{aligned}
D_{ij}(\mathbf{x})\partial_i'\partial_j'\delta(\mathbf{x}'-\mathbf{x}) =& D_{ij}(\bar{\mathbf{x}})\frac{\partial^2}{\partial u_i\partial u_j}\delta(\mathbf{u}) + 2a\left(\frac{\partial}{\partial\bar{x}_j}D_{ij}(\bar{\mathbf{x}})\right)\frac{\partial}{\partial u_i}\delta(\mathbf{u}) \\
&+ a^2\left(\frac{\partial^2}{\partial\bar{x}_i\partial\bar{x}_j}D_{ij}(\bar{\mathbf{x}})\right)\delta(\mathbf{u}) \\
=& D_{ij}(\bar{\mathbf{x}})\partial_i'\partial_j'\delta(\mathbf{x}'-\mathbf{x}) + 2a\left(\frac{\partial}{\partial\bar{x}_j}D_{ij}(\bar{\mathbf{x}})\right)\partial_i'\delta(\mathbf{x}'-\mathbf{x}) \\
&+ a^2\left(\frac{\partial^2}{\partial\bar{x}_i\partial\bar{x}_j}D_{ij}(\bar{\mathbf{x}})\right)\delta(\mathbf{x}'-\mathbf{x})
\end{aligned}
$$

We then have

$$
\begin{aligned}
P(\mathbf{x}',t+dt|\mathbf{x},t) =& \int\frac{d\mathbf{y}}{(2\pi)^N}\,e^{-i\mathbf{y}\cdot(\mathbf{x}'-\mathbf{x})}\Big[1+(dt)iy_iA_i(\bar{\mathbf{x}})-(dt)a\frac{\partial A_i(\bar{\mathbf{x}})}{\partial\bar{x}_i} \\
&-(dt)D_{ij}(\bar{\mathbf{x}})y_iy_j - 2a(dt)iy_i\frac{\partial}{\partial\bar{x}_j}D_{ij}(\bar{\mathbf{x}}) + a^2\frac{\partial^2}{\partial\bar{x}_i\partial\bar{x}_j}D_{ij}(\bar{\mathbf{x}})\Big] \\
=& \int\frac{d\mathbf{y}}{(2\pi)^N}\,\exp\Big\{-(dt)\Big[y_iD_{ij}(\bar{\mathbf{x}})y_j + iy_i\left(\frac{x_i'-x_i}{dt} - A_i(\bar{\mathbf{x}}) + 2a\frac{\partial}{\partial\bar{x}_j}D_{ij}(\bar{\mathbf{x}})\right) \\
&+ a\frac{\partial A_i(\bar{\mathbf{x}})}{\partial\bar{x}_i} - a^2\frac{\partial^2}{\partial\bar{x}_i\partial\bar{x}_j}D_{ij}(\bar{\mathbf{x}})\Big]\Big\}
\end{aligned}
$$

Response Functions

Consider again for some i

$$\dot{x}_i = f_i(\mathbf{x}) + \underbrace{\lambda_i(t)}_{perturbation} + \xi_i(t)$$

- Response of an average of a local observable $\langle \mathcal{A}[\mathbf{x}(t)] \rangle$ at t due to a perturbation $\lambda_i(t')$ at t'.
- Linear response

$$R^i_{\mathcal{A}}(t,t') = \left. \frac{\delta \langle \mathcal{A}[\mathbf{x}(t)] \rangle}{\delta \lambda_i(t')} \right|_{\lambda=0}$$

- Nonlinear responses

$$R^i_{\mathcal{A}}(t;t',t'') = \left. \frac{\delta^2 \langle \mathcal{A}[\mathbf{x}(t)] \rangle}{\delta \lambda_i(t') \delta \lambda_i(t'')} \right|_{\lambda=0}, \quad \text{etc.}$$

- Causality: $R^i_{\mathcal{A}}(t,t') = 0$ if $t < t'$. $R^i_{\mathcal{A}}(t;t',t'') = 0$ if $t < t'$ or $t < t''$.

$$\langle \mathcal{A}[\mathbf{x}(t)] \rangle = \int dt' \; R^i_{\mathcal{A}}(t,t') \lambda_i(t') + \frac{1}{2} \int dt' \int dt'' \; R^i_{\mathcal{A}}(t;t',t'') \lambda_i(t') \lambda_i(t'') + \cdots$$

Response Field Formalism

- In the action S_0, we have an additional term $-i\int dt\hat{x}_i(t)\lambda_i(t)$.
- Taking a derivative w.r.t. $\lambda_i(t')$ brings down a factor of $i\hat{x}_i(t')$ in front of the exponential.
- $\hat{x}(t)$: Response Field
- No need to introduce λ; All averages are w.r.t. the unperturbed action.

