

Lecture 11

Recall the FP equation:

$$\frac{\partial p}{\partial t} = - \partial^i (F_i p) + \frac{1}{2} \partial^i [G_{ij} (\partial^j p)] \quad (*)$$

Define $\vec{v}(\vec{x}; \lambda)$ and $\vec{A}(\vec{x}; \lambda)$ as:

$$\begin{cases} v^i = 2 \Gamma^{ij} F_j, \\ A^i = v^i + \partial^i \varphi. \end{cases} \quad \Leftarrow p_s = e^{-\varphi}$$

Eq. (*) becomes

$$\frac{\partial p}{\partial t} = - \partial^i J_i, \quad \text{where}$$

$$J_i = \frac{1}{2} G_{ij} (v^j - \partial^j) p.$$

Indeed, $J_i = \underbrace{G_{ij} \Gamma^{jk}}_{\delta_i^k} F_k p - \frac{1}{2} G_{ij} \partial^j p =$
 $= F_i p - \frac{1}{2} G_{ij} \partial^j p,$
 as in Eq. (*)

At SS, $J_i^s \Big|_{\substack{\uparrow \\ p_s = e^{-\varphi}}} = [F_i + \frac{1}{2} G_{ij} (\partial^j \varphi)] e^{-\varphi} =$
 $= \frac{1}{2} G_{ij} A^j e^{-\varphi}.$

Note that $\partial^i J_i^s = 0$ since $\frac{\partial p_s}{\partial t} = 0.$

$$\text{If } \vec{v}(\vec{x}; \lambda) = -\vec{\nabla} u(\vec{x}; \lambda),$$

$$p_s = \frac{e^{-u}}{z} \quad \text{yields}$$

$$J_i^s = \frac{1}{2} G_{ij} (-\partial^j u + \partial^j u) \underbrace{\frac{e^{-u}}{z}}_{\Downarrow} = 0, \quad \text{s.t.}$$

$$\partial^i J_i^s = 0 \quad \text{trivially.}$$

$$e^{-\underbrace{(u + \log z)}_{\text{"y"}}}$$

It follows that

$$A^i = -\partial^i u + \partial^i (u + \log z) = 0.$$

This is the case when conservative forces ($v^i = -\partial^i u$) imply detailed balance ($J_i^s = 0$), s.t. p_s becomes

$$p_{eq} = \frac{e^{-u}}{z}.$$

↖ equil. canonical distribution

Conversely, if v^i cannot be represented as a gradient of a scalar potential,

$$J_i^s \neq 0 \text{ \& } A^i \neq 0 \text{ and } p_s \neq p_{eq}.$$

Thus, $\vec{A}$ can serve as an indicator of conservative/non-conservative forces.

Another way of perturbing the equilibrium is through explicit time dependence: $\lambda \rightarrow \lambda_t$.

$\lambda = \text{const}(t)$ autonomous dynamics

$\lambda = \lambda_t$ non-autonomous dynamics

We will consider $-\tau \leq t \leq \tau$, with

$$p(\vec{x}, -\tau) = \underbrace{e^{-\mathcal{G}(\vec{x}; \lambda_{-\tau})}}_{S'S \text{ distribution}}$$

—○—

Next, note that

$$\frac{\partial p}{\partial t} = \mathcal{L}_\lambda p = -\partial^i (J_i^S e^{\mathcal{G}} p) + \frac{1}{2} \partial^i [G_{ij} e^{-\mathcal{G}} \partial^j (e^{\mathcal{G}} p)]$$

Indeed,

$$\begin{aligned} J_i^S &= J_i^S e^{\mathcal{G}} p - \frac{1}{2} G_{ij} e^{-\mathcal{G}} \partial^j (e^{\mathcal{G}} p) = \\ &= \left[F_i + \frac{1}{2} G_{ij} (\partial^j \mathcal{G}) \right] p - \frac{1}{2} G_{ij} (\partial^j \mathcal{G}) p - \\ &\quad - \frac{1}{2} G_{ij} (\partial^j p) = F_i p - \frac{1}{2} G_{ij} (\partial^j p), \\ &\quad \text{as expected.} \end{aligned}$$

If $p \rightarrow p_S = e^{-\mathcal{G}}$, $\mathcal{L}_\lambda p_S = 0$ automatically
[recall that $\partial^i J_i^S = 0$]

We will be especially interested in contrasting $\mathcal{I}_\lambda: \{\vec{J}^S, \mathcal{V}, G\}$ with $\hat{\mathcal{I}}_\lambda: \{-\vec{J}^S, \mathcal{V}, G\}$.

