Introduction to

Stochastic Thermodynamics

Lecture 4

The 22nd KIAS-APCTP Winter School on Statistical Physics

January 6 ~10, 2025

Jae Sung Lee

Korea Institute for Advanced Study

Eigenfunction of Fokker-Planck Equation

1. Another form of FP operator

$$\partial_t P(x,t) = L_{\mathrm{FP}} P(x,t)$$

$$L_{\mathrm{FP}} = -\partial_x A + \partial_x^2 D$$

$$= \partial_x D e^{-\Phi} \underline{\partial_x e^{\Phi}} \qquad \text{where} \quad \Phi \equiv \ln D - \int^x dx' \frac{A(x')}{D(x')}$$

$$= e^{\Phi}(\partial_x \Phi) + e^{\Phi}\partial_x = e^{\Phi}[(\partial_x \Phi) + \partial_x]$$

$$= \partial_x D[\underline{(\partial_x \Phi)} + \partial_x]$$

$$= \frac{(\partial_x D)}{D} - \frac{A}{D}$$

$$= -\partial_x A + \underline{\partial_x(\partial_x D) + \partial_x D \partial_x}$$

$$= \partial_x[(\partial_x D) + D\partial_x]$$

$$= \partial_x^2 D$$

Eigenfunction of Fokker-Planck Equation

$$\partial_t P(x,t) = L_{\mathrm{FP}} P(x,t)$$

$$L_{\mathrm{FP}} = -\partial_x A + \partial_x^2 D = \partial_x D e^{-\Phi} \partial_x e^{\Phi} \qquad \text{where} \quad \Phi \equiv \ln D - \int^x dx' \frac{A(x')}{D(x')}$$

2. Adjoint operator of FP operator

inner product: $\langle \psi | \phi \rangle \equiv \int dx\, \psi \phi$

$L_{\mathrm{FP}}^{\dagger}$: adjoint operator of L_{FP} $\rightarrow \langle \psi | L_{\mathrm{FP}} \phi \rangle = \langle L_{\mathrm{FP}}^{\dagger} \psi | \phi \rangle$

$$\langle \psi | L_{\mathrm{FP}} \phi \rangle \equiv \int dx\, \psi L_{\mathrm{FP}} \phi = \int dx\, \psi \partial_x D e^{-\Phi} \partial_x e^{\Phi} \phi$$

$$= -\int dx\, (\partial_x \psi) D e^{-\Phi} \partial_x e^{\Phi} \phi \quad \text{(integration by parts)}$$

$$= \int dx\, [\partial_x D e^{-\Phi} (\partial_x \psi)] e^{\Phi} \phi \quad \text{(integration by parts)}$$

$$= \int dx\, [e^{\Phi} \partial_x D e^{-\Phi} (\partial_x \psi)] \phi$$

$$= \int dx\, (L_{\mathrm{FP}}^{\dagger} \psi) \phi \qquad L_{\mathrm{FP}}^{\dagger} = e^{\Phi} \partial_x D e^{-\Phi} \partial_x = A \partial_x + D \partial_x^2$$

Eigenfunction of Fokker-Planck Equation

$$\partial_t P(x,t) = L_{\mathrm{FP}} P(x,t)$$

$$L_{\mathrm{FP}} = -\partial_x A + \partial_x^2 D = \partial_x D e^{-\Phi} \partial_x e^{\Phi} \qquad \text{where} \quad \Phi \equiv \ln D - \int^x dx' \frac{A(x')}{D(x')}$$

$$L_{\mathrm{FP}}^\dagger = e^{\Phi} \partial_x D e^{-\Phi} \partial_x = A \partial_x + D \partial_x^2$$

3. Eigenfunction of FP operator

$$L_{\mathrm{FP}} \phi_n = \lambda_n \phi_n \qquad L_{\mathrm{FP}}^\dagger \phi_n^\dagger = \lambda_n^\dagger \phi_n^\dagger$$

1) $\lambda_n = \lambda_n^\dagger$

$$\lambda_n \langle \phi_n^\dagger | \phi_n \rangle = \langle \phi_n^\dagger | L_{\mathrm{FP}} \phi_n \rangle = \langle L_{\mathrm{FP}}^\dagger \phi_n^\dagger | \phi_n \rangle = \lambda_n^\dagger \langle \phi_n^\dagger | \phi_n \rangle$$

