# Some bounds on entropy production stronger than the second law of thermodynamics

Naoto Shiraishi (Gakushuin University)

N. Shiraishi, K. Saito, and H. Tasaki, PRL 117, 190601 (2016).
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).

# Outline

Motivation

Brief review of stochastic thermodynamics

Finite-speed processes

Relaxation processes

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**Motivation**

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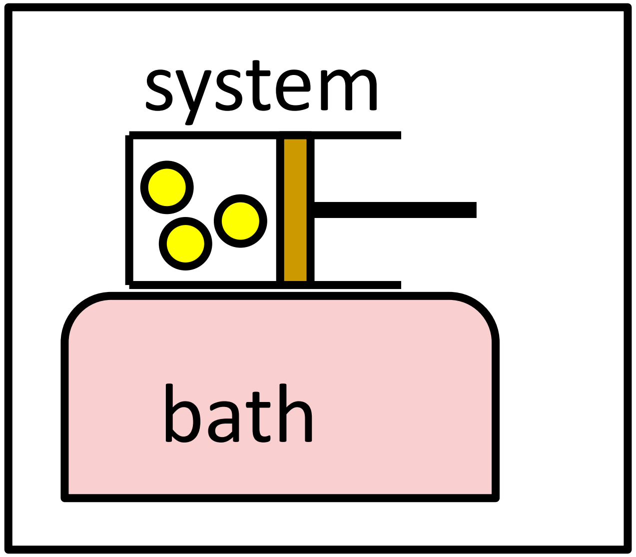
# Second law of thermodynamics




Entropy production

$$\sigma := \Delta S_{\mathrm{system}} + \Delta S_{\mathrm{bath}}$$

Second law of thermodynamics

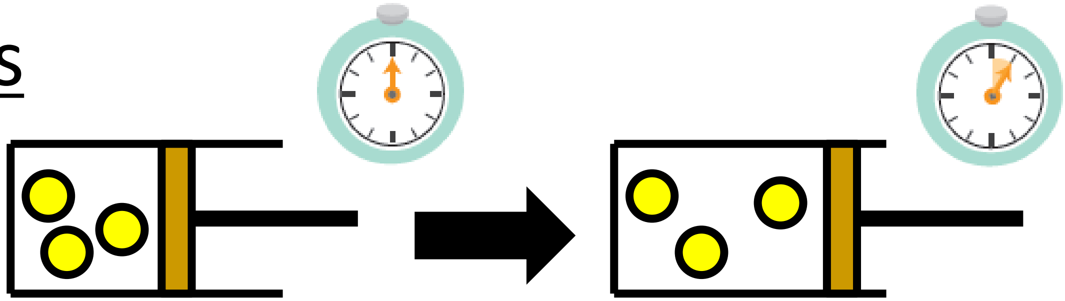
$$\boldsymbol{\sigma \geq 0}$$

Quasi-static operation achieves equality.

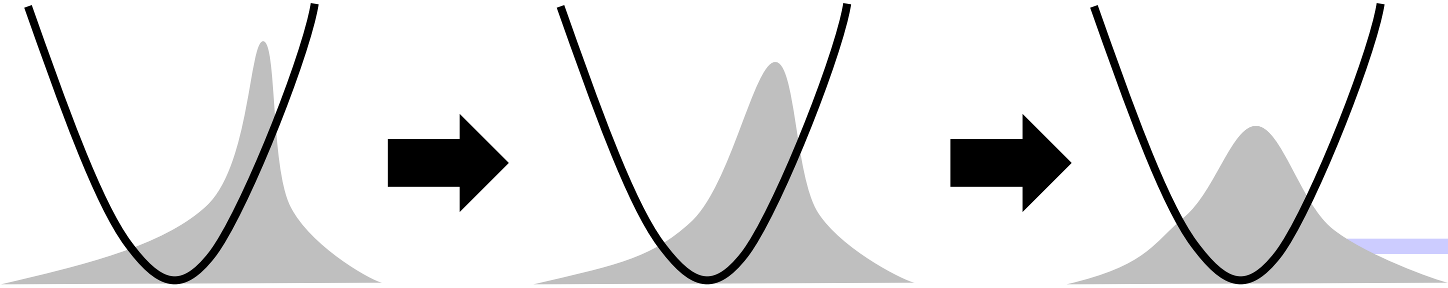
# Non quasi-static processes

Various NOT quasi-static processes:

Finite speed process

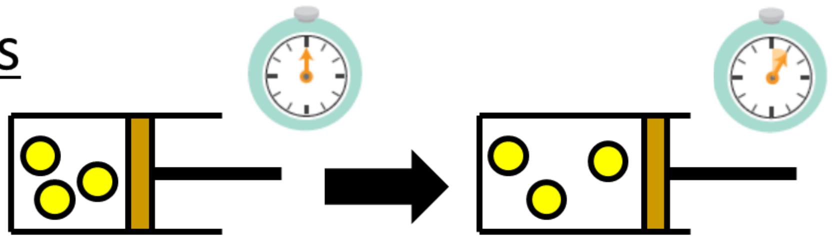


Relaxation process

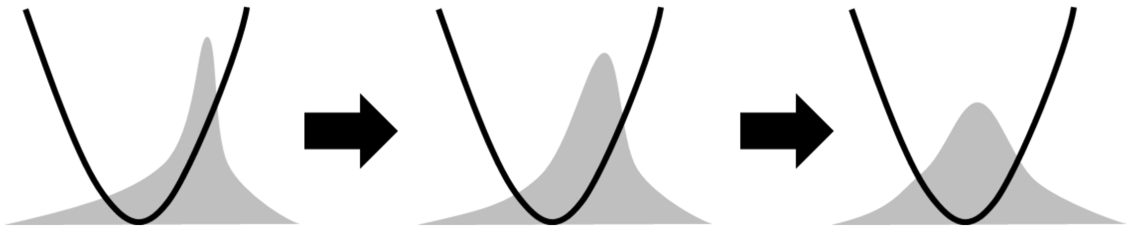


# Stronger bound than the second law?

Finite speed process



Relaxation process



Entropy production must be strictly larger than zero!

**But we still do not know a better bound than the second law $\sigma \geq 0$!**

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**Brief review of stochastic thermodynamics**

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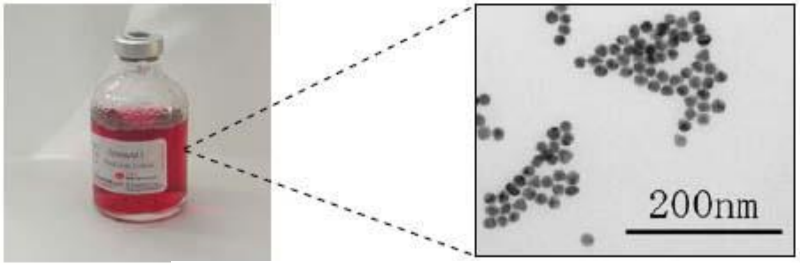
# Setup of stochastic thermodynamics

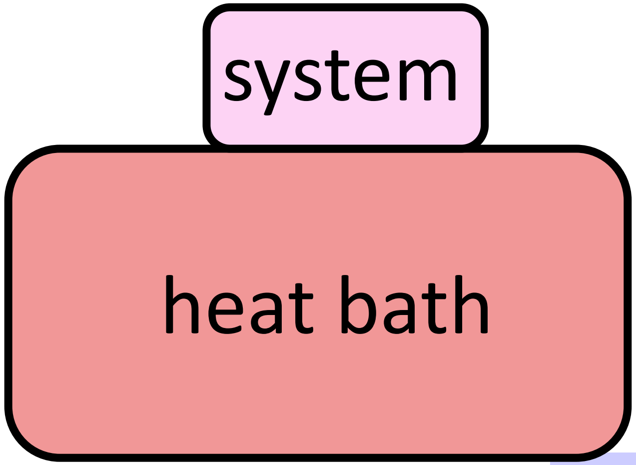
System evolves stochastically due to thermal noise




Colloidal particle

<u>Setup throughout this talk</u>

- Heat bath is in equilibrium
  →describe as **Markov process**
- Consider classical system



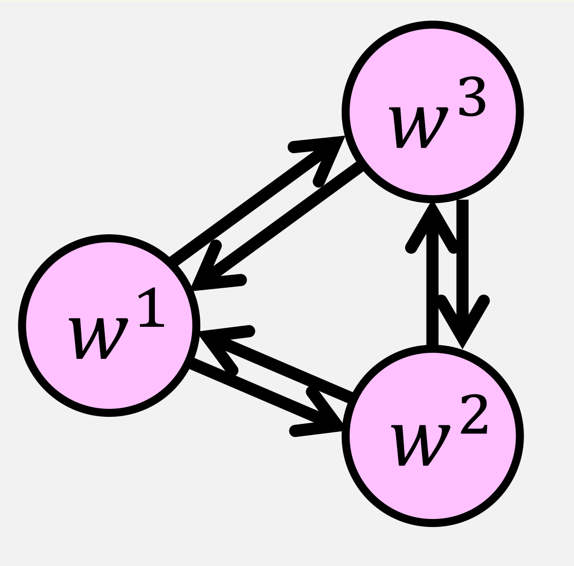
# Description of classical stochastic process

State: **probability distribution $\boldsymbol{p}$**.

