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

- The effect of a weak external forcing on a system at equilibrium.
  - $\hookrightarrow$ response of the system to the forcing.
  - based on perturbation theory $\to$ linear response $\begin{cases} \text{fluctuation-dissipation thm} \\ \text{Green-Kubo formula} \end{cases}$

1. Motivating Examples

Example The Langevin Eq. $\ddot{q} = -\nabla V(q) - \gamma \dot{q} + \sqrt{2\gamma\beta}\,\dot{W}$ $\quad \begin{cases} dq_t = p_t\,dt \\ dp_t = -\nabla V(q_t)\,dt - \gamma p_t\,dt + \sqrt{2\gamma\beta}\,dW_t \end{cases}$

- Assume V is a confining potential $\left(e^{-\beta V} \in L^1,\ \lim_{|x|\to\infty} V(x) = +\infty\right)$

$\Rightarrow$ Ergodic w/ stationary distr. $f_\infty(p,q) \propto e^{-\beta H(p,q)}$, $H(p,q) = \frac{1}{2}p^2 + V(q)$.

① Perturb the drift: Exp 9.3

$$dp_t = -\nabla V(q_t)\,dt - \gamma p_t\,dt + \varepsilon F(t) + \sqrt{2\gamma\beta}\,dW_t \qquad \varepsilon \ll 1.$$

② Perturb the temperature (diffusion) Exp 9.4

$$dp_t = -\nabla V(q_t)\,dt - \gamma p_t\,dt + \sqrt{2\gamma\beta(1+\varepsilon T(t))}\,dW_t$$

Question: How will an observable change? observable: a function of (p,q). $L^2(f_\infty)$

$A: \mathbb{R}^{2d} \to \mathbb{R}$

In general:

$$dX_t = h(X_t)\,dt + \sigma(X_t)\,dW_t \qquad \text{ergodic \& stationary} \qquad \text{(SDE)}$$

$$dX_t^\varepsilon = h(X_t)\,dt + \varepsilon F(t)\,dt + \sigma(X_t)\,dW_t \qquad \text{or } [\sigma(X_t) + \varepsilon T_t]\,dW_t. \qquad (\text{SDE}_\varepsilon)$$

What is the change in mean? $A(t) = \langle A(X_t^\varepsilon)\rangle - \langle A(X_t)\rangle_{Eq}$. $\to$ An estimation for all ε & F, T?

$= \mathbb{E}[A(X_t^\varepsilon)] - \mathbb{E}[A(X_t)]$ $\quad$ ($\varepsilon \ll 1$, F, T "reasonable")

2. Linear response theory

Let X_t denote a stationary dynamical system w/ invariant measure $\mu(dx) = f_\infty(x)dx$; $\quad f_t \equiv f_\infty$

Let X_t^ε denote the perturbed system, w/ density f_t^ε.

Assume that f_t^ε satisfies a linear kinetic equ.: $\boxed{\partial_t f_t^\varepsilon = L^{*,\varepsilon} f_t^\varepsilon; \quad f_{t_0}^\varepsilon = f_\infty}$

$$L^{*\varepsilon} f = -\nabla(hf) + \frac{1}{2}\nabla^2 : (\sigma\sigma^T f) - \varepsilon F(t)\cdot\nabla f \qquad L_1^* = F(t)\cdot\mathcal{D}, \quad \mathcal{D} = -\nabla.$$

$$= L^* f + \varepsilon L_1^* f \qquad L^{*\varepsilon} = L^* + \varepsilon L_1^*$$

- Note that since X_t is ergodic: $\quad L^* f_\infty = 0 \quad$ and f_∞ is the unique solu. to $L^* f = 0$.
- In the case of temperature perturbation $\quad \mathcal{D} = \varphi\beta^{-1}\Delta_p$.

Let $f_t^\varepsilon = f_t^0 + \varepsilon f_t^1 + \cdots$. Then $\quad \partial_t f_t^\varepsilon = \partial_t f_t^0 + \varepsilon\partial_t f_t^1 + \cdots \qquad \forall \varepsilon \ll 1$

$(f_0^0 = f_\infty;\ f_0^1 \equiv 0, \cdots) \qquad \overset{\shortparallel}{L^{*\varepsilon} f_t^\varepsilon} = L^*(f_t^0 + \varepsilon f_t^1 + \cdots) + \varepsilon L_1^*(f_t^0 + \varepsilon f_t^1 + \cdots)$

$\Rightarrow O(1)$: $\quad \partial_t f_t^0 = L^* f_t^0 \quad f_0^0 = f_\infty \Rightarrow \quad f_t^0 \equiv f_\infty$

$O(\varepsilon)$: $\quad \partial_t f^1 = L^* f^1 + L_1^* f^0 = L^* f^1 + F(t)\mathcal{D} f_\infty \quad \Rightarrow \boxed{f_t^1 - \cancel{f_0^1} = \int_0^t e^{L^*(t-s)} F(s)\mathcal{D} f_\infty\, ds.}$

$f_0^1 \equiv 0$

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

$$\mathbb{E}[A(X_t^\varepsilon)] - \mathbb{E}[A(X_t)] = \int A(x)[f_t^\varepsilon(x) - f_\infty(x)]\,dx$$

$$= \varepsilon\int A(x)\int_0^t e^{L^*(t-s)} F(s)\mathcal{D} f_\infty(x)\,ds\,dx + O(\varepsilon).$$

Assume integrability conditions. $\quad = \varepsilon\int_0^t \underbrace{\int A(x) e^{L^*(t-s)} F(s)\mathcal{D} f_\infty(x)\,dx}\,ds + O(\varepsilon)$

Define the Response function:

$$R_{L,A}(t) = \int A(x) e^{L^* t}\mathcal{D} f_\infty(x)\,dx \qquad \text{Linear response}$$

we have: $\boxed{\mathbb{E}[A(X_t^\varepsilon)] - \mathbb{E}[A(X_t)] = \varepsilon\int_0^t R_{L,A}(t-s)F(s)\,ds + O(\varepsilon)} \qquad (17)$

Note that: $\quad R_{L,A}(t) = \int A(x) e^{L^* t}\mathcal{D} f_\infty(x)\,dx = \int e^{Lt}A(x)\,\mathcal{D} f_\infty(x)\frac{f_\infty}{f_\infty}\,dx$

$$= \mathbb{E}[\mathbb{E}^{X_0}[A(X_t)]\mathcal{D} f_\infty/f_\infty(X_0)] = \mathbb{E}[A(X_t)\frac{\mathcal{D}f_\infty}{f_\infty}(X_0)] \qquad (26)$$

$\Rightarrow \quad \underline{\mathbb{E}[A(X_t^\varepsilon)] - \mathbb{E}[A(X_t)] = \varepsilon\int_0^t \mathbb{E}[A(X_t)\frac{\mathcal{D}f_\infty}{f_\infty}(X_0)]F(s)\,ds + O(\varepsilon)}$ **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."