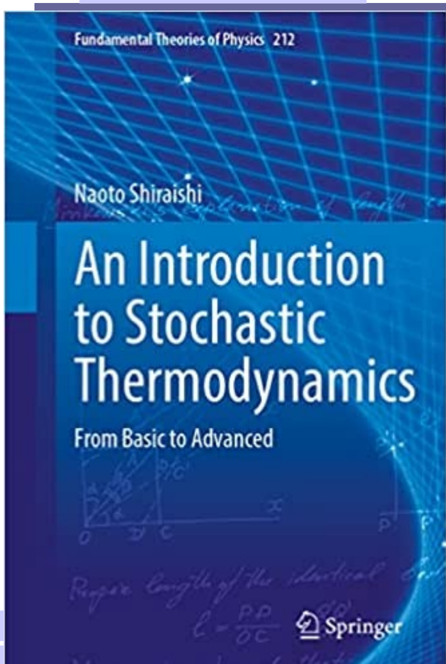
Entropy production bounds (almost) everything



Naoto Shiraishi (University of Tokyo)

N. Shiraishi, K Funo, and K. Saito, PRL 121, 070601 (2018).
N. Shiraishi and K. Saito, J. Stat. Phys. 174, 433 (2019).
N. Shiraishi and K. Saito, PRL 123, 110603 (2019).
N. Shiraishi, J. Stat. Phys. 185, 19 (2021).
N. Shiraishi, arXiv:2304.12775

N. Shiraishi, "An introduction to stochastic thermodynamics" Springer (2023)

Outline

Brief review of stochastic thermodynamics

Part 1: Finite-speed processes

Part 2: Relaxation processes

Part 3: Oscillation phenomena

Outline

Brief review of stochastic thermodynamics

Part 1: Finite-speed processes

Part 2: Relaxation processes

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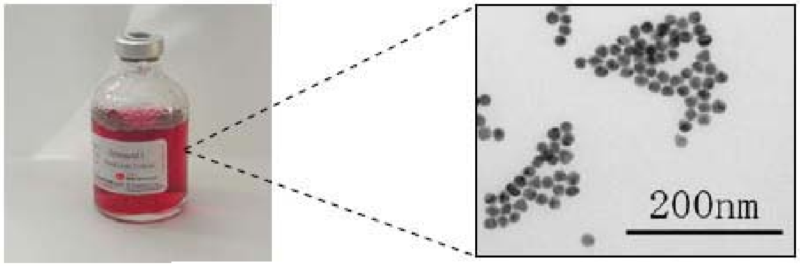
Setup of stochastic thermodynamics

Consider classical small systems evolving stochastically due to thermal noise.

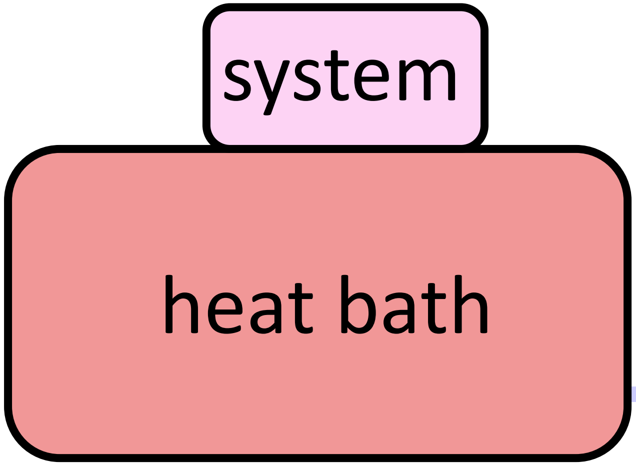


Colloidal particle

Setup throughout this talk

Heat bath is in equilibrium

→describe as **Markov process**

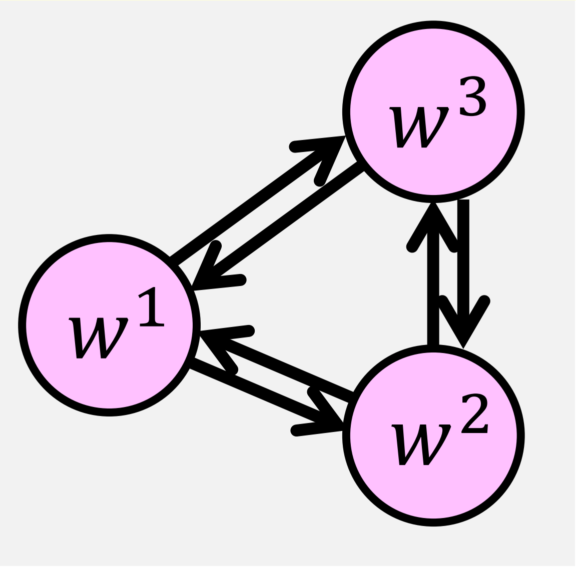


Description of classical stochastic process

Probability distribution $\boldsymbol{p}$ evolves according to the **master equation.**

$$\frac{d}{dt}p_{w,t} = \sum_{w'} R_{ww'} p_{w',t}$$

transition matrix



normalization condition: $\sum_w \boldsymbol{R_{ww'}} = \boldsymbol{0}$

(only $R_{w'w'}$ is negative, others are nonnegative)

Definition of entropy production rate

Entropy production rate (single heat bath)

$$\dot{\sigma} = -\sum_{w} \beta E_w \frac{dp_w}{dt} + \frac{d}{dt}\left(-\sum_{w} p_w \ln p_w\right)$$

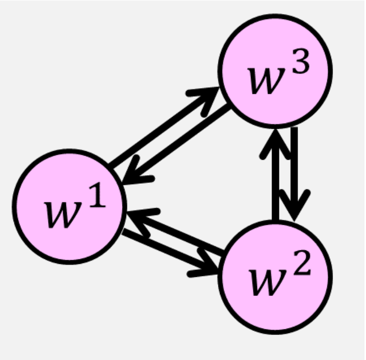
Entropy increase of bath (dQ/T)

(Shannon) entropy increase of system

Local detailed-balance condition

Local detailed-balance (LDB)
If distribution is canonical (equilibrium), there is no microscopic probability current.

$$\frac{R_{ww'}}{R_{w'w}} = e^{-\beta\left(E_w - E_{w'}\right)}$$



(For case of multiple baths, LDB is imposed on each single bath)

Definition of entropy production rate

Entropy production rate (single heat bath)

$$\dot{\sigma} = -\sum_{w} \beta E_w \frac{dp_w}{dt} + \frac{d}{dt}\left(-\sum_{w} p_w \ln p_w\right)$$

$$= \sum_{w,w'} R_{w'w} p_w \ln \frac{R_{w'w} p_w}{R_{ww'} p_{w'}}$$

Assuming local detailed-balance (LDB)

Pseudo entropy production Π

$$\dot{\sigma} = \sum_{w \neq w'} R_{w'w} P_w \ln \frac{R_{w'w} P_w}{R_{ww'} P_{w'}}$$

$$= \frac{1}{2} \sum_{w \neq w'} (R_{w'w} P_w - R_{ww'} P_{w'}) \ln \frac{R_{w'w} P_w}{R_{ww'} P_{w'}}$$

$$\geq \sum_{w \neq w'} \frac{(R_{w'w} P_w - R_{ww'} P_{w'})^2}{R_{w'w} P_w + R_{ww'} P_{w'}}$$

$$=: \dot{\Pi}$$

pseudo entropy production rate

(N. Shiraishi, J. Stat. Phys. 185, 19 (2021))

Second law

Integration of entropy production rate is entropy production (entropy increase)

$$\sigma = \int_0^\tau dt\, \dot{\sigma}$$

$\dot{\sigma} \geq 0$ implies $\sigma \geq 0$.

