Lecture 11

Recall the FP equation:

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

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

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

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, $J_i^s \underset{\uparrow}{=} [F_i + \frac{1}{2}G_{ij}(\partial^j\varphi)]e^{-\varphi} =$

$p_s = e^{-\varphi}$ $\quad = \boxed{\frac{1}{2}G_{ij}A^j e^{-\varphi}}$.

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

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

$$p_s = \frac{e^{-\mathcal{U}}}{Z} \quad \text{yields}$$

$$J_i^s = \frac{1}{2} G_{ij} (-\partial^j \mathcal{U} + \partial^j \mathcal{U}) \underbrace{\frac{e^{-\mathcal{U}}}{Z}}_{\Downarrow \; e^{-\underbrace{(\mathcal{U} + \log Z)}_{= \varphi}}} = 0, \quad \text{s.t.}$$

$\partial^i J_i^s = 0$ trivially.

It follows that

$$A^i = -\partial^i \mathcal{U} + \partial^i (\mathcal{U} + \log Z) = 0.$$

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

$$p_{eq} = \frac{e^{-\mathcal{U}}}{Z}.$$

equil. canonical distribution

Conversely, if v^i cannot be represented as a gradient of a scalar potential, $J_i^s \neq 0$ & $A^i \neq 0$ 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: $\lambda \to \lambda_t$.

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

$\lambda = \lambda_t$ non-autonomous dynamics

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

$$p(\vec{x}, -\tau) = \underbrace{e^{-\varphi(\vec{x};\, \lambda_{-\tau})}}_{SS \text{ distribution}}$$

Next, note that

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

Indeed,

$$J_i = J_i^s e^{\varphi} p - \frac{1}{2} G_{ij} e^{-\varphi} \partial^j (e^{\varphi} p) =$$

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

$$- \frac{1}{2} G_{ij} (\partial^j p) = F_i p - \frac{1}{2} G_{ij} (\partial^j p),$$

as expected.

If $p \to p_s = e^{-\varphi}$, $\mathcal{L}_\lambda p_s = 0$ automatically [recall that $\partial^i J_i^s = 0$]

We will be especially interested in contrasting $\mathcal{I}_\lambda : \{\vec{J}^s, \varphi, G\}$ with

$$\hat{\mathcal{I}}_\lambda : \{-\vec{J}^s, \varphi, G\}.$$

Note that $\left[\hat{F}_i + \frac{1}{2} G_{ij}(\partial^j \varphi)\right] e^{-\varphi} =$

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

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

Note that if $\vec{J}^s = 0$, $\mathcal{I}_\lambda = \hat{\mathcal{I}}_\lambda$ and

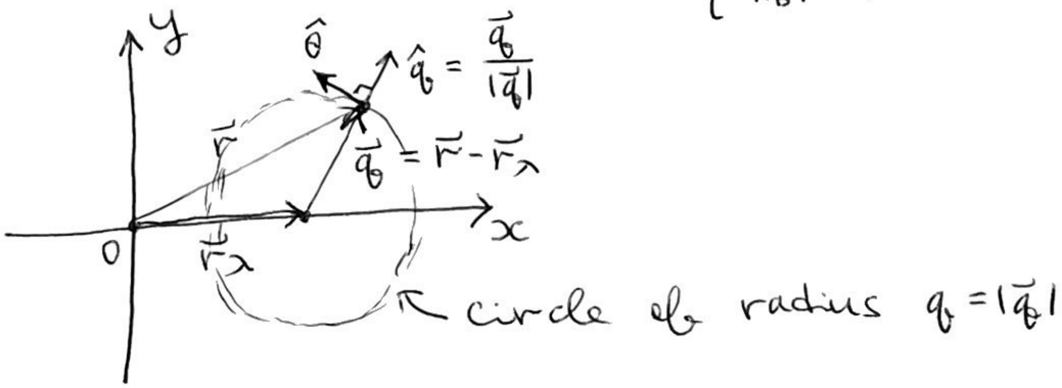
$F_i = \hat{F}_i$ trivially.

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

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

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

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



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

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

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

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

Next, $A^i = 2\underbrace{\Gamma^{ij}F_j}_{\frac{\gamma}{2}\delta^{ij}F_j = \frac{\gamma}{2}F^i} + \partial^i\varphi$.