Time evolution of $p$ is given by **master equation.**

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

transition matrix




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

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

# Definition of entropy production rate

Entropy production rate (single heat bath)

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

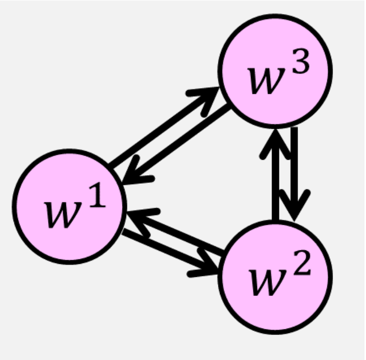
Entropy increase of bath $(dQ/T)$

(Shannon) entropy increase of system

# Detailed balance condition

**<u>Detailed balance (DB)</u>**
If distribution is canonical (equilibrium), there is no <u>microscopic</u> probability current.

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




(For case of multiple baths, DB 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 detailed balance (DB)

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# Background: Efficiency and power - longstanding open problem

Key quantity of heat engine: **efficiency** and **power**.

Expectation: High efficiency implies less power.

But there has been no general proof…

Even worse, a very basic problem
“**Does finite power engine attain Carnot efficiency?**”
has still been an open problem!

# Present situation (before our result)

- **General frameworks** (thermodynamics, linear irreversible thermodynamics) **do not prohibit** an engine with CE at finite power.

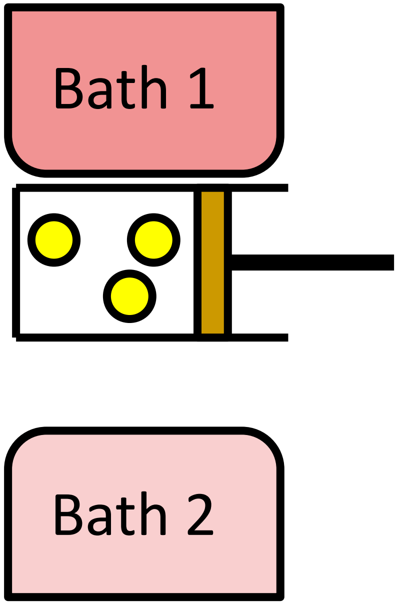
  G. Benenti, K. Saito, and G. Casati, PRL 106, 230602 (2011).

- **In analyses on concrete models in linear regime,** all models do not attain CE with finite power.

  K. Brandner, K. Saito, and U. Seifert, PRL 110, 070603 (2013).
  V. Balachandran, G. Beneti, and G. Casati, PRB 87, 165419 (2013).
  K. Brandner, K. Saito, and U. Seifert, PRX 5, 031019 (2015).
  K. Proesmans and C. Van den Broeck, PRL 115, 090601 (2015).

- General trade-off relation between power and efficiency has completely been elusive.

# Setup of our result




Assumption

- Dynamics of the engine is described by classical Markov process
- Canonical distribution is invariant under the stochastic process

Remarks

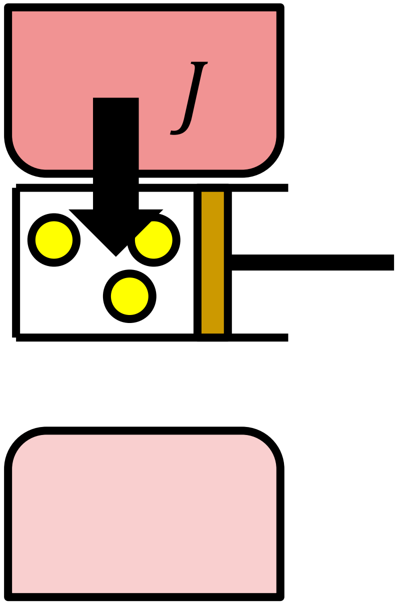
- Broken time-reversal symmetry → OK
- No detailed-balance → OK
- Nonlinear regime → OK
- Transient process → OK

# Main result (Inequality between heat flux entropy production)

Key quantities

$J$: heat flux between bath and engine (in general, flux of conserved quantities)

$\dot{\sigma}$:entropy production rate




Then, the following relation holds (case of single bath)