Response Field Formalism

$$R^i_{\mathcal{A}}(t,t') = \langle \mathcal{A}[\mathbf{x}(t)]i\hat{x}_i(t')\rangle.$$

$$R^i_{\mathcal{A}}(t;t',t'') = \langle \mathcal{A}[\mathbf{x}(t)]i\hat{x}_i(t')i\hat{x}_i(t'')\rangle, \quad \text{etc.}$$

1 Langevin Equations

2 Generalized Langevin Equations

3 Fokker-Planck Equation

4 Fluctuation-Response Relations
  - Fokker-Planck equation
  - Liouville Equation

5 FDR and Time-Reversal Symmetry
  - Martin-Siggia-Rose-Janssen-De Dominicis Formalism
  - Time-Reversal Transformations

$\mathcal{R}$-transformation

$$\mathcal{T}: \begin{cases} \mathbf{x}(t) & \to & \mathbf{x}^{\mathrm{R}}(t) \equiv \mathbf{x}(\tau - t) \\ \hat{\mathbf{x}}(t) & \to & \hat{\mathbf{x}}^{\mathrm{R}}(t) \equiv \hat{\mathbf{x}}(\tau - t) - i\mathrm{D}^{-1} \cdot \frac{d}{dt}\mathbf{x}(\tau - t) \end{cases}$$

- Integration measure:

$$\mathcal{D}\mathbf{x}\mathcal{D}\hat{\mathbf{x}} = \mathcal{D}\mathbf{x}^{\mathrm{R}}\mathcal{D}\hat{\mathbf{x}}^{\mathrm{R}}$$

- Jacobian

$$\begin{aligned} S_J[\mathbf{x}] \to S_J[\mathbf{x}^{\mathrm{R}}] &= \theta(0)\int_0^\tau dt\, \sum_i \frac{\partial}{\partial x_i^{\mathrm{R}}} f_i(\mathbf{x}^{\mathrm{R}}) \\ &= \theta(0)\int_0^\tau dt\, \sum_i \frac{\partial}{\partial x_i(\tau - t)} f(\mathbf{x}(\tau - t)) \\ &= S_J[\mathbf{x}] \end{aligned}$$

after changing the integration variable from $t \to t' = \tau - t$.

$$
\begin{aligned}
S_0[\mathbf{x}^{\mathrm{R}},\hat{\mathbf{x}}^{\mathrm{R}}] &= \int_0^{\tau} dt\Big[\{\hat{\mathbf{x}}(\tau-t) - i\mathtt{D}^{-1}\cdot\frac{d}{dt}\mathbf{x}(\tau-t)\}\cdot\mathtt{D} \\
&\qquad\qquad \cdot\{\hat{\mathbf{x}}(\tau-t) - i\mathtt{D}^{-1}\cdot\frac{d}{dt}\mathbf{x}(\tau-t)\} \\
&\quad + i\{\hat{\mathbf{x}}(\tau-t) - i\mathtt{D}^{-1}\cdot\frac{d}{dt}\mathbf{x}(\tau-t)\}\cdot\{\frac{d}{dt}\mathbf{x}(\tau-t) - \mathbf{f}(\mathbf{x}(\tau-t))\}\Big] \\
&= \int_0^{\tau} dt[\{\hat{\mathbf{x}}(t) + i\mathtt{D}^{-1}\cdot\frac{d}{dt}\mathbf{x}(t)\}\cdot\mathtt{D}\cdot\{\hat{\mathbf{x}}(t) + i\mathtt{D}^{-1}\cdot\frac{d}{dt}\mathbf{x}(t)\} \\
&\quad + i\{\hat{\mathbf{x}}(t) + i\mathtt{D}^{-1}\cdot\frac{d}{dt}\mathbf{x}(t)\}\cdot\{-\frac{d}{dt}\mathbf{x}(t) - \mathbf{f}(\mathbf{x}(t))\}] \\
&= S_0[\mathbf{x},\hat{\mathbf{x}}] + \underbrace{\int_0^{\tau} dt\,\dot{\mathbf{x}}(t)\cdot\mathtt{D}^{-1}\cdot\mathbf{f}(\mathbf{x}(t))}_{\equiv\Delta S[\mathbf{x}]}
\end{aligned}
$$