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

$$A^q = 2\frac{\gamma}{2}F^q + \frac{\partial\varphi}{\partial q} = 2\frac{\gamma}{2}\left(-\frac{k}{\gamma}q\right) + kq = 0.$$

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

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

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

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

Thus, our ansatz indeed yields a SS with non-zero current. If $f(q)=0$, $\vec{A}=\vec{0}$ & $\vec{J}^s=\vec{0}$ $\Rightarrow$ thermal equilibrium with detailed balance

Note that in this case,

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

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

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 $\lambda^F_{-\tau}$ to λ^F_τ in a forward process, we obtain:

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

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

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

Now, consider a <u>reverse process</u>:

$$\begin{array}{ccc} \lambda^F_\tau & \rightarrow & \lambda^F_{-\tau} \\ \| & & \| \\ \lambda^R_{-\tau} & \rightarrow & \lambda^R_\tau \end{array} \quad \text{s.t.} \quad \lambda^R_t = \lambda^F_{-t}.$$

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

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

$$P^R[X] = p^s(\vec{x}_{-\tau}; \underset{\lambda^F_\tau}{\underset{\|}{\lambda^R_{-\tau}}})\, P^R[X \mid \vec{x}_{-\tau}].$$

Now, consider the time-reversed trajectory:

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

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

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

$$\underset{\uparrow\, dt \to -dt}{=} \mathcal{N} e^{-\int_{-\tau}^{\tau} dt\, \underbrace{S_{-}(\vec{x}_{t}, \dot{\vec{x}}_{t}; \lambda^{F}_{t})}_{= S_{+}(\vec{x}_{t}, -\dot{\vec{x}}_{t}; \lambda^{F}_{t})}}$$

Next, consider

$$S_{+} - S_{-} = \frac{1}{2}(\dot{x}_{i} - F_{i}) \Gamma^{ij} (\dot{x}_{j} - F_{j}) + \frac{1}{2} \partial^{i} F_{i} -$$

$$- \frac{1}{2}(-\dot{x}_{i} - F_{i}) \Gamma^{ij} (-\dot{x}_{j} - F_{j}) - \frac{1}{2} \partial^{i} F_{i} = $$

$$= 2\frac{1}{2}(-\dot{x}_{i} \Gamma^{ij} F_{j}) - 2\frac{1}{2}(F_{i} \Gamma^{ij} \dot{x}_{j}) \overset{\Gamma^{ij} = \Gamma^{ji}}{=}$$

$$= -2 \dot{x}_{i} \Gamma^{ij} F_{j} = -\dot{x}_{i} v^{i} = -\dot{x}_{i}(A^{i} - \partial^{i} \varphi).$$

Now, $$\frac{p^{F}[X | \vec{x}_{-\tau}]}{p^{R}[X^{+} | \underbrace{\vec{x}^{+}_{-\tau}}_{= \vec{x}_{\tau}}]} = \underbrace{\frac{\mathcal{N}[X]}{\mathcal{N}[X^{+}]}}_{\substack{=1 \\ \text{by construction}}} e^{\int_{F} dt\, \dot{x}_{i} v^{i}}$$

$\int_{F}$: $\int_{-\tau}^{\tau} dt$ with λ^{F}_{t}

Furthermore,

$$\frac{P^F[X]}{P^R[X^+]} = \frac{P^F[X|\vec{x}_{-\tau}]\, p_s(\vec{x}_{-\tau};\lambda^F_{-\tau})}{P^R[X^+|\vec{x}_{\tau}]\, p_s(\vec{x}_{\tau};\lambda^F_{\tau})} =$$

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

$$\Delta\varphi = \varphi(\vec{x}_\tau;\lambda^F_\tau) - \varphi(\vec{x}_{-\tau};\lambda^F_{-\tau}) =$$

$$= \int_{-\tau}^{\tau} dt \Big[\underbrace{\dot{\lambda}^F_t \frac{\partial\varphi}{\partial\lambda} + \dot{x}_i \partial^i\varphi}_{\frac{d\varphi}{dt}} \Big] .$$

Define $Y^F = \int_{-\tau}^{\tau} dt\, \dot{\lambda}^F_t \frac{\partial\varphi}{\partial\lambda}$, then