（Both inequalities are called the second law）

$(\dot{\Pi} \geq 0$ implies $\Pi = \int dt \dot{\Pi} \geq 0)$

Outline

Brief review of stochastic thermodynamics

Part 1: Finite-speed processes

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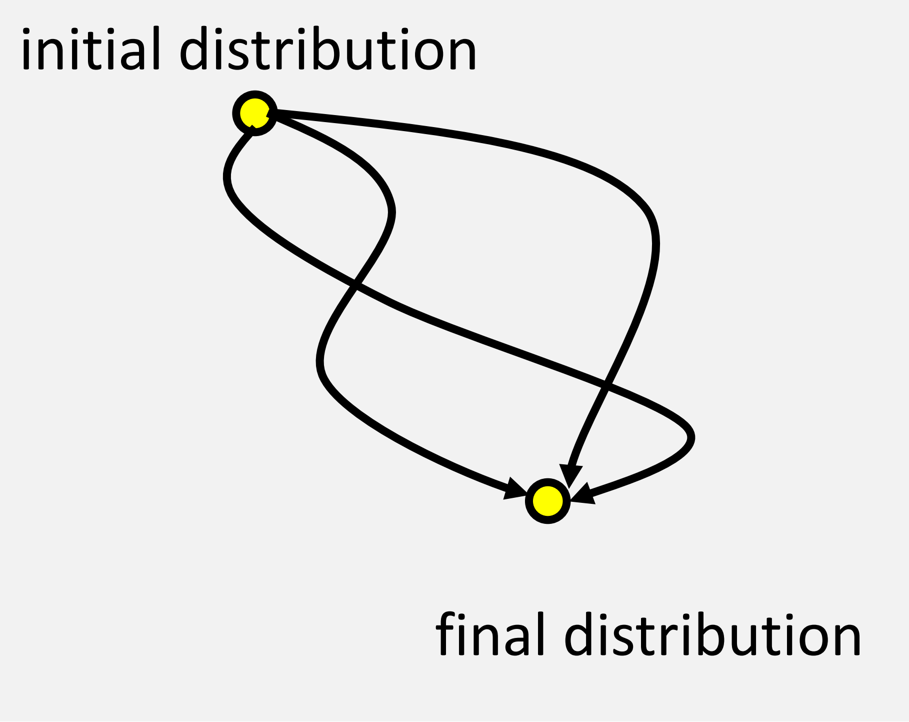
Part 3: Oscillation phenomena

Speed limit: problem

<u>Problem</u>: Given Initial and final distributions.

How quick can we transform this distribution?

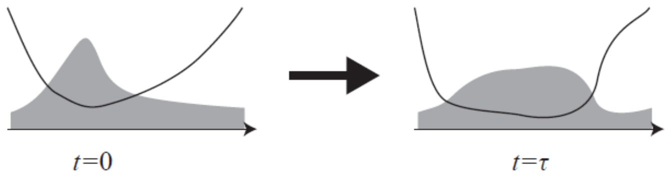
We can tune how to change the control parameters.



Speed limits: some attempts

Overdamped Langevin systems

K. Sekimoto and S.-i. Sasa, J. Phys. Soc. Jpn. 66, 3326 (1997).
E. Aurell, et.al., J. Stat. Phys. 147, 487 (2012).



Entropy production is a cost of quick state transformation.

Physical picture is clear.
But system (and derivation) is specific to overdamped Langevin systems.

Main result (Part 1)

For any Markov jump process with LDB, we have

$$\frac{\mathcal{L}(p,p')^2}{2\sigma\langle A\rangle} \leq \tau$$

(N. Shiraishi, K Funo, and K. Saito, PRL 121, 070601 (2018))

$\mathcal{L}(p,p') \coloneqq \sum_w |p_w - p'_w|$: total variation distance

$\langle A\rangle$: averaged dynamical activity $\int_0^\tau dt A(t)$

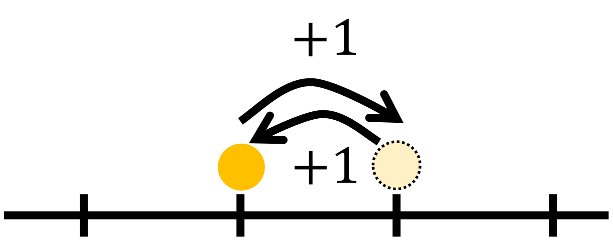
What is dynamical activity?

Dynamical activity: How frequently jumps occur.

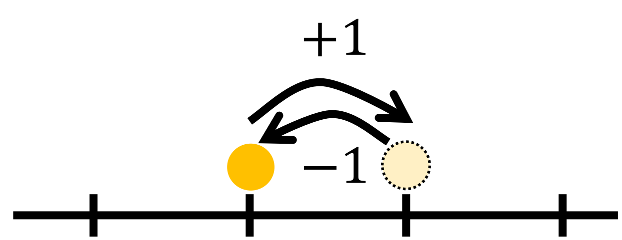
$$A(t) := \sum_{w \neq w'} R_{w'w} p_w(t)$$

Activity determines **time-scale of dynamics**.

Activity



cf) Current



Glassy dynamics: J. P. Garrahan, et al., PRL 98, 195702 (2007).

Nonequilibrium steady state: M. Baiesi, et al., PRL 103, 010602 (2009).

Physical meaning of this inequality

Length between initial and final distributions

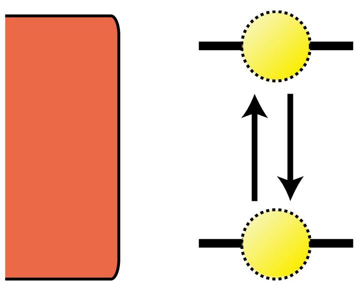
$$\frac{\mathcal{L}(p,p')^2}{2\sigma\langle A\rangle} \leq \tau$$

<u>Entropy production</u>: Cost of quick state transformation

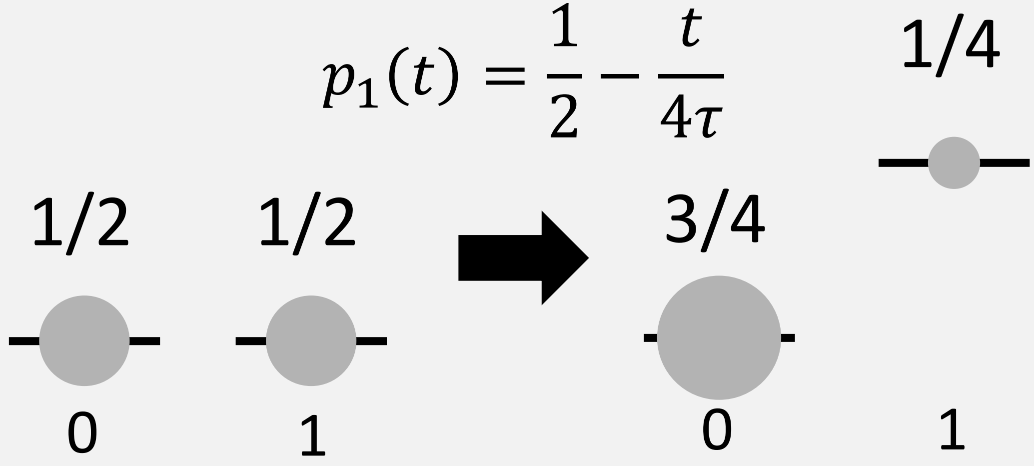
Time-scale of dynamics

Numerical demonstration

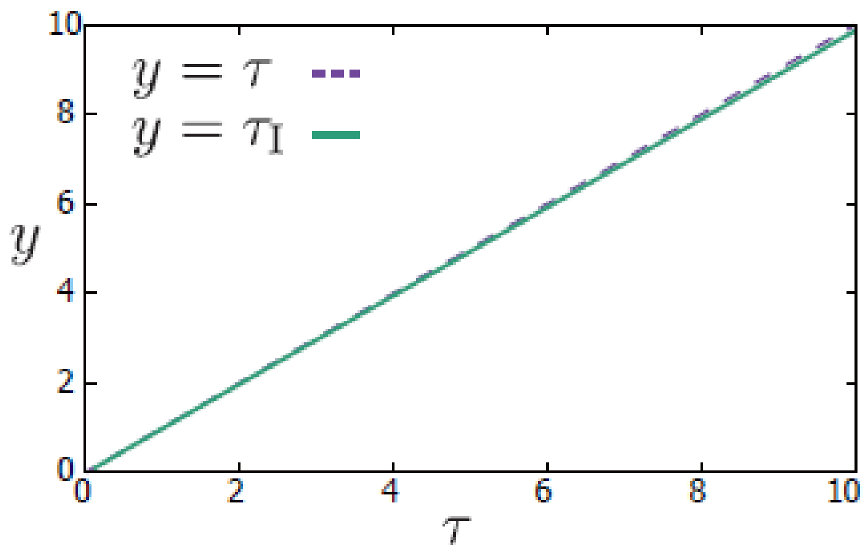
2-state system



$$p_1(t) = \frac{1}{2} - \frac{t}{4\tau}$$



$$\tau_I := \frac{\mathcal{L}(p, p')^2}{2\sigma\langle A \rangle} \leq \tau$$



Derivation (instantaneous quantities)