Suppose that $\mathbf{f} = \mathbf{f}^{\mathrm{ir}}$ and that the DB condition holds

$$\mathbf{f}(\mathbf{x}) = -\mathtt{D} \cdot \boldsymbol{\nabla}\phi(\mathbf{x}), \qquad P^{\mathrm{s}}(\mathbf{x}) = e^{-\phi(\mathbf{x})}$$

Then

$$\Delta S[\mathbf{x}] = -\int_0^\tau dt\, \dot{\mathbf{x}}(t) \cdot \boldsymbol{\nabla}\phi(\mathbf{x}) = -\int_0^\tau dt\, \frac{d}{dt}\phi(\mathbf{x}(t)) = -[\phi(\mathbf{x}(\tau)) - \phi(\mathbf{x}(0))].$$

Now suppose that $P_i(\mathbf{x}(0)) = \exp(-\phi(\mathbf{x}(0)))$. Then

$$\begin{aligned}
\langle \mathcal{O}[\mathbf{x}, \hat{\mathbf{x}}] \rangle &= \int \mathcal{D}\mathbf{x} \int \mathcal{D}\hat{\mathbf{x}}\, \mathcal{O}[\mathbf{x}, \hat{\mathbf{x}}] e^{-S_0[\mathbf{x},\hat{\mathbf{x}}] - S_J[\mathbf{x}]} P_i(\mathbf{x}(0)) \\
&= \int \mathcal{D}\mathbf{x}^{\mathrm{R}} \int \mathcal{D}\hat{\mathbf{x}}^{\mathrm{R}}\, \mathcal{O}[\mathbf{x}^{\mathrm{R}}, \hat{\mathbf{x}}^{\mathrm{R}}] e^{-S_0[\mathbf{x}^{\mathrm{R}},\hat{\mathbf{x}}^{\mathrm{R}}] - S_J[\mathbf{x}^{\mathrm{R}}]} P_i(\mathbf{x}^{\mathrm{R}}(0)) \\
&= \int \mathcal{D}\mathbf{x} \int \mathcal{D}\hat{\mathbf{x}}\, \mathcal{O}[\mathbf{x}^{\mathrm{R}}, \hat{\mathbf{x}}^{\mathrm{R}}] e^{-S_0[\mathbf{x},\hat{\mathbf{x}}] - \Delta S[\mathbf{x}] - S_J[\mathbf{x}]} P_i(\mathbf{x}(\tau)) \\
&= \int \mathcal{D}\mathbf{x} \int \mathcal{D}\hat{\mathbf{x}}\, \mathcal{O}[\mathbf{x}^{\mathrm{R}}, \hat{\mathbf{x}}^{\mathrm{R}}] e^{-S_0[\mathbf{x},\hat{\mathbf{x}}] - S_J[\mathbf{x}] + \{\phi(\mathbf{x}(\tau)) - \phi(\mathbf{x}(0))\}} P_i(\mathbf{x}(\tau)) \\
&= \int \mathcal{D}\mathbf{x} \int \mathcal{D}\hat{\mathbf{x}}\, \mathcal{O}[\mathbf{x}^{\mathrm{R}}, \hat{\mathbf{x}}^{\mathrm{R}}] e^{-S_0[\mathbf{x},\hat{\mathbf{x}}] - S_J[\mathbf{x}]} P_i(\mathbf{x}(0)) \\
&= \langle \mathcal{O}[\mathbf{x}^{\mathrm{R}}, \hat{\mathbf{x}}^{\mathrm{R}}] \rangle
\end{aligned}$$

In particular

$$\langle \mathcal{A}[\mathbf{x}(t)]\hat{x}_i(t')]\rangle = \left\langle \mathcal{A}[\mathbf{x}(\tau-t)] \left\{ \hat{x}_i(\tau-t') - i\sum_j [D^{-1}]_{ij}\frac{d}{dt'}x_j(\tau-t') \right\} \right\rangle$$

or

$$R^i_{\mathcal{A}}(t,t') = R^i_{\mathcal{A}}(\tau-t,\tau-t') + \sum_j [D^{-1}]_{ij}\frac{d}{dt'}\langle \mathcal{A}[\mathbf{x}(\tau-t)]x_j(\tau-t')\rangle$$