Note that $[\hat{F}_i + \frac{1}{2} G_{ij} (\partial^j \mathcal{V})] e^{-\mathcal{V}} = -[F_i + \frac{1}{2} G_{ij} (\partial^j \mathcal{V})] e^{-\mathcal{V}}$ yields

$$\hat{F}_i = -F_i - G_{ij} (\partial^j \mathcal{V}).$$

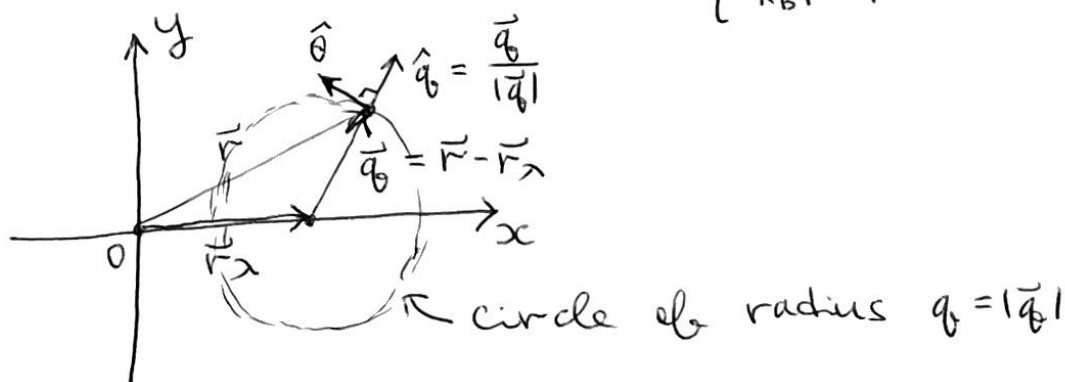
Note that if $\vec{J}^S = 0$, $\mathcal{I}_\lambda = \hat{\mathcal{I}}_\lambda$ and $F_i = \hat{F}_i$ trivially.

Ex. Consider a particle in 2D: $\vec{r} = (x, y)$

$$\vec{F}(\vec{r}; \lambda) = -\frac{k}{r} \vec{q} + \frac{1}{r} f(q) \hat{\theta}, \quad \text{where}$$

$$\vec{q} = \vec{r} - \vec{r}_\lambda, \quad \vec{r}_\lambda = (\lambda, 0)$$

$$\begin{cases} k > 0, & \text{spring const} \\ \gamma > 0, & \text{friction coeff.} \\ k_B T = 1 \end{cases}$$



If $f(q) = 0$, this is a particle in a quadratic potential. If $f(q) \neq 0$, the particle is subject to an additional angular force around $\vec{r}_\lambda$.

Finally, $G_{ij}(\vec{r}; \lambda) = \frac{2}{r} \delta_{ij},$

$$T^{ij}(\vec{r}; \lambda) = \frac{r}{2} \delta^{ij}.$$

For this system, $p_s = p_{eq} = \frac{e^{-\frac{kq^2}{2}}}{Z} = e^{-\underbrace{\left(\frac{kq^2}{2} + \log Z\right)}_{\psi}}.$

$$J_i^s = \frac{1}{r} \delta_{ij} A^j e^{-\psi} = \frac{1}{r} A_i e^{-\psi}.$$

Next, $A^i = 2 \underbrace{T^{ij} F_j}_{\frac{r}{2} \delta^{ij} F_j} + \partial^i \psi.$

In polar coords, $A^q = 2 \frac{r}{2} F^q + \frac{\partial \psi}{\partial q} =$
 $= 2 \frac{r}{2} \left(-\frac{k}{r} q\right) + kq = 0.$

$$\vec{\nabla} = \left(\frac{\partial}{\partial q}, \frac{1}{q} \frac{\partial}{\partial \theta} \right)$$

$$A^\theta = r F^\theta + \frac{1}{q} \frac{\partial \psi}{\partial \theta} = f(q).$$