$$\sum_w \left| \frac{d}{dt} p_w \right|$$

$$= \sum_w \left| \sum_{w'(\neq w)} (R_{w'w} P_w - R_{ww'} P_{w'}) \right|$$

$$\leq \sum_w \sqrt{\sum_{w'(\neq w)} (R_{w'w} P_w + R_{ww'} P_{w'}) \cdot \sum_{w'(\neq w)} \frac{(R_{w'w} P_w - R_{ww'} P_{w'})^2}{R_{w'w} P_w + R_{ww'} P_{w'}}}$$

Schwarz inequality $|\sum_i a_i b_i|^2 \leq (\sum_i a_i^2)(\sum_i b_i^2)$

Derivation (instantaneous quantities)

$$\sum_w \left| \frac{d}{dt} p_w \right|$$

$$= \sum_w \left| \sum_{w'(\neq w)} (R_{w'w} P_w - R_{ww'} P_{w'}) \right|$$

$$\leq \sum_w \sqrt{\sum_{w'(\neq w)} (R_{w'w} P_w + R_{ww'} P_{w'}) \cdot \sum_{w'(\neq w)} \frac{(R_{w'w} P_w - R_{ww'} P_{w'})^2}{R_{w'w} P_w + R_{ww'} P_{w'}}}$$

$$\leq \sqrt{\sum_{w' \neq w} (R_{w'w} P_w + R_{ww'} P_{w'}) \cdot \sum_{w' \neq w} \frac{(R_{w'w} P_w - R_{ww'} P_{w'})^2}{R_{w'w} P_w + R_{ww'} P_{w'}}}$$

$$= \sqrt{2A\dot{\Pi}} \leq \sqrt{2A\dot{\sigma}}$$

Derivation (time integration)

$$\mathcal{L}(p_i, p_f) \leq \sum_w \int_0^\tau dt \left| \frac{d}{dt} p_w \right|$$

$$\leq \int_0^\tau dt \sqrt{2\dot{\sigma}A} \leq \sqrt{2\tau\sigma\langle A \rangle}$$

This is the desired result!

$$\boldsymbol{\frac{\mathcal{L}(p, p')^2}{2\sigma\langle A \rangle} \leq \frac{\mathcal{L}(p, p')^2}{2\Pi\langle A \rangle} \leq \tau}$$

Note: some development

Using Wasserstein distance $\mathcal{W}(p,p')$ (a distance defined in optimal transport theory), we have

$$\frac{\mathcal{W}(p,p')^2}{2\Pi\langle A\rangle} \leq \tau$$

and its equality is achievable (tight).

(A. Dechant, J. Phys. A Math. Theor. 55, 094001 (2022))

Its derivation is more technical and complicated.

Outline

Brief review of stochastic thermodynamics

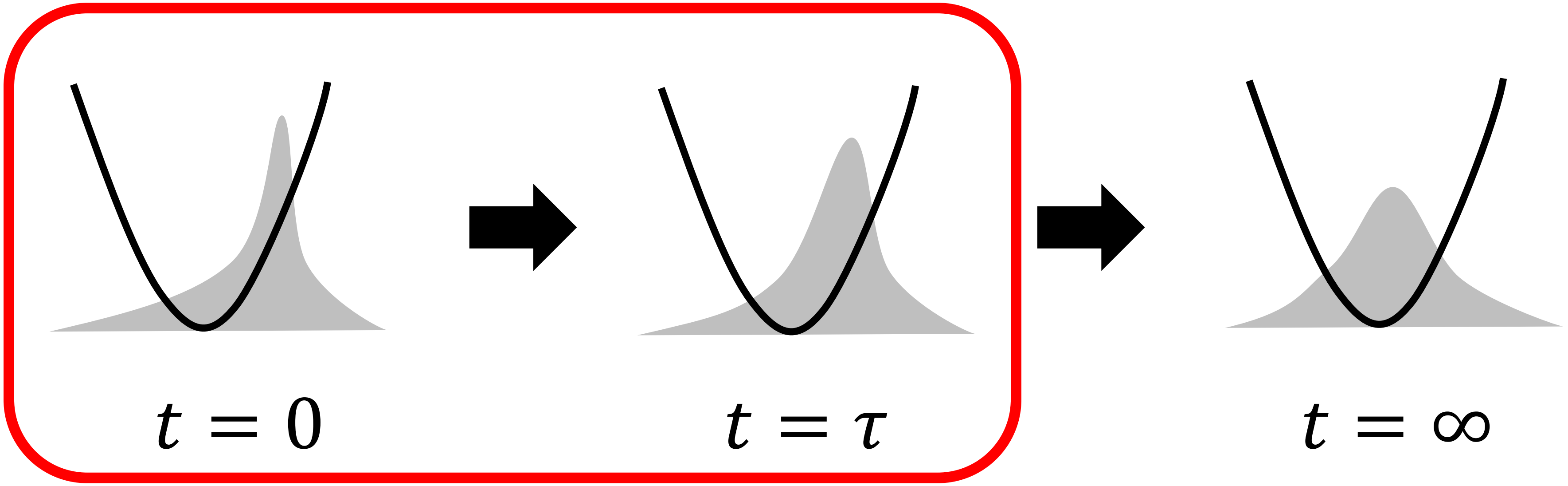
Part 1: Finite-speed processes

Part 2: Relaxation processes

Part 3: Oscillation phenomena

Problem: entropy production in thermal relaxation process

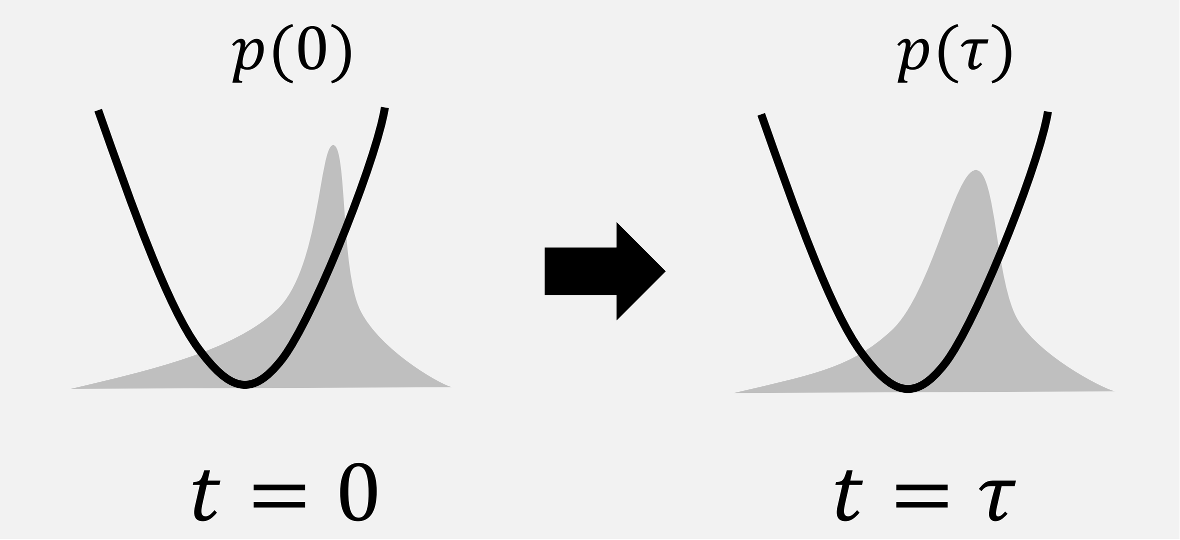
Situation：relaxation process with a single heat bath in continuous time. We assume LDB.