By changing $\tau - t \to t$ and $\tau - t' \to t'$,

FDR 1 (DB)

$$R^i_{\mathcal{A}}(t,t') - R^i_{\mathcal{A}}(\tau-t,\tau-t') = \sum_j [D^{-1}]_{ij}\langle \mathcal{A}[\mathbf{x}(t)]\dot{x}_j(t')\rangle$$

$\mathcal{U}$-transformation

$$\mathcal{U}:\left\{\begin{array}{lcl}\mathbf{x}(t) & \rightarrow & \mathbf{x}^{\mathrm{U}}(t)\equiv\mathbf{x}(\tau-t)\\ \hat{\mathbf{x}}(t) & \rightarrow & \hat{\mathbf{x}}^{\mathrm{U}}(t)\equiv-\hat{\mathbf{x}}(\tau-t)+i\mathrm{D}^{-1}\cdot\mathbf{f}(\mathbf{x}(\tau-t))\end{array}\right.$$

- One can show again with the same ΔS that (see next page)

$$S_0[\mathbf{x}^{\mathrm{U}},\hat{\mathbf{x}}^{\mathrm{U}}]=S_0[\mathbf{x},\hat{\mathbf{x}}]+\Delta S[\mathbf{x}]$$

- The Jacobians and the measure are invariant as well.
- If the DB holds and the initial state is given by the stationary state, then

$$\langle\mathcal{O}[\mathbf{x},\hat{\mathbf{x}}]\rangle=\langle\mathcal{O}[\mathbf{x}^{\mathrm{U}},\hat{\mathbf{x}}^{\mathrm{U}}]\rangle$$

$$\langle\mathcal{A}[\mathbf{x}(t)]\hat{x}_i(t')]\rangle=\left\langle\mathcal{A}[\mathbf{x}(\tau-t)]\left\{-\hat{x}_i(\tau-t')+i\sum_j[D^{-1}]_{ij}f_j(\mathbf{x}(\tau-t'))\right\}\right\rangle$$

FDR 2 (DB)

$$R^i_{\mathcal{A}}(t,t')+R^i_{\mathcal{A}}(\tau-t,\tau-t')=-\sum_j[D^{-1}]_{ij}\left\langle\mathcal{A}[\mathbf{x}(t)]f_j(\mathbf{x}(t'))\right\rangle$$

$$
\begin{aligned}
S_0[\mathbf{x}^{\mathrm{U}}, \hat{\mathbf{x}}^{\mathrm{U}}] &= \int_0^\tau dt \Big[\{-\hat{\mathbf{x}}(\tau - t) + i\mathtt{D}^{-1} \cdot \mathbf{f}(\mathbf{x}(\tau - t))\} \cdot \mathtt{D} \\
&\qquad\qquad \cdot \{-\hat{\mathbf{x}}(\tau - t) + i\mathtt{D}^{-1} \cdot \mathbf{f}(\mathbf{x}(\tau - t))\} \\
&\quad + i\{-\hat{\mathbf{x}}(\tau - t) + i\mathtt{D}^{-1} \cdot \mathbf{f}(\mathbf{x}(\tau - t))\} \cdot \{\frac{d}{dt}\mathbf{x}(\tau - t) - \mathbf{f}(\mathbf{x}(\tau - t))\}\Big] \\
&= \int_0^\tau dt [\{\hat{\mathbf{x}}(t) - i\mathtt{D}^{-1} \cdot \mathbf{f}(\mathbf{x}(t))\} \cdot \mathtt{D} \cdot \{\hat{\mathbf{x}}(t) - i\mathtt{D}^{-1} \cdot \mathbf{f}(\mathbf{x}(t))\} \\
&\quad + i\{-\hat{\mathbf{x}}(t) + i\mathtt{D}^{-1} \cdot \mathbf{f}(\mathbf{x}(t))\} \cdot \{-\frac{d}{dt}\mathbf{x}(t) - \mathbf{f}(\mathbf{x}(t))\}] \\
&= S_0[\mathbf{x}, \hat{\mathbf{x}}] + \underbrace{\int_0^\tau dt\, \dot{\mathbf{x}}(t) \cdot \mathtt{D}^{-1} \cdot \mathbf{f}(\mathbf{x}(t))}_{\equiv \Delta S[\mathbf{x}]}
\end{aligned}
$$