2) orthogonality (assuming no degeneracy)

$$\lambda_m \langle \phi_n^\dagger | \phi_m \rangle = \langle \phi_n^\dagger | L_{\mathrm{FP}} \phi_m \rangle = \langle L_{\mathrm{FP}}^\dagger \phi_n^\dagger | \phi_m \rangle = \lambda_n \langle \phi_n^\dagger | \phi_m \rangle \qquad \rightarrow (\lambda_m - \lambda_n) \langle \phi_n^\dagger | \phi_m \rangle = 0$$

$$\Rightarrow \langle \phi_n^\dagger | \phi_m \rangle = \delta_{nm}$$

3) $\phi_n^\dagger = e^{\Phi} \phi_n$

$$L_{\mathrm{FP}}^\dagger e^{\Phi} \phi_n = e^{\Phi} \underbrace{\partial_x D e^{-\Phi} \partial_x e^{\Phi}}_{= L_{\mathrm{FP}}} \phi_n = e^{\Phi} L_{\mathrm{FP}} \phi_n = \lambda_n e^{\Phi} \phi_n$$

Eigenfunction of Fokker-Planck Equation

$$\partial_t P(x,t) = L_{\mathrm{FP}} P(x,t)$$

$$L_{\mathrm{FP}} = -\partial_x A + \partial_x^2 D \;= \partial_x D e^{-\Phi} \partial_x e^{\Phi} \qquad \text{where} \quad \Phi \equiv \ln D - \int^x dx' \frac{A(x')}{D(x')}$$

$$L_{\mathrm{FP}}^\dagger = e^{\Phi} \partial_x D e^{-\Phi} \partial_x \;= A\partial_x + D\partial_x^2$$

3. Eigenfunction of FP operator

$$L_{\mathrm{FP}} \phi_n = \lambda_n \phi_n \qquad\qquad L_{\mathrm{FP}}^\dagger \phi_n^\dagger = \lambda_n^\dagger \phi_n^\dagger$$

1) $\lambda_n = \lambda_n^\dagger$

2) orthogonality (assuming no degeneracy) $\Rightarrow \langle \phi_n^\dagger | \phi_m \rangle = \delta_{nm}$

3) $\phi_n^\dagger = e^{\Phi} \phi_n$

4) nonpositivity of λ_n (≤ 0)

$$\lambda_n = \lambda_n \langle \phi_n^\dagger | \phi_n \rangle = \int dx \, \underbrace{\phi_n^\dagger}_{= e^{\Phi}\phi_n} L_{\mathrm{FP}} \phi_n \;= \int dx \, e^{\Phi} \phi_n \partial_x D e^{-\Phi} \partial_x e^{\Phi} \phi_n$$

$$= -\int dx \, (\partial_x e^{\Phi} \phi_n) D e^{-\Phi} \partial_x e^{\Phi} \phi_n$$

$$= -\int dx \, D e^{-\Phi} (\partial_x e^{\Phi} \phi_n)^2 \leq 0$$

$$(0 \geq \lambda_0 > \lambda_1 > \lambda_2 > \cdots)$$

Eigenfunction of Fokker-Planck Equation

$$\partial_t P(x,t) = L_{\rm FP} P(x,t)$$

$$L_{\rm FP} = -\partial_x A + \partial_x^2 D = \partial_x D e^{-\Phi} \partial_x e^{\Phi} \qquad \text{where} \quad \Phi \equiv \ln D - \int^x dx' \frac{A(x')}{D(x')}$$

$$L_{\rm FP}^\dagger = e^{\Phi} \partial_x D e^{-\Phi} \partial_x = A\partial_x + D\partial_x^2$$

3. Eigenfunction of FP operator

$$L_{\rm FP}\phi_n = \lambda_n \phi_n \qquad L_{\rm FP}^\dagger \phi_n^\dagger = \lambda_n^\dagger \phi_n^\dagger$$

1) $\lambda_n = \lambda_n^\dagger$

2) orthogonality (assuming no degeneracy) $\Rightarrow \langle \phi_n^\dagger | \phi_m \rangle = \delta_{nm}$

3) $\phi_n^\dagger = e^{\Phi}\phi_n$

4) nonpositivity of λ_n (≤ 0) $(0 \geq \lambda_0 > \lambda_1 > \lambda_2 > \cdots)$

5) $\lambda_0 = 0$ (largest eigenvalue)

$$\phi_0 = e^{-\Phi} \rightarrow L_{\rm FP} e^{-\Phi} = \partial_x D e^{-\Phi} \partial_x 1 = 0$$

$$\phi_0^\dagger = e^{\Phi}\phi_0 = 1$$

Summary 1

1. Adjoin operator of FP operator

$$\partial_t P(x,t) = L_{\mathrm{FP}} P(x,t)$$

$$L_{\mathrm{FP}} = -\partial_x A + \partial_x^2 D = \partial_x D e^{-\Phi} \partial_x e^{\Phi} \qquad \text{where} \quad \Phi \equiv \ln D - \int^x dx' \frac{A(x')}{D(x')}$$

$$L_{\mathrm{FP}}^\dagger = e^{\Phi} \partial_x D e^{-\Phi} \partial_x = A \partial_x + D \partial_x^2$$