Goal：Deriving lower bound of entropy production within $0 \leq t \leq \tau$ (denoted by $\sigma_{[0,\tau]}$)

Main result (Part 2)

$$\boldsymbol{\sigma_{[0,\tau]} \geq D(p(0)||p(\tau))}$$



$D(p||q) := \sum_i p_i \ln \frac{p_i}{q_i}$: Kullback-Leibler divergence

(a kind of (pseudo-)distance)

(N. Shiraishi and K. Saito, PRL 123, 110603 (2019))

Significance

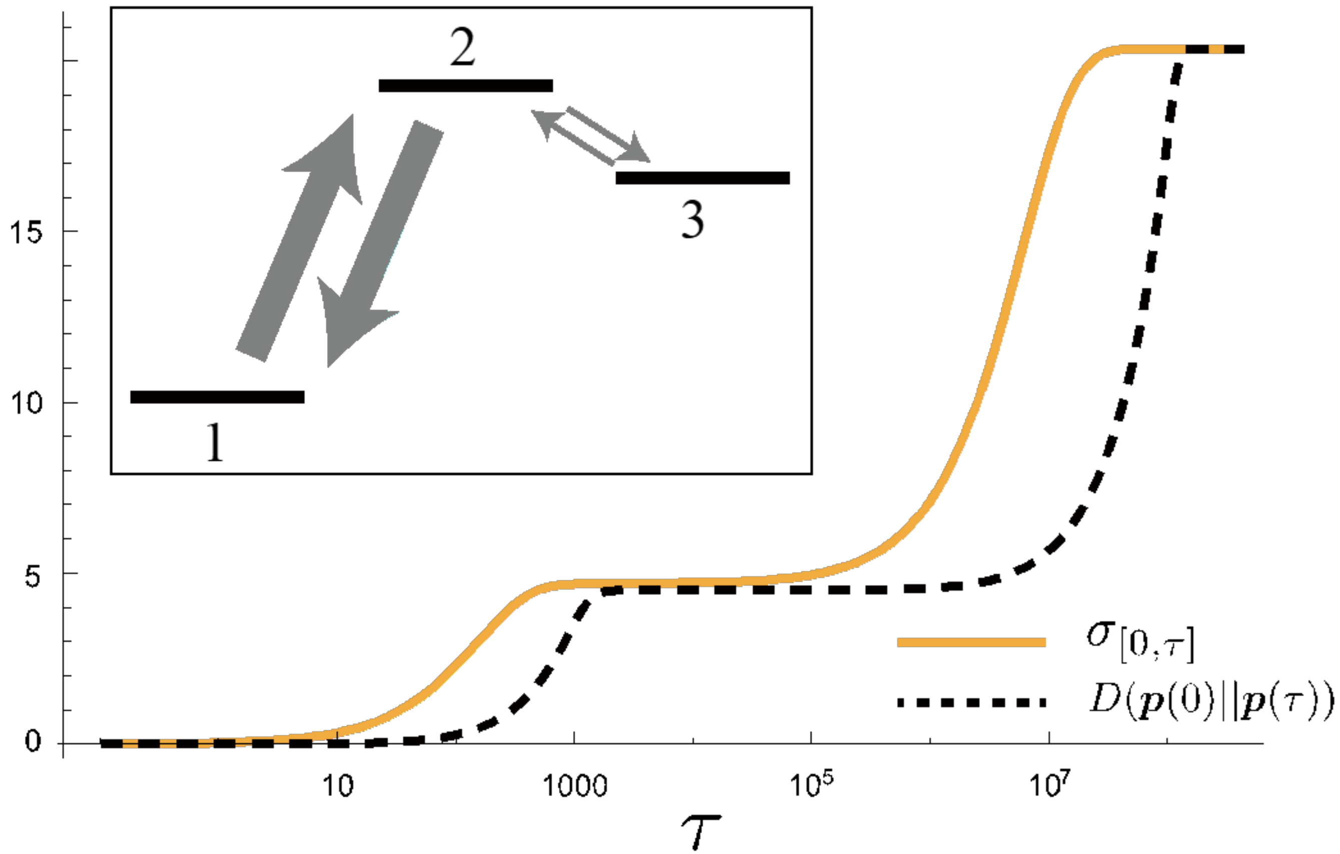
$$\boldsymbol{\sigma}_{[\mathbf{0},\boldsymbol{\tau}]} \geq \boldsymbol{D}(\boldsymbol{p}(\mathbf{0})||\boldsymbol{p}(\boldsymbol{\tau}))$$

- Only for relaxation processes (It does not hold in general process).
- Equality holds for both $\tau = 0$ and $\boldsymbol{\tau} = \infty$.
- It does not hold in discrete time Markov chain.

Numerical demonstration

<u>Setup</u>：three-state model

Take a system with anomalous (two-step) relaxation.

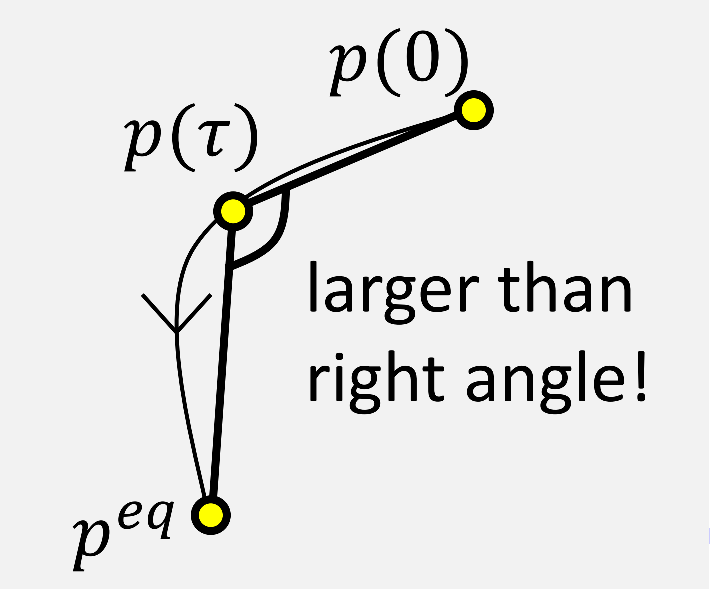


Geometric visualization

Relation $\boldsymbol{\sigma_{[0,\tau]} = D(p(0)||p^{eq}) - D(p(\tau)||p^{eq})}$ implies