In other words, $\vec{A} = f(q) \hat{\theta}.$

Then $\vec{J}^s = \frac{1}{r} f(q) e^{-\psi} \hat{\theta}.$

Finally, $\partial^i J_i^s = \underbrace{\frac{\partial J_q^s}{\partial q}}_0 + \frac{1}{q} \frac{\partial}{\partial \theta} \left[\frac{1}{r} f(q) e^{-\psi(q)} \right] = 0, \text{ as expected.}$

Thus, our ansatz indeed yields a SS current. If $f(q) = 0$, thermal equilibrium with detailed balance

with non-zero $\vec{A} = \vec{0}$ & $\vec{J}^s = \vec{0} \Rightarrow$

Note that in this case,

$$\mathcal{I}_\lambda: \{k, \gamma, f(q)\}$$

$$\hat{\mathcal{I}}_\lambda: \{k, \gamma, -f(q)\}$$

Path integral formalism

Consider $X = \{\vec{x}_t\}_{-\tau}^{\tau} \Rightarrow$ system trajectory from $-\tau$ to τ

If $\lambda = \text{const}(t)$,

$$P_\lambda[X | \underbrace{\vec{x}_{-\tau}}_{\text{IC}}] = \mathcal{N} e^{-\int_{-\tau}^{\tau} dt S_+(\vec{x}_t, \dot{\vec{x}}_t; \lambda)},$$

where $S_+(\vec{x}, \dot{\vec{x}}; \lambda) = \frac{1}{2} (\dot{x}_i - F_i) \Gamma^{ij} (\dot{x}_j - F_j) + \frac{1}{2} \partial^i F_i$.

If $\lambda = \lambda_t$ and varies from $\lambda_{-\tau}^F$ to λ_τ^F in a forward process, we obtain:

$$P^F[X | \vec{x}_{-\tau}] = \mathcal{N} e^{-\int_{-\tau}^{\tau} dt S_+(\vec{x}_t, \dot{\vec{x}}_t; \lambda_t^F)}$$

If $p_s(\vec{x}; \lambda_{-\tau}^F)$ is used to sample $\vec{x}_{-\tau}$,
one can write:

$$\underbrace{P^F[X]}_{\text{unconditional prob. of observing } X} = P^F[X | \vec{x}_{-\tau}] p_s(\vec{x}_{-\tau}; \lambda_{-\tau}^F)$$

Now, consider a reverse process:
 $\lambda_{\tau}^F \rightarrow \lambda_{-\tau}^F$ s.t. $\lambda_t^R = \lambda_{-t}^F$.
 $\lambda_{-\tau}^R \rightarrow \lambda_{\tau}^R$

Then (the time evolution is still from
 $-\tau$ to τ):

$$P^R[X | \vec{x}_{-\tau}] = \mathcal{N} e^{-\int_{-\tau}^{\tau} dt S_+(\vec{x}_t, \dot{\vec{x}}_t; \lambda_t^R)},$$

$$P^R[X] = p^s(\vec{x}_{-\tau}; \lambda_{-\tau}^R) P^R[X | \vec{x}_{-\tau}].$$

λ_{τ}^F

Now, consider the time-reversed trajectory:

$$\vec{x}_t^+ = \vec{x}_{-t} \quad , \quad \text{s.t.} \quad X^+ = \{ \vec{x}_t^+ \}_{-\tau}^{\tau}$$

$$\vec{x}_{-\tau}^+ \rightarrow \vec{x}_{\tau}^+ \quad \text{implies} \quad \vec{x}_{\tau} \rightarrow \vec{x}_{-\tau} \quad \text{backward evolution}$$

$$\text{Then } \text{PR}[X^+ | \vec{x}_{-\tau}^+] = \mathcal{N} e^{-\int_{-\tau}^{\tau} dt S_+(\vec{x}_t^+, \dot{\vec{x}}_t^+; \lambda_t^R)} \quad \textcircled{=}$$

$$\textcircled{=} \mathcal{N} e^{-\int_{-\tau}^{\tau} dt \underbrace{S_-(\vec{x}_t, \dot{\vec{x}}_t; \lambda_t^F)}_{\substack{\uparrow dt \rightarrow -dt \\ S_+(\vec{x}_t, -\dot{\vec{x}}_t; \lambda_t^F)}}$$