2. Eigenfunction of FP operator

$$L_{\mathrm{FP}} \phi_n = \lambda_n \phi_n \qquad L_{\mathrm{FP}}^\dagger \phi_n^\dagger = \lambda_n^\dagger \phi_n^\dagger$$

1) $\lambda_n = \lambda_n^\dagger$

2) orthogonality (assuming no degeneracy) $\Rightarrow \langle \phi_n^\dagger | \phi_m \rangle = \delta_{nm}$

3) $\phi_n^\dagger = e^{\Phi} \phi_n$

4) nonpositivity of λ_n (≤ 0) $(0 \geq \lambda_0 > \lambda_1 > \lambda_2 > \cdots)$

5) $\lambda_0 = 0$ (largest eigenvalue) $\phi_0 = e^{-\Phi}$ $\phi_0^\dagger = e^{\Phi} \phi_0 = 1$

Calculation of Mean & Variance of Observables

Observable: $\Theta(\tau) = \int_0^\tau dt\Lambda(x,t) \circ \dot{x}(t)$

Generating function: $G_h(x,\tau) = \left\langle e^{h\Theta(\tau)} \right\rangle_{x_0=x}$

Cumulant generating function: $C(h) = \lim_{\tau\to\infty} \frac{1}{\tau} \ln G_h(x,\tau)$

m-th cumulant: $\partial_h^m C(h)\,|_{h=0}$

ex) 1st cumulant: $\partial_h C(h)\,|_{h=0} = \lim_{\tau\to\infty} \left.\frac{\langle \Theta_\tau e^{h\Theta_\tau}\rangle}{\tau\langle e^{h\Theta_\tau}\rangle}\right|_{h=0} = \lim_{\tau\to\infty} \frac{\langle \Theta_\tau \rangle}{\tau} = \langle \dot{\Theta} \rangle_{\mathrm{ss}}$

2nd cumulant: $\partial_h^2 C(h)\,|_{h=0} = \lim_{\tau\to\infty} \left.\frac{\langle \Theta_\tau^2 e^{h\Theta_\tau}\rangle - \langle \Theta_\tau e^{h\Theta_\tau}\rangle^2}{\tau\langle e^{h\Theta_\tau}\rangle^2}\right|_{h=0}$

$$= \lim_{\tau\to\infty} \frac{\langle \Theta_\tau^2 \rangle - \langle \Theta_\tau \rangle^2}{\tau} = \mathscr{D}$$

Calculation of Mean & Variance of Observables

Observable: $\Theta(\tau) = \int_0^\tau dt \Lambda(x,t) \circ \dot{x}(t)$

Generating function: $G_h(x,\tau) = \left\langle e^{h\Theta(\tau)} \right\rangle_{x_0=x}$

Cumulant generating function: $C(h) = \lim_{\tau\to\infty} \frac{1}{\tau} \ln G_h(x,\tau)$

m-th cumulant: $\partial_h^m C(h)\,|_{h=0}$ $\qquad \partial_h C(h)\,|_{h=0} = \langle \dot{\Theta} \rangle_{\mathrm{ss}}$

$$\partial_h^2 C(h)\,|_{h=0} = \lim_{\tau\to\infty} \frac{\langle \Theta_\tau^2 \rangle - \langle \Theta_\tau \rangle^2}{\tau} = \mathscr{D}$$

how to calculate $C(h)$

1) find equation for $G_h(x,t)$: $\partial_t G_h(x,t) = L_h^\dagger G_h(x,t)$

2) find the largest eigenvalue of $L_h^\dagger$: $\lambda(h)$ $\to C(h) = \lambda(h)$

formal solution of $\partial_t G_h(x,t) = L_h^\dagger G_h(x,t)$: $G_h(x,t) = e^{L_h^\dagger t} G_h(x,0)$

eigenfunction expansion of $G_h(x,0)$: $G_h(x,0) = \sum_{n=0}^{\infty} a_n \phi_n^\dagger$ $\qquad (L_h^\dagger \phi_n^\dagger = \lambda_n \phi_n^\dagger)$

$\to G_h(x,t) = \sum_{n=0}^{\infty} e^{\lambda_n t} a_n \phi_n^\dagger \approx e^{\lambda_0 t} a_0 \phi_0^\dagger \quad (t \gg 1)$ $\qquad (\lambda_0 > \lambda_1 > \lambda_2 > \cdots)$