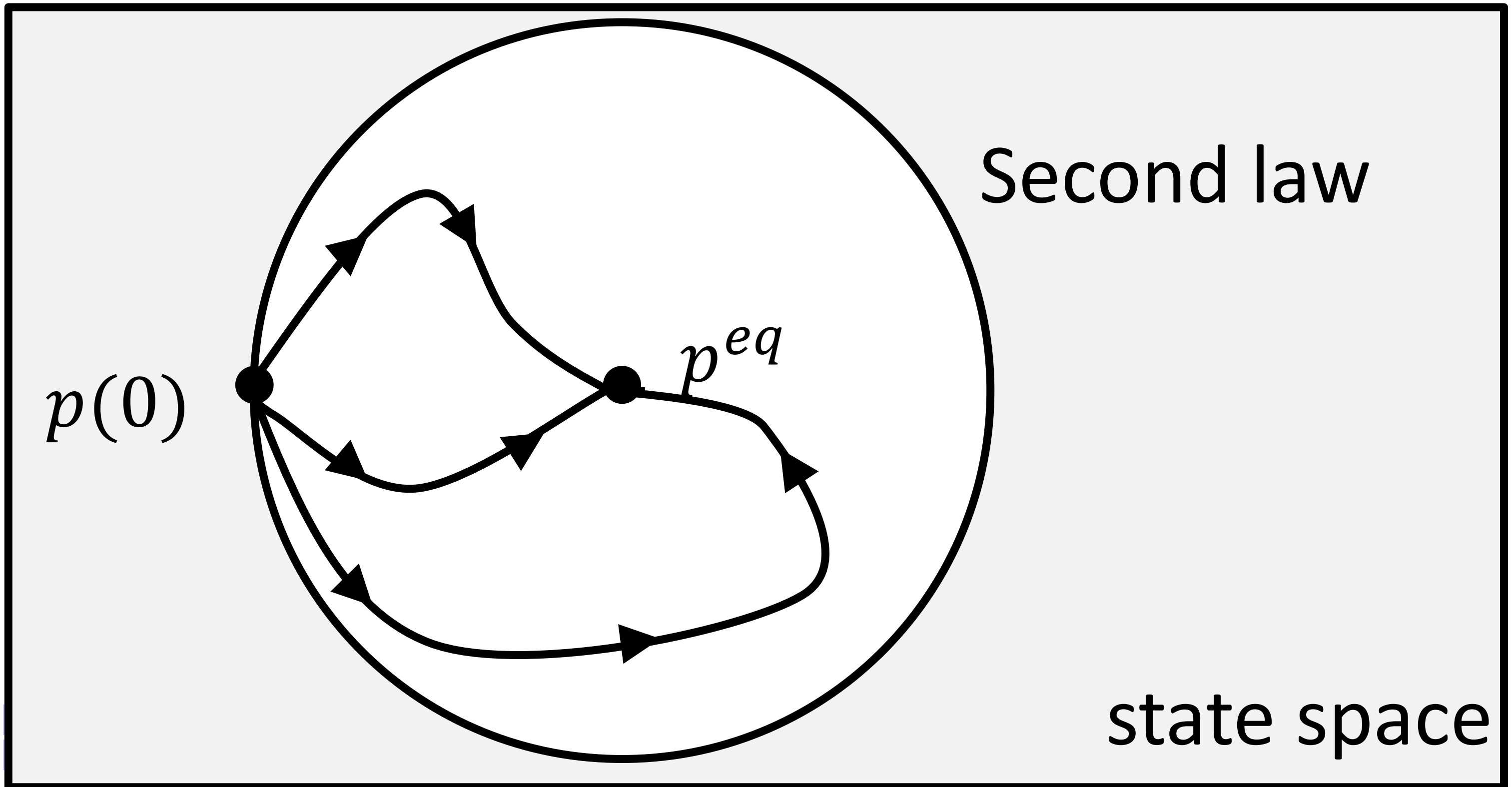
$$\boldsymbol{D(p(0)||p^{eq}) \geq D\big(p(0)\big|\big|p(\tau)\big) + D(p(\tau)||p^{eq})}$$

<ins>Remark</ins>:
KL-divergence ↔ square of distance



Restriction on possible trajectory

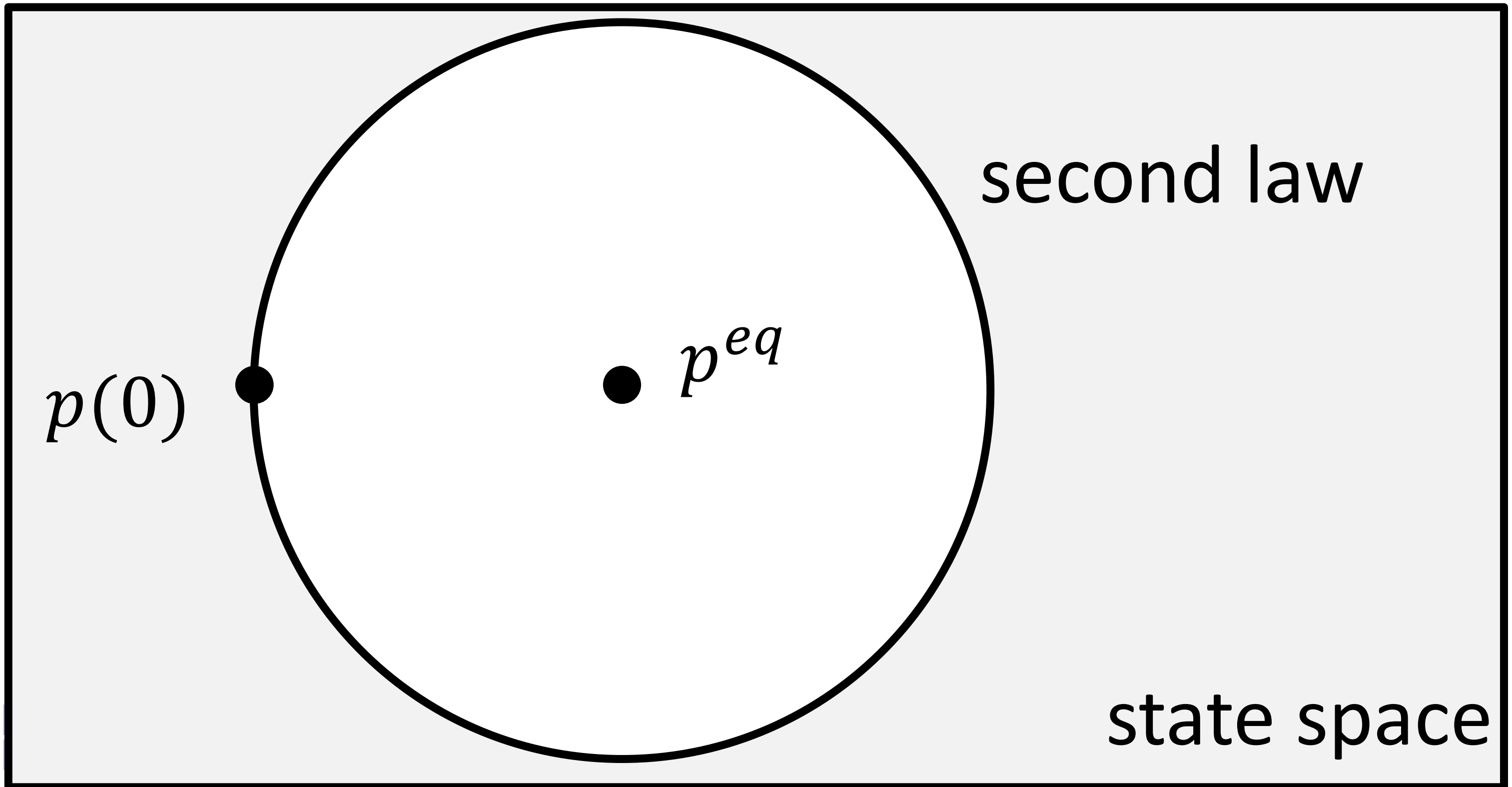
Given both initial and equilibrium distribution.
What is possible pass of relaxation processes?