Next, consider

$$S_+ - S_- = \frac{1}{2} (\dot{x}_i - F_i) \Gamma^{ij} (\dot{x}_j - F_j) + \frac{1}{2} \partial^i F_i -$$

$$- \frac{1}{2} (-\dot{x}_i - F_i) \Gamma^{ij} (-\dot{x}_j - F_j) - \frac{1}{2} \partial^i F_i =$$

$$= 2 \frac{1}{2} (-\dot{x}_i \Gamma^{ij} F_j) - 2 \frac{1}{2} (F_i \Gamma^{ij} \dot{x}_j) = \quad \leftarrow \Gamma^{ij} = \Gamma^{ji}$$

$$= -2 \dot{x}_i \Gamma^{ij} F_j = -\dot{x}_i v^i = -\dot{x}_i (A^i - \partial^i \phi)$$

$$\text{Now, } \frac{\text{PF}[X | \vec{x}_{-\tau}]}{\text{PR}[X^+ | \vec{x}_{-\tau}^+]} = \underbrace{\frac{\mathcal{N}[X]}{\mathcal{N}[X^+]}}_{\substack{\text{"1"} \\ \text{by construction}}} e^{\int_{-\tau}^{\tau} dt \dot{x}_i v^i} \quad \text{with } \lambda_t^F$$

Furthermore,

$$\frac{P^F[X]}{P^R[X^+]} = \frac{P^F[X|\vec{x}_{-\tau}] p_S(\vec{x}_{-\tau}; \lambda_{-\tau}^F)}{P^R[X^+|\vec{x}_{\tau}] p_S(\vec{x}_{\tau}; \lambda_{\tau}^F)} =$$

$$= e^{\Delta\mathcal{G} + \int_F dt \dot{x}_i v^i}, \quad \text{where}$$

$$\Delta\mathcal{G} = \mathcal{G}(\vec{x}_{\tau}; \lambda_{\tau}^F) - \mathcal{G}(\vec{x}_{-\tau}; \lambda_{-\tau}^F) =$$

$$= \int_{-\tau}^{\tau} dt \underbrace{\left[\dot{\lambda}_t^F \frac{\partial \mathcal{G}}{\partial \lambda} + \dot{x}_i \partial^i \mathcal{G} \right]}_{\frac{d\mathcal{G}}{dt}}.$$

Define $Y^F = \int_{-\tau}^{\tau} dt \dot{\lambda}_t^F \frac{\partial \mathcal{G}}{\partial \lambda}$, then

$$\frac{P^F[X]}{P^R[X^+]} = e^{Y^F + \int_{-\tau}^{\tau} dt \dot{x}_i \partial^i \mathcal{G} + \int_{-\tau}^{\tau} dt \dot{x}_i (A^i - \partial^i \mathcal{G})} =$$

$$= e^{Y^F + \underbrace{\int_{-\tau}^{\tau} dt \dot{x}_i A^i}_{\int_F d\vec{x} \cdot \vec{A}}} \quad \Leftarrow \quad \begin{array}{l} \text{Define} \\ R^F[X] = Y^F[X] + \int_F d\vec{x} \cdot \vec{A} \end{array}$$

$$\frac{P^F[X]}{P^R[X^+]} = e^{R^F[X]}$$

If the dynamics are autonomous ($\dot{\lambda}_t^F = 0$)
and the forces conservative ($\vec{A} = \vec{0}$),
we obtain: $P^F[X] = P^R[X^+]$, consistent
with DB.