$\therefore C(h) = \lambda_0(h)$ $\qquad$ (ex: full counting statistics…)

Calculation of Mean & Variance of Observables

Setup

(N dim) $\dot{x}_i = F_i(\boldsymbol{x}) + \sum_{j=1}^{N} B_{ij}\xi_j$ $\qquad \mathsf{D} = \frac{1}{2}\mathsf{B}\mathsf{B}^{\mathrm{T}}$ $\qquad F_i(\boldsymbol{x}) = -\sum_{j=1}^{N} A_{ij}x_j$

Observable: $\Theta(\tau) = \int_0^{\tau} dt\, \boldsymbol{\Lambda}(x,t)^{\mathrm{T}} \circ \dot{\boldsymbol{x}}(t)$ $\qquad \Lambda_i = \sum_{j=1}^{N} W_{ij}x_j$

Generating function

Touchette, Physica A 504 (2018) 5–19

Chun, Fischer, Seifert, PRE 99, 042128 (2019)

$\partial_t G_h(x,t) = L_h^{\dagger} G_h(x,t)$

tilted FP operator: $L_h^{\dagger} = \boldsymbol{F}^{\mathrm{T}}(\nabla + h\boldsymbol{\Lambda}) + (\nabla + h\boldsymbol{\Lambda})^{\mathrm{T}}\mathsf{D}(\nabla + h\boldsymbol{\Lambda})$ $\qquad (L_{h=0}^{\dagger} = L_{\mathrm{FP}}^{\dagger})$

$\lambda(h)$: largest eigenvalue of $L_h^{\dagger}$ $\;\rightarrow \lambda(0) = \lambda_0 = 0$: largest eigenvalue of $L_{\mathrm{FP}}^{\dagger}$

$\phi^{\dagger}(h)$: eigenfunction associated with $\lambda(h)$ $\;\rightarrow \phi^{\dagger}(0) = \phi_0^{\dagger} = 1$: first eigenfunction of $L_{\mathrm{FP}}^{\dagger}$

Trial solution

$\phi^{\dagger}(h) = \exp\left[-\frac{1}{2}\boldsymbol{x}^{\mathrm{T}}\mathsf{G}(h)\boldsymbol{x}\right]$

$\mathsf{G}(h)$: symmetric

note :$\phi^{\dagger}(0) = 1 \rightarrow \mathsf{G}(0) = 0$

$$L_h^{\dagger}\phi^{\dagger}(h) = \left[-\boldsymbol{x}^{\mathrm{T}}\mathsf{A}^{\mathrm{T}}(\nabla + h\mathsf{W}\boldsymbol{x}) + (\nabla + h\mathsf{W}\boldsymbol{x})^{\mathrm{T}}\mathsf{D}(\nabla + h\mathsf{W}\boldsymbol{x})\right]\phi^{\dagger}(h)$$

Calculation of Mean & Variance of Observables

Generating function

$$\partial_t G_h(x,t) = L_h^\dagger G_h(x,t) \;\; \to \lambda(0) = \lambda_0 = 0 : \text{largest eigenvalue of } L_{\mathrm{FP}}^\dagger$$

Trial solution

$$\phi^\dagger(h) = \exp\left[-\frac{1}{2}\boldsymbol{x}^{\mathrm{T}}\mathsf{G}(h)\boldsymbol{x}\right]$$

$\mathsf{G}(h)$: symmetric

note :$\phi^\dagger(0) = 1 \to \mathsf{G}(0) = 0$

$$L_h^\dagger \phi^\dagger(h) = \left[-\boldsymbol{x}^{\mathrm{T}}\mathsf{A}^{\mathrm{T}}(\nabla + h\mathsf{W}\boldsymbol{x}) + (\nabla + h\mathsf{W}\boldsymbol{x})^{\mathrm{T}}\mathsf{D}(\nabla + h\mathsf{W}\boldsymbol{x})\right]\phi^\dagger(h)$$

$$= \left[-\boldsymbol{x}^{\mathrm{T}}\mathsf{A}^{\mathrm{T}}(-\mathsf{G} + h\mathsf{W})\boldsymbol{x} + (\nabla + h\mathsf{W}\boldsymbol{x})^{\mathrm{T}}\mathsf{D}(-\mathsf{G} + h\mathsf{W})\boldsymbol{x}\right]\phi^\dagger(h)$$