Restriction on possible trajectory

Obtained relation

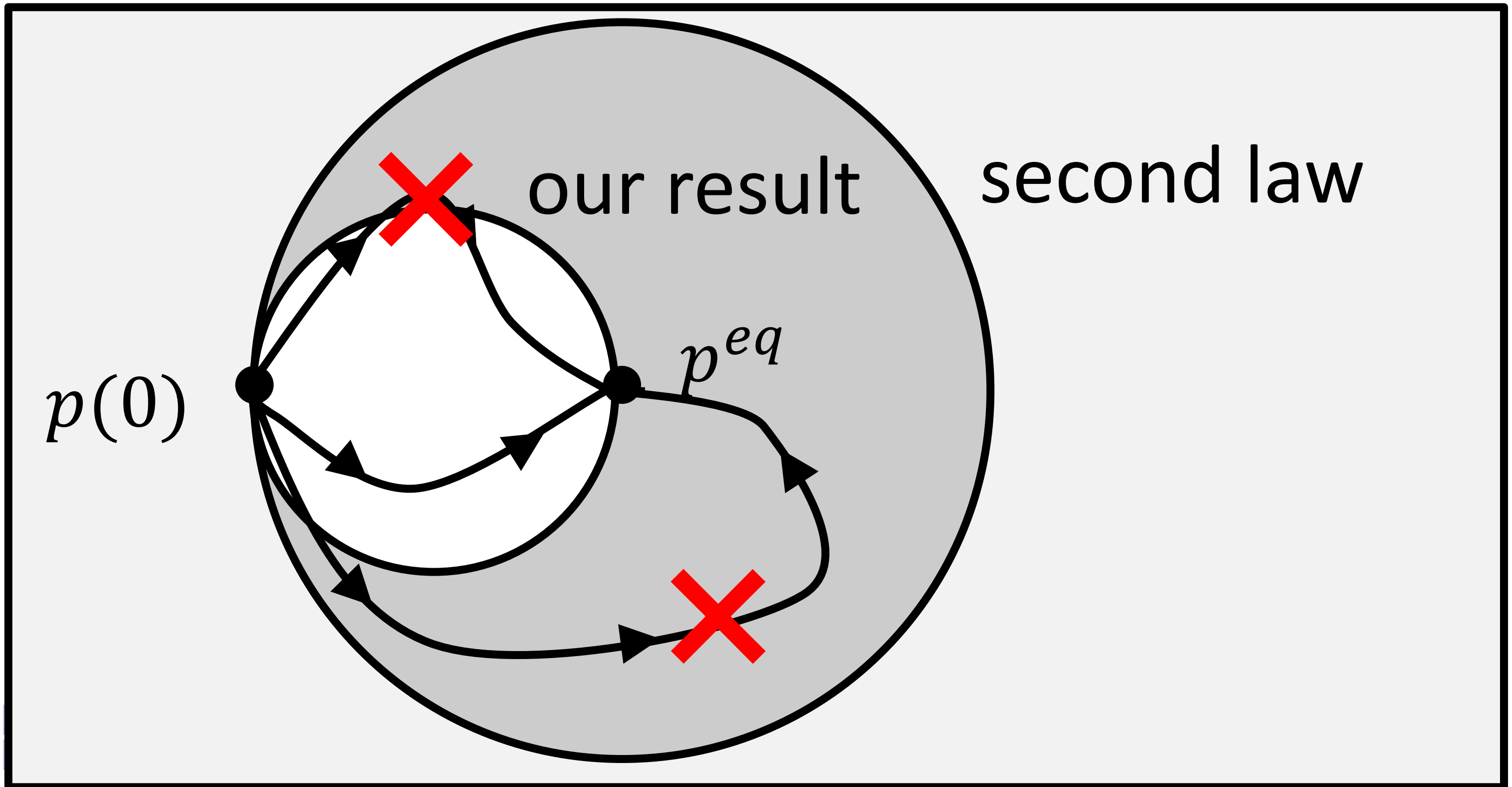
$$D(p(0)||p^{eq}) \geq D(p(0)\,\big\|\,p(\tau)\big) + D(p(\tau)||p^{eq})$$



Restriction on possible trajectory

Obtained relation

$$\boldsymbol{D(p(0)||p^{eq}) \geq D(p(0)\big\|p(\tau)\big) + D(p(\tau)||p^{eq})}$$



Key relation: variational expression of entropy production rate

$$\dot{\sigma} = -\frac{d}{dt} D(p(t)||p^{eq})$$

Because right-hand side equals

$$-\frac{d}{dt}\left[\sum_i p_i \ln p_i - p_i \ln \frac{e^{-\beta E_i}}{Z}\right] = \frac{d}{dt} H(\boldsymbol{p}) + \frac{d}{dt}\langle E \rangle = \dot{\sigma}$$

Key relation: variational expression of entropy production rate

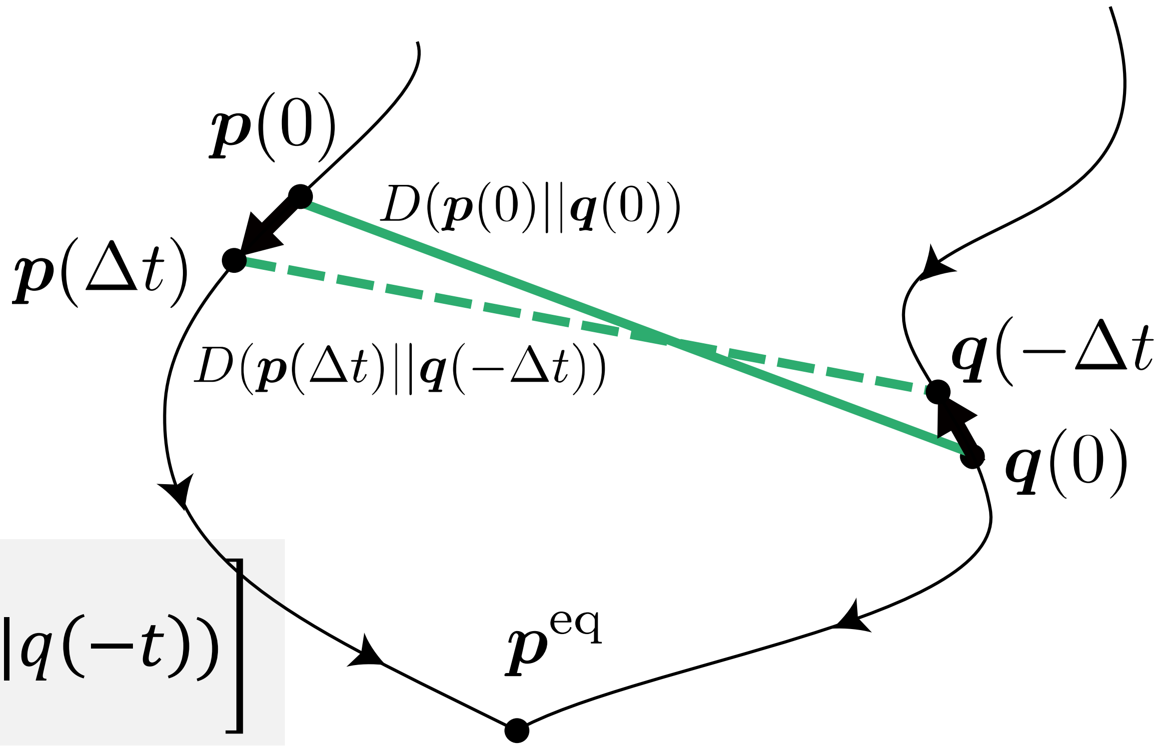
$$\dot{\sigma} = -\frac{d}{dt} D(p(t)||p^{eq})$$

$$= \max_{q} \left[-\frac{d}{dt} D(p(t)||q(-t)) \right]$$

$q(-t)$: distribution evolves backward in time under the same transition matrix as $p(t)$.

(N. Shiraishi and K. Saito, PRL 123, 110603 (2019))

Schematic of variational expression



$$\dot{\sigma} = \max_{q}\left[-\frac{d}{dt}D(p(t)||q(-t))\right]$$

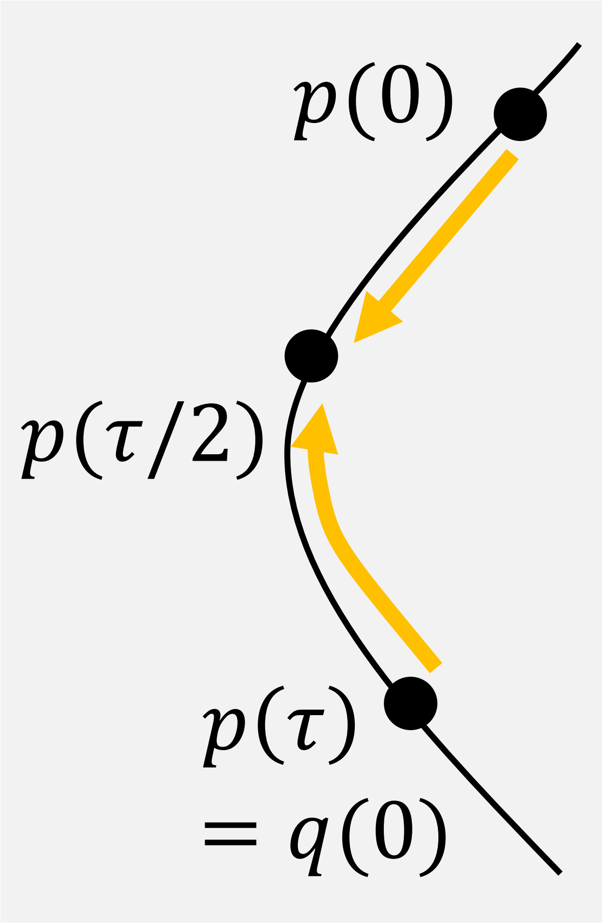
Green lines：KL divergence $D(p||q)$

Difference between solid line and dashed line takes maximum when $q = p^{eq}$.