For the reverse process, we define:

$$Y^R[X^+] = \int_R dt \dot{\lambda}_t^R \frac{\partial \mathcal{L}}{\partial \lambda} \Rightarrow Y^R[X^+] = -Y^F[X]$$

$$R^R[X^+] = Y^R[X^+] + \int_R d\vec{x} \cdot \vec{A} \Rightarrow R^R[X^+] = -R^F[X]$$

—○—

Next, consider sum over all paths

$$p^F(R) = \int \mathcal{D}X P^F[X] \delta(R - R^F[X]) \quad \text{①}$$

prob. of R , forward process

$$\mathcal{D}X = \prod_{k=0}^K d\vec{x}_k$$

$$\text{②} \int \mathcal{D}X P^R[X^+] e^{R^F[X]} \delta(R - R^F[X]) =$$

$$= e^R \underbrace{\int \mathcal{D}X^+ P^R[X^+] \delta(R + R^R[X^+])}_{\int \mathcal{D}X = \int \mathcal{D}X^+} \quad p^R(-R) = \text{prob. of } -R, \text{ reverse process}$$

Thus,
$$\boxed{\frac{p^F(+R)}{p^F(-R)} = e^R}$$

Here, we assumed that

$$\begin{cases} \frac{dx_i}{dt} = F_i(\vec{x}; \lambda_t^F) + \mathcal{L}_i(t, \vec{x}; \lambda_t^F), \\ \frac{dx_i}{dt} = F_i(\vec{x}; \lambda_t^R) + \mathcal{L}_i(t, \vec{x}; \lambda_t^R). \end{cases}$$

reverse trajectory but the forces are the same

$$\{\mathcal{I}_\lambda, \lambda_t^F\}_{\text{forward}} \rightarrow \{\mathcal{I}_\lambda, \lambda_t^R\}_{\text{reverse}}$$

If we now take

$$\frac{dx_i}{dt} = \underbrace{\hat{F}_i(\bar{x}; \lambda_t^R)}_{"-F_i - G_{ij} \partial^j y"} + \ell_i(t, \bar{x}; \lambda_t^R)$$

Thus, we now have

$$\{\mathcal{I}_\lambda, \lambda_t^F\} \rightarrow \{\hat{\mathcal{I}}_\lambda, \lambda_t^R\}.$$

Then $\hat{P}^R[X^+ | \underbrace{\bar{x}_{-\tau}^+}_{\text{"}\bar{x}_\tau\text{"}}] = \mathcal{N} e^{-\int_{-\tau}^{\tau} dt \hat{S}_+(\bar{x}_t^+, \dot{\bar{x}}_t^+; \lambda_t^R)}$ $\hat{F}_i$ replaced by $\hat{F}_i$ $\textcircled{=}$

$$\textcircled{=} \mathcal{N} e^{-\int_{-\tau}^{\tau} dt \underbrace{\hat{S}_{-}(\bar{x}_t, \dot{\bar{x}}_t; \lambda_t^F)}_{\hat{S}_{+}(\bar{x}_t, -\dot{\bar{x}}_t; \lambda_t^F)}}$$

$$\begin{aligned} \text{Now, } S_+ - \hat{S}_- &= \frac{1}{2} (\dot{x}_i - F_i) T^{ij} (\dot{x}_j - F_j) + \frac{1}{2} \partial^i F_i - \\ &- \frac{1}{2} (-\dot{x}_i - \hat{F}_i) T^{ij} (-\dot{x}_j - \hat{F}_j) - \frac{1}{2} \partial^i \hat{F}_i = \\ &= -\frac{1}{2} 2 \dot{x}_i T^{ij} F_j + \frac{1}{2} F_i T^{ij} F_j + \frac{1}{2} \partial^i F_i - \\ &- \frac{1}{2} 2 \dot{x}_i T^{ij} \hat{F}_j - \frac{1}{2} \hat{F}_i T^{ij} \hat{F}_j - \frac{1}{2} \partial^i \hat{F}_i \quad \textcircled{=}\end{aligned}$$

$$\begin{aligned} \textcircled{=} & - \dot{x}_i \cancel{\Gamma^{ij}} F_j + \frac{1}{2} F_i \cancel{\Gamma^{ij}} F_j + \frac{1}{2} \partial^i F_i + \\ & + \dot{x}_i \cancel{\Gamma^{ij}} F_j + \underbrace{\dot{x}_i \Gamma^{ij} G_{jk}}_{\delta^i_k} \partial^k y - \frac{1}{2} F_i \cancel{\Gamma^{ij}} F_j \textcircled{-} \end{aligned}$$