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

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

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

If the dynamics are autonomous ($\dot{\lambda}^F_t = 0$) 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:

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

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

Next, consider sum over all paths

$$\underbrace{p^F(R)}_{\text{prob. of } R,\text{ forward process}} = \int \mathcal{D}X\, P^F[X]\, \delta(R - R^F[X]) \circled{=}$$

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

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

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

$$\int \mathcal{D}X = \int \mathcal{D}X^+$$

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

Here, we assumed that

$$\begin{cases} \dfrac{dx_i}{dt} = F_i(\vec{x};\lambda^F_t) + \xi_i(t,\vec{x};\lambda^F_t), \\ \dfrac{dx_i}{dt} = F_i(\vec{x};\lambda^R_t) + \xi_i(t,\vec{x};\lambda^R_t). \end{cases}$$

reverse trajectory but the forces are the same

$$\underbrace{\{\mathcal{I}_\lambda, \lambda^F_t\}}_{\text{forward}} \rightarrow \underbrace{\{\mathcal{I}_\lambda, \lambda^R_t\}}_{\text{reverse}}$$

If we now take

$$\frac{dx_i}{dt} = \underbrace{\hat F_i(\vec x; \lambda^R_t)}_{= -F_i - G_{ij}\partial^j \varphi} + \xi_i(t, \vec x; \lambda^R_t)$$

Thus, we now have

$$\{\mathcal{J}_x, \lambda^F_t\} \to \{\hat{\mathcal{J}}_x, \lambda^R_t\}.$$

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

F_i replaced by $\hat F_i$

$$\underset{dt=-dt}{=} \mathcal{N} e^{-\int_{-\tau}^{\tau} dt\, \underbrace{\hat S_-(\vec x_t, \dot{\vec x}_t; \lambda^F_t)}_{= \hat S_+(\vec x_t, -\dot{\vec x}_t; \lambda^F_t)}}.$$

Now, $S_+ - \hat S_- = \frac{1}{2}(\dot x_i - F_i)\Gamma^{ij}(\dot x_j - F_j) + \frac{1}{2}\partial^i F_i -$

$$- \frac{1}{2}(-\dot x_i - \hat F_i)\Gamma^{ij}(-\dot x_j - \hat F_j) - \frac{1}{2}\partial^i \hat F_i =$$

$$= -\frac{1}{2}2\dot x_i \Gamma^{ij} F_j + \frac{1}{2}F_i\Gamma^{ij}F_j + \frac{1}{2}\partial^i F_i -$$

$$- \frac{1}{2}2\dot x_i \Gamma^{ij}\underbrace{\hat F_j}_{= -F_j - G_{jk}\partial^k\varphi} - \frac{1}{2}\hat F_i \Gamma^{ij}\hat F_j - \frac{1}{2}\partial^i \hat F_i =$$

$$= -\dot x_i \cancel{\Gamma^{ij}} F_j + \frac{1}{2}F_i \cancel{\Gamma^{ij}} F_j + \underline{\frac{1}{2}\partial^i F_i} +$$

$$+ \dot x_i \cancel{\Gamma^{ij}} F_j + \dot x_i \underbrace{\Gamma^{ij} G_{jk}}_{\delta^i{}_k}\partial^k\varphi - \frac{1}{2}\cancel{F_i\Gamma^{ij}}F_j =$$

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

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

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

On the other hand,

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

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

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

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

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

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

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

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

$$\frac{P^F[X]}{\hat{P}^R[X^+]} = e^{\underbrace{\Delta \varphi}_{\substack{\shortparallel \\ \int_{-\tau}^{\tau} dt \left[\dot{\lambda}^F_t \frac{\partial \varphi}{\partial \lambda} + \dot{x}_j\, \partial^j \varphi \right]}} - \int_{-\tau}^{\tau} dt\, \dot{x}_j\, \partial^j \varphi} = e^{Y^F}.$$

We immediately obtain:

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

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

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

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. $A_i = 0$, $\dot{\lambda}_t \neq 0$

   $\mathcal{I}_\lambda = \hat{\mathcal{I}}_\lambda$; $Y = R = \int_{-\tau}^{\tau} dt\, \dot{\lambda}_t \frac{\partial \varphi}{\partial \lambda}$.

   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