Variational expression leads to bound on relaxation processes

$$\sigma_{[0,\tau/2]} \geq -\int_0^{\tau/2} dt \frac{d}{dt} D(p(t)||q(-t))$$

$$= D(p(0)||p(\tau))$$



From $\sigma_{[0,\tau]} \geq \sigma_{[0,\tau/2]}$, we have

$$\boldsymbol{\sigma_{[0,\tau]} \geq D(p(0)||p(\tau))}$$

Proof of variational expression

It suffices to prove

$$\frac{d}{dt}\left[D\big(p(t)\big|\big|q(-t)\big) - D\big(p(t)\big|\big|p^{eq}\big)\right] \geq 0$$

for any q.

The left-hand side is equal to

$$\frac{d}{dt}\left[\sum_i p_i(t)\ln\frac{p_i^{eq}}{q_i(-t)}\right]$$

Proof of variational expression

$$\frac{d}{dt}\left[\sum_i p_i(t)\ln\left(\frac{p_i^{\rm eq}}{q_i(-t)}\right)\right]$$

$$=\sum_i\sum_j R_{ij}p_j\ln\left(\frac{p_i^{\rm eq}}{q_i}\right)+\sum_i p_i\sum_j\frac{R_{ij}q_j}{q_i}$$

We used $\sum_{i(\neq j)} R_{ij}p_j\ln\left(\frac{q_j}{p_j^{\rm eq}}\right)=-R_{jj}p_j\ln\left(\frac{q_j}{p_j^{\rm eq}}\right)$

Proof of variational expression

$$\frac{d}{dt}\left[\sum_i p_i(t)\ln\left(\frac{p_i^{\mathrm{eq}}}{q_i(-t)}\right)\right]$$

$$= \sum_i \sum_j R_{ij} p_j \ln\left(\frac{p_i^{\mathrm{eq}}}{q_i}\right) + \sum_i p_i \sum_j \frac{R_{ij} q_j}{q_i}$$

$$+ \sum_i R_{ii} p_i \qquad = \sum_{i \neq j} R_{ij} p_j \ln\left(\frac{p_i^{\mathrm{eq}} q_j}{p_j^{\mathrm{eq}} q_i}\right) + \sum_{i \neq j} p_i \frac{R_{ij} q_j}{q_i} -$$

(We used $x - 1 - \ln x \geq 0$)

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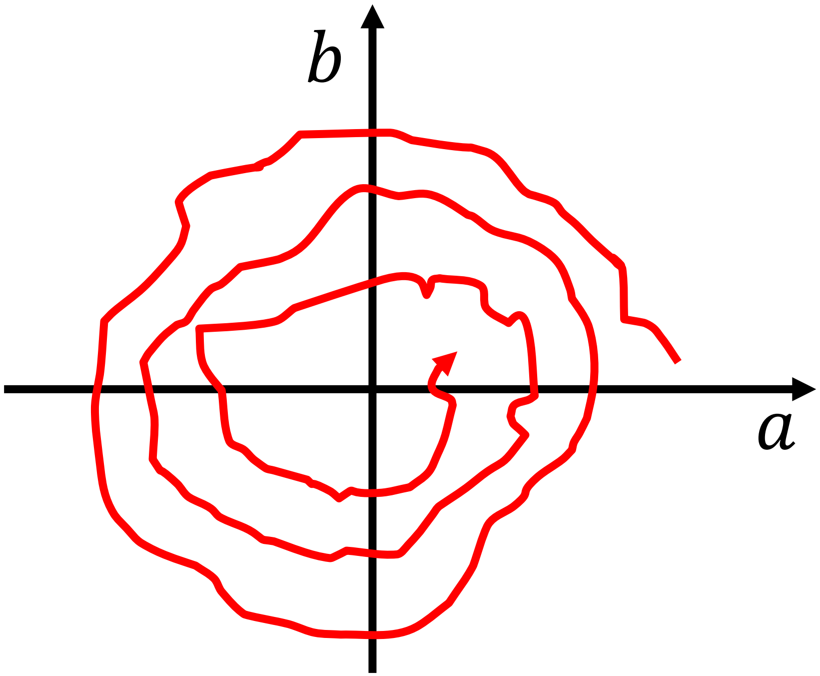
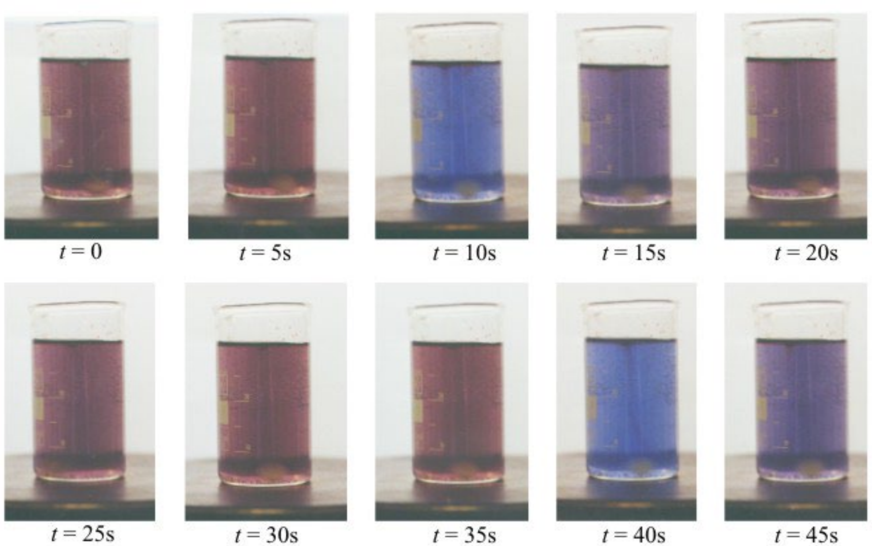
Fluctuation oscillation phenomena

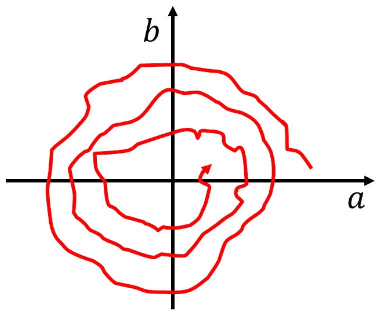


a, b: state variable

Fluctuation oscillates in a-b plane.



Quantifying oscillation



Oscillation is quantified by

$$\boldsymbol{\alpha_{ab} := \langle a\dot{b} - b\dot{a} \rangle}$$

To normalize the speed of oscillation by relaxation speed, we introduce autocorrelation:

$$D_a := -\langle a\dot{a} \rangle = \frac{1}{2}\sum_{i,j}\left(a_i - a_j\right)^2 R_{ij} p_j^{ss}$$

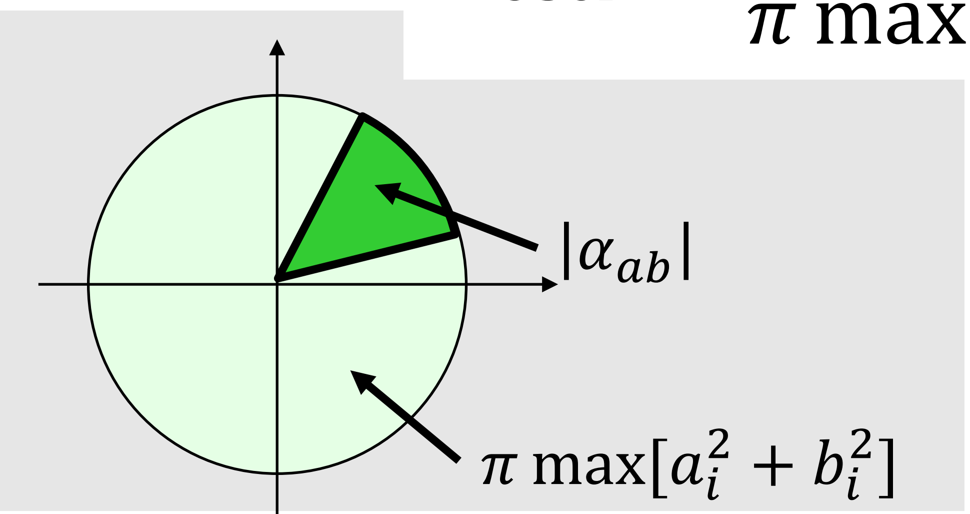
Task: Bound $\dfrac{2\alpha_{ab}}{D_a + D_b}$ by entropy production.