$$= \left[-\boldsymbol{x}^{\mathrm{T}}\mathsf{A}^{\mathrm{T}}(-\mathsf{G} + h\mathsf{W})\boldsymbol{x} + \boldsymbol{x}^{\mathrm{T}}(-\mathsf{G} + h\mathsf{W})^{\mathrm{T}}\mathsf{D}(\nabla + h\mathsf{W}\boldsymbol{x}) + \mathrm{tr}\{\mathsf{D}(-\mathsf{G} + h\mathsf{W})\}\right]\phi^\dagger(h)$$

$$= \underline{\boldsymbol{x}^{\mathrm{T}}\left[-\mathsf{A}^{\mathrm{T}}(-\mathsf{G} + h\mathsf{W}) + (-\mathsf{G} + h\mathsf{W})^{\mathrm{T}}\mathsf{D}(-\mathsf{G} + h\mathsf{W})\right]\boldsymbol{x}}\phi^\dagger(h) + \mathrm{tr}\{\mathsf{D}(-\mathsf{G} + h\mathsf{W})\}\phi^\dagger(h)$$

$$= \lambda(h)\phi^\dagger(h) \qquad = \boldsymbol{x}^{\mathrm{T}}\mathsf{Q}\boldsymbol{x} = 0 \;\; \to \mathsf{Q}^{\mathrm{T}} = -\mathsf{Q}$$

$$\mathsf{A}^{\mathrm{T}}(h\mathsf{W} - \mathsf{G}) + (h\mathsf{W} - \mathsf{G})^{\mathrm{T}}\mathsf{A} = 2(h\mathsf{W} - \mathsf{G})^{\mathrm{T}}\mathsf{D}(h\mathsf{W} - \mathsf{G})$$

$$\lambda(h) = \mathrm{tr}\{\mathsf{D}(-\mathsf{G} + h\mathsf{W})\} \qquad \text{check} : \lambda(0) = 0$$

Calculation of Mean & Variance of Observables

Generating function

$\partial_t G_h(x,t) = L_h^\dagger G_h(x,t) \;\to \lambda(0) = \lambda_0 = 0$: largest eigenvalue of $L_{\mathrm{FP}}^\dagger$

→ $\mathsf{A}^{\mathrm{T}}(h\mathsf{W}-\mathsf{G}) + (h\mathsf{W}-\mathsf{G})^{\mathrm{T}}\mathsf{A} = 2(h\mathsf{W}-\mathsf{G})^{\mathrm{T}}\mathsf{D}(h\mathsf{W}-\mathsf{G})$

$\lambda(h) = \mathrm{tr}\{\mathsf{D}(-\mathsf{G}+h\mathsf{W})\}$

We have to obtain G (not easy in general)

We are interested in small h : $\partial_h \lambda(h)|_{h=0}$ $\quad \partial_h^2 \lambda(h)|_{h=0}$

expansion $\to \mathsf{G} = \mathsf{G}_1 h + \mathsf{G}_2 h^2 + O(h^3)$

$$\mathsf{A}^{\mathrm{T}}(h\mathsf{W}-\mathsf{G}) + (h\mathsf{W}-\mathsf{G})^{\mathrm{T}}\mathsf{A} = 2(h\mathsf{W}-\mathsf{G})^{\mathrm{T}}\mathsf{D}(h\mathsf{W}-\mathsf{G}) \quad \leftarrow \mathsf{G} = \mathsf{G}_1 h + \mathsf{G}_2 h^2$$

$$O(h): \;\; \mathsf{A}^{\mathrm{T}}(\mathsf{W}-\mathsf{G}_1) + (\mathsf{W}-\mathsf{G}_1)^{\mathrm{T}}\mathsf{A} = 0$$

$$O(h^2): \;\; \mathsf{A}^{\mathrm{T}}(-\mathsf{G}_2) + (-\mathsf{G}_2)^{\mathrm{T}}\mathsf{A} = 2(\mathsf{W}-\mathsf{G}_1)^{\mathrm{T}}\mathsf{D}(\mathsf{W}-\mathsf{G}_1)$$

$$\langle \dot{\Theta} \rangle_{\mathrm{ss}} = \partial_h \lambda(h)|_{h=0} = \mathrm{tr}\{\mathsf{D}(\mathsf{W}-\mathsf{G}_1)\}$$

$$\mathscr{D} = \partial_h^2 \lambda(h)|_{h=0} = -2\,\mathrm{tr}\{\mathsf{D}\mathsf{G}_2\}$$

→ TUR: $\mathscr{Q} = \dfrac{\mathscr{D}}{\langle \dot{\Theta} \rangle^2}\langle \dot{S}_{\mathrm{tot}} \rangle \geq 2k_{\mathrm{B}}$