Chp 9 (Pruinino 14)  Linear response theory for diffusion process

- The effect of a weak external forcing on a system at equilibrium.
- "Response of the system to the forcing."
- Based on perturbation theory \( \rightarrow \) linear response / fluctuation-dissipation theorem / Green-Kubo formula

1. Motivating Examples

Example: The Langevin Eq. \( \dot{q} = -V(q) - \gamma \dot{q} + \sqrt{2\gamma} \dot{W} \)

Assume \( V \) is a confining potential \( (e^{-V(x)}/Z_0, \text{int.}=0) \)
\( \Rightarrow \) Equilib. w stationary distr. \( f_\mu (p,\beta) \propto e^{-\beta H(p,\beta)} \), \( H(p,\beta) = \frac{1}{2} p^2 + V(p) \).

- Perturb the drift: Exp. 9.3
  \[ \dot{p}_t = -V(p) \dot{p}_t - \gamma \dot{p}_t + \xi(t) \Rightarrow \]
  \[ \dot{p}_t = -V(p) \dot{p}_t - \gamma \dot{p}_t + \xi(t) \]
  \( \varepsilon \ll 1 \).

- Perturb the temperature (diffusion): Exp. 9.4
  \[ \dot{p}_t = -V(p) \dot{p}_t - \gamma \dot{p}_t + \xi(t) \]
  \( \varepsilon \ll 1 \).

Question: How well an observable change? \( \Rightarrow \) Observable: a function of \((p,\beta)\), \( \mathcal{L}(f_{\mu}) \)

In general:
\[ d\mu = h(x) dx + \sigma(x) dW \]
\( \Rightarrow \) equilibrium stationary (SPE)
\[ \sigma_t = h(x) dx + \xi(t) dt + \sigma_t(x) dW \]
\( \text{or} \ (\sigma(x) + \xi(t)) dW \) (SDE).\nThe change in mean:
\[ \Delta E = \mathcal{E}[A(x)] - \mathcal{E}[A(x)] \]
\( \Rightarrow \) An estimation for all \( E \in [F,T] \)
\( \Delta E \ll 1, F,T \) "reasonable"
2. Linear response theory

Let \( \Phi_t \) denote a stationary dynamical system w/ invariant measure \( \mu(\Phi_t) = f(\Phi_t) d\mu \), \( \int f = \int f_0 \).

Let \( \Phi_t^\varepsilon \) denote the perturbed system, w/ density \( f_t^\varepsilon \).

Assume that \( f_t^\varepsilon \) satisfies a linear kinetic equ.:

\[
L_t^\varepsilon f_t^\varepsilon = -V(\h f_t^\varepsilon) + \frac{1}{2} \nabla^2 \cdot (\nabla^\varepsilon f_t^\varepsilon) + \varepsilon F_t f_t, \quad L_t^\varepsilon = L_t + \varepsilon L_t^\varepsilon
\]

\[
L_t^\varepsilon f_t^\varepsilon = L_t^\varepsilon f_t^0 + \varepsilon L_t^\varepsilon f_t^1 + \cdots
\]

(\( f_t^0 = f_0, f_t^0 = f_0, \ldots \))

\[
L_t^\varepsilon f_t^0 = L_t^\varepsilon f_t^0 + \varepsilon L_t^\varepsilon f_t^1 + \cdots
\]

\( \Rightarrow O(\varepsilon) \):

\[
\partial_t f_t^0 = L_t^\varepsilon f_t^0 \Rightarrow f_t^0 = f_0, \quad f_t^0 = f_0
\]

\( O(\varepsilon) \):

\[
\partial_t f_t^1 = L_t^\varepsilon f_t^1 + L_t^\varepsilon f_t^0 = L_t^\varepsilon f_t^1 + F(t) df_t^0 \Rightarrow f_t^1 = \int_0^t e^{L_t(t-s)} F(s) df_t^0 \, ds.
\]

Then, we can compute the change in mean of observable as:

\[
IE[A(\Phi)] - IE[A(\Phi^\varepsilon)] = \int A(\Phi^\varepsilon) [f_t^0(\Phi^\varepsilon) - f_0(\Phi^\varepsilon)] d\mu
\]

\[
= \varepsilon \int A(\Phi) \int_0^t e^{L_t(t-s)} F(s) df_t^0(\Phi^\varepsilon) d\mu \, ds + O(\varepsilon).
\]

Assume ergodicity condition:

\[
= \varepsilon \int_0^t \int A(\Phi) e^{L_t(t-s)} F(s) df_t^0(\Phi^\varepsilon) d\mu \, ds + O(\varepsilon)
\]

Define the Response function:

\[
R_{L_t}(t) = \int A(\Phi) e^{L_t(t-s)} df_t^0(\Phi^\varepsilon) \, d\mu.
\]

Linear response:

\[
IE[A(\Phi^\varepsilon)] - IE[A(\Phi)] = \varepsilon \int R_{L_t}(t-s) F(s) \, ds + O(\varepsilon)
\]

Note that:

\[
R_{L_t}(t) = \int A(\Phi) e^{L_t(\Phi^\varepsilon)} df_t^0(\Phi^\varepsilon) \, d\mu = \int e^{L_t(\Phi^\varepsilon)} df_t^0(\Phi^\varepsilon) \, d\mu
\]

\[
= IE [e^{L_t(\Phi^\varepsilon)} df_t^0(\Phi^\varepsilon)] = IE [A(\Phi^\varepsilon) df_t^0(\Phi^\varepsilon)]
\]

\[
= IE [A(\Phi^\varepsilon) df_t(\Phi^\varepsilon)] = IE [A(\Phi^\varepsilon) df_t(\Phi^\varepsilon)]
\]

\[
= \varepsilon \int IE [A(\Phi^\varepsilon) df_t(\Phi^\varepsilon)] F(s) \, ds + O(\varepsilon)
\]

Fluctuation dissipation theorem

"It forms one of the cornerstones of nonequilibrium statistical mechanics. In particular, it enables us to calculate equilibrium correlation functions by measuring the response of the system to a weak external forcing."