Main result (Part 3)

$$\frac{2|\alpha_{ab}|}{D_a + D_b} \leq \frac{\dot{\sigma}}{2\pi w_{\mathrm{osci}}}$$

w_{osci} is a characteristic maximum angular speed of oscillation:

$$w_{\mathrm{osci}} := \frac{|\alpha_{ab}|}{\pi \max[a_i^2 + b_i^2]}$$



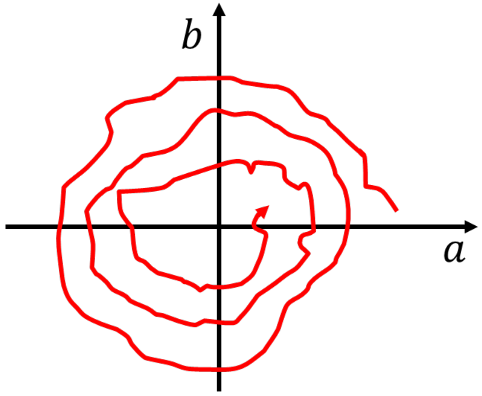
(N. Shiraishi, arXiv:2304.12775)

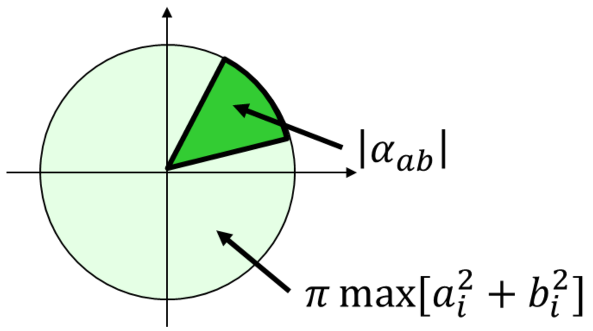
Physical meaning of main result

$$\frac{2|\alpha_{ab}|}{D_a + D_b} \leq \frac{\dot{\sigma}}{2\pi w_{\mathrm{osci}}}$$

Strength of oscillation (relative to relaxation)

Entropy production per single oscillation





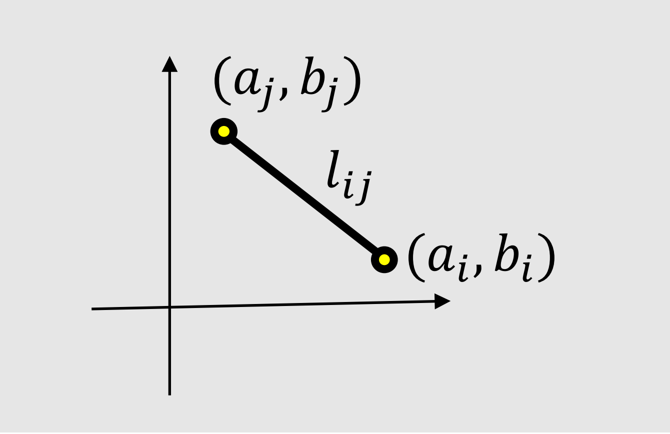
Geometric interpretation 1

Autocorrelation is written as $\frac{D_a + D_b}{2} = \frac{1}{2}\sum_{(i,j)} A_{ij} l_{ij}^2$

A_{ij}: activity

(N. Ohga, et al., arXiv:2303.13116)

$l_{ij} \coloneqq \sqrt{(a_i - a_j)^2 + (b_i - b_j)^2}$: length from i to j



(Intuitive: autocorrelation = average squared displacement)

Geometric interpretation 2

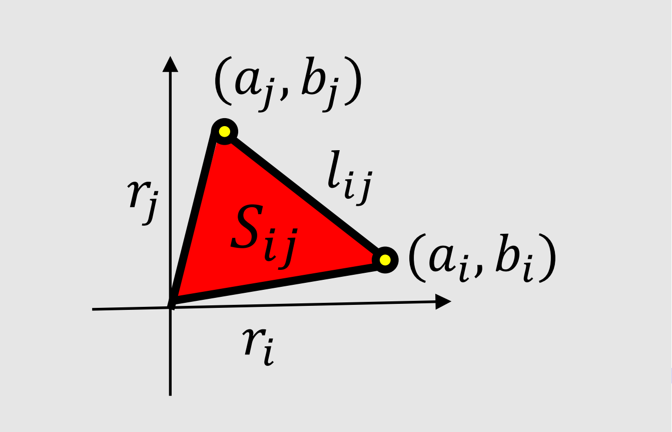
Fluctuation oscillation is evaluated as

$$\alpha_{ab} = \sum_{i,j} (a_i b_j - b_i a_j) R_{ij} p_j^{ss} = \sum_{(i,j)} S_{ij} J_{ij}$$

We define length from origin as $r_i := \sqrt{a_i^2 + b_i^2}$.

Important evaluation:

$$\boldsymbol{S_{ij} \leq \frac{1}{2} r_i l_{ij} \leq \frac{1}{2} r_{\max} l_{ij}}$$



Proof

$$\frac{2\left|\alpha_{ab}^2\right|}{D_a + D_b} = \frac{2\left(\sum_{(i,j)} J_{ij} S_{ij}\right)^2}{\sum_{(i,j)} A_{ij} l_{ij}^2} \leq \frac{r_{\max}^2}{2} \frac{\left(\sum_{(i,j)} J_{ij} l_{ij}\right)^2}{\sum_{(i,j)} A_{ij} l_{ij}^2}$$

$$\leq \frac{r_{\max}^2}{2} \sum_{(i,j)} \frac{J_{ij}^2}{A_{ij}}$$

Schwarz inequality: $\left(\sum_{(i,j)} J_{ij} l_{ij}\right)^2 \leq \left(\sum_{(i,j)} A_{ij} l_{ij}^2\right)\left(\sum_{(i,j)} \frac{J_{ij}^2}{A_{ij}}\right)$

Proof

$$\frac{2\left|\alpha_{ab}^2\right|}{D_a + D_b} = \frac{2\left(\sum_{(i,j)} J_{ij} S_{ij}\right)^2}{\sum_{(i,j)} A_{ij} l_{ij}^2} \le \frac{r_{\max}^2}{2} \frac{\left(\sum_{(i,j)} J_{ij} l_{ij}\right)^2}{\sum_{(i,j)} A_{ij} l_{ij}^2}$$

$$\le \frac{r_{\max}^2}{2} \sum_{(i,j)} \frac{J_{ij}^2}{A_{ij}}$$

$$= \frac{r_{\max}^2}{2} \dot{\Pi} \le \frac{r_{\max}^2}{2} \dot{\sigma}$$

Summary

- Trade-off relation between speed and entropy production: $$\frac{\mathcal{L}(p,p')^2}{2\sigma\langle A\rangle} \leq \tau$$
- Bound on entropy production in relaxation process: $$\sigma \geq D(p(0)||p(\tau))$$
- Trade-off between oscillation and entropy production $$\frac{2|\alpha_{ab}|}{D_a + D_b} \leq \frac{\dot{\sigma}}{2\pi w_{\mathrm{osci}}}$$

END