$$\ominus \frac{1}{2} G_{ik} \partial^k \varphi \underbrace{\Gamma^{ij} G_{jl}}_{\delta^i_l} \partial^l \varphi - F_i \underbrace{\Gamma^{ij} G_{jk}}_{\delta^i_k} \partial^k \varphi + \frac{1}{2} \partial^i F_i +$$

$$+ \frac{1}{2} \partial^i (G_{ik} \partial^k \varphi) = \partial^i F_i + \dot{x}_i \partial^i \varphi - \frac{1}{2} G_{ik} \partial^k \varphi \partial^i \varphi -$$

$$- F_i \partial^i \varphi + \frac{1}{2} \partial^i (G_{ik} \partial^k \varphi).$$

On the other hand,

$$e^{\varphi} \partial^i \left[(F_i - \frac{1}{2} G_{ij} \partial^j \varphi) e^{-\varphi} \right] = \partial^i F_i + e^{\varphi} F_i (-\partial^i \varphi) e^{-\varphi} +$$

$$+ e^{\varphi} \partial^i [G_{ij} (-\partial^j \varphi) e^{-\varphi}] \left(-\frac{1}{2}\right) = \partial^i F_i - F_i \partial^i \varphi +$$

$$+ \frac{1}{2} \left[\partial^i [G_{ij} (\partial^j \varphi)] + G_{ij} (\partial^j \varphi) (-\partial^i \varphi) \right] =$$

$$= \partial^i F_i - F_i \partial^i \varphi - \frac{1}{2} G_{ij} (\partial^i \varphi) (\partial^j \varphi) + \frac{1}{2} \partial^i (G_{ij} \partial^j \varphi).$$

Hence, $S_+ - \hat{S}_- = \dot{x}_i \partial^i \varphi + e^{\varphi} \partial^i \left[(F_i - \frac{1}{2} G_{ij} \partial^j \varphi) e^{-\varphi} \right].$

$$(F_i + \frac{1}{2} G_{ij}'' (\partial^j \varphi)) e^{-\varphi} =$$

$$= J_i^S$$

Since $\partial^i J_i^S = 0,$

$$S_+ - \hat{S}_- = \dot{x}_i \partial^i \varphi$$

Then $\frac{P^F[X|\vec{x}_-, \tau]}{\hat{P}^R[X^+|\vec{x}_-, \tau]} = e^{-\int_{-\tau}^{\tau} dt \dot{x}_j \partial^j \varphi},$ or

$$\frac{P^F[X]}{\hat{P}^R[X^+]} = e^{\Delta \varphi - \int_{-\tau}^{\tau} dt \dot{x}_j \partial^j \varphi} = e^{Y^F} \quad \left[\int_{-\tau}^{\tau} dt \left[\dot{\lambda}_t^F \frac{\partial \varphi}{\partial \lambda} + \dot{x}_j \partial^j \varphi \right] \right]$$

We immediately obtain:

$$\frac{p^F(+Y)}{\hat{p}^R(-Y)} = e^Y, \text{ where}$$

$p^F(\tilde{Y})$ = distr'n of $\tilde{Y}$ values for the forward process $(\mathcal{I}_\lambda, \lambda_t^F)$
 $\hat{p}^R(\tilde{Y})$ = distr'n of $\tilde{Y}$ values for the reverse process $(\hat{\mathcal{I}}_\lambda, \lambda_t^R)$.

Summary =

- ① Non-conservative forces, autonomous dynamics : $A_i \neq 0, \dot{\lambda}_t = 0$

$Y=0$ always, use $\frac{p^F(R)}{p^R(-R)} = e^R, R = \int d\vec{x} \cdot \vec{A}$.

- ② $A_i = 0, \dot{\lambda}_t \neq 0$
 $\mathcal{I}_\lambda = \hat{\mathcal{I}}_\lambda; Y=R = \int_{-\tau}^{\tau} dt \dot{\lambda}_t \frac{\partial \mathcal{L}}{\partial \lambda}$

Again, use $\frac{p^F(R)}{p^R(-R)} = e^R$.

- ③ $A_i \neq 0, \dot{\lambda}_t \neq 0$
 Both "Y" and "R" fluctuation theorems can be considered