$\mathcal{E}$-transformation

$$\mathcal{E}: \begin{cases} \mathbf{x}(t) & \rightarrow & \mathbf{x}^{\mathrm{E}}(t) \equiv \mathbf{x}(t) \\ \hat{\mathbf{x}}(t) & \rightarrow & \hat{\mathbf{x}}^{\mathrm{E}}(t) \equiv -\hat{\mathbf{x}}(t) - i\mathtt{D}^{-1} \cdot (\dot{\mathbf{x}}(t) - \mathbf{f}(\mathbf{x}(t))) \end{cases}$$

- Unlike $\mathcal{R}$ and $\mathcal{U}$, they don't involve time reversal.
- One can show that it is an exact symmetry: (see next page)

$$S_0[\mathbf{x}^{\mathrm{E}}, \hat{\mathbf{x}}^{\mathrm{E}}] = S_0[\mathbf{x}, \hat{\mathbf{x}}]$$

Without assuming DB or stationary initial distribution, we have

$$\langle \mathcal{O}[\mathbf{x}, \hat{\mathbf{x}}] \rangle = \langle \mathcal{O}[\mathbf{x}^{\mathrm{E}}, \hat{\mathbf{x}}^{\mathrm{E}}] \rangle$$

It follows that

$$\begin{aligned} \left\langle \mathcal{A}[\mathbf{x}(t)] \hat{x}_i(t')] \right\rangle = &- \left\langle \mathcal{A}[\mathbf{x}(t)] \hat{x}_i(t') \right\rangle \\ &- i \sum_j [D^{-1}]_{ij} \left\langle \mathcal{A}[\mathbf{x}(t)] \dot{x}_j(t') \right\rangle + i \sum_j [D^{-1}]_{ij} \left\langle \mathcal{A}[\mathbf{x}(t)] f_j(\mathbf{x}(t')) \right\rangle \end{aligned}$$

$$
\begin{aligned}
S_0[\mathbf{x}^{\mathrm{E}}, \hat{\mathbf{x}}^{\mathrm{E}}] &= \int_0^{\tau} dt \Big[\{ -\hat{\mathbf{x}}(t) - i\mathtt{D}^{-1} \cdot (\dot{\mathbf{x}}(t) - \mathbf{f}(\mathbf{x}(t)) \} \cdot \mathtt{D} \\
&\qquad\qquad\qquad \cdot \{ -\hat{\mathbf{x}}(t) - i\mathtt{D}^{-1} \cdot (\dot{\mathbf{x}}(t) - \mathbf{f}(\mathbf{x}(t)) \} \\
&\quad + i \{ -\hat{\mathbf{x}}(t) - i\mathtt{D}^{-1} \cdot (\dot{\mathbf{x}}(t) - \mathbf{f}(\mathbf{x}(t)) \} \cdot \{ \frac{d}{dt}\mathbf{x}(t) - \mathbf{f}(\mathbf{x}(t)) \} \Big] \\
&= S_0[\mathbf{x}, \hat{\mathbf{x}}]
\end{aligned}
$$

Identity (DB or non-DB)

$$2\sum_j D_{ij} R^j_{\mathcal{A}}(t,t') = \langle \mathcal{A}[\mathbf{x}(t)]\,\dot{x}_i(t')\rangle - \langle \mathcal{A}[\mathbf{x}(t)]\,f_i(\mathbf{x}(t'))\rangle$$

- This nonperturbative relation can also be obtained from the identity

$$\begin{aligned} 0 &= \int \mathcal{D}\mathbf{x}(t) \int \mathcal{D}\hat{\mathbf{x}}(t)\, \frac{\delta}{\delta \hat{x}_i(t')} \left[\mathcal{A}[\mathbf{x}] e^{-S_0[\mathbf{x},\hat{\mathbf{x}}]-S_J[\mathbf{x}]} P_i(\mathbf{x}(0)) \right] \\ &= -2\sum_j D_{ij} \left\langle \mathcal{A}[\mathbf{x}(t)]\hat{x}_j(t')\right\rangle - i\left\langle \mathcal{A}[\mathbf{x}(t)]\dot{x}_i(t')\right\rangle + i\left\langle \mathcal{A}[\mathbf{x}(t)] f_i(\mathbf{x}(t'))\right\rangle \end{aligned}$$

- This relation can be used to study the violation of the FDR in nonequilibrium