$$|J| \leq \sqrt{\Theta \dot{\sigma}}$$

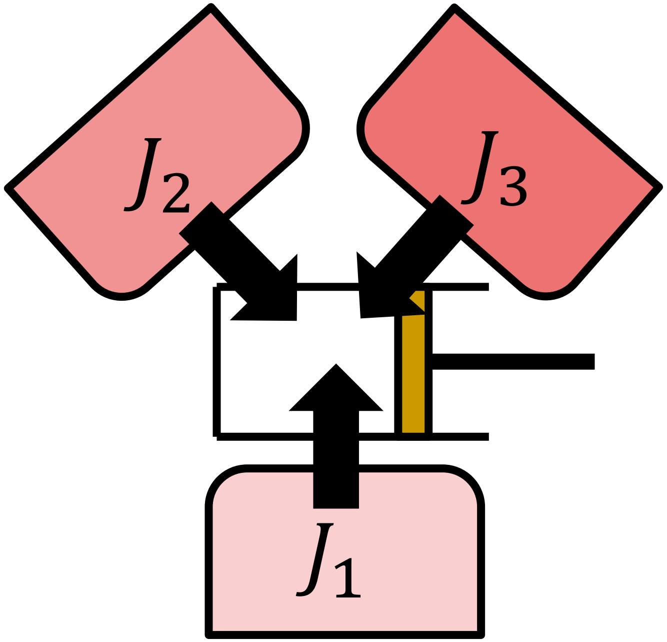
($\Theta$: coefficient depending on state defined later)

(N. Shiraishi, K. Saito, and H. Tasaki, PRL 117, 190601 (2016))

# Multi-bath case

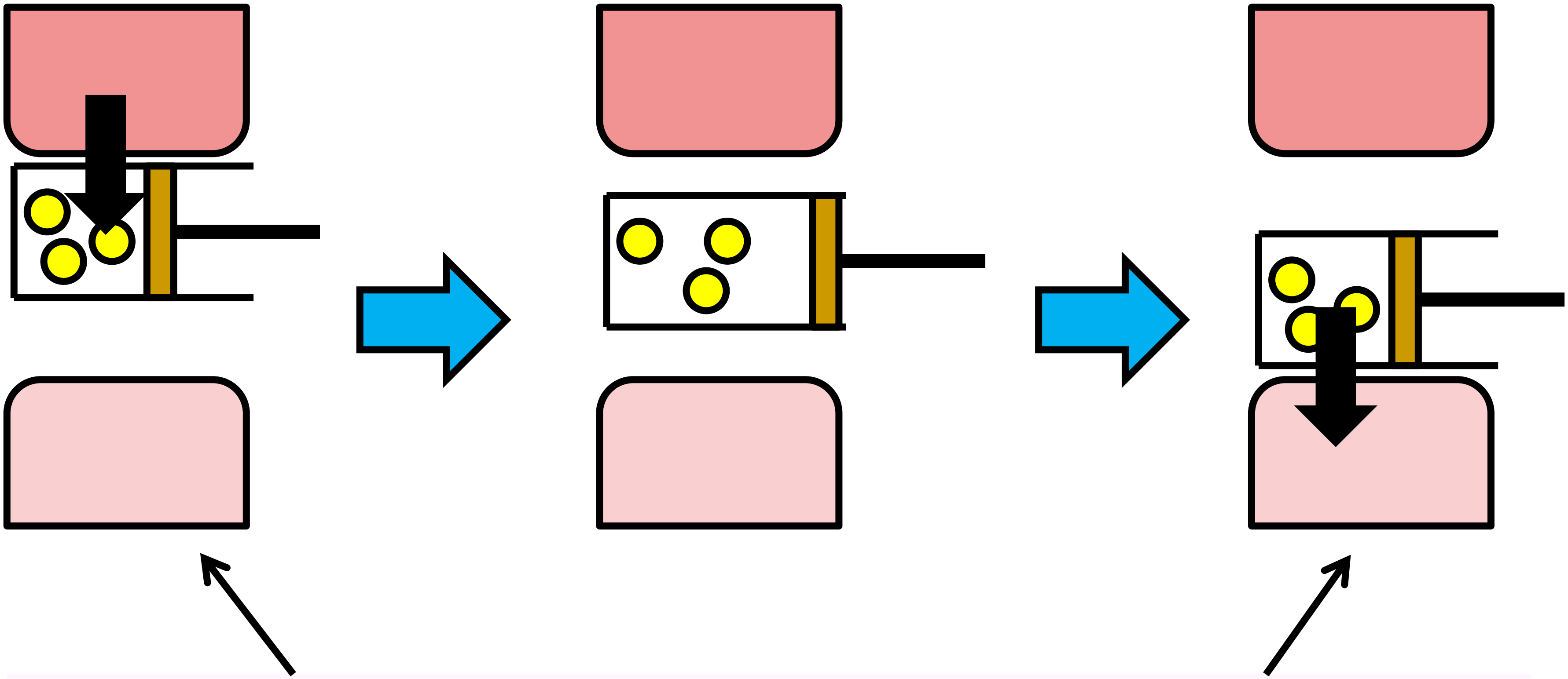
In a similar manner, $\Theta := \sum_\nu \Theta_\nu$, satisfies

$$\sum_\nu |J_\nu| \le \sqrt{\Theta \dot{\sigma}}$$



# Power and efficiency (schematics)

Cyclic process with two baths



There must exist isothermal processes, and they possess inevitable dissipation.

# Main result (Inequality between power and efficiency)

Cyclic process with two baths, work $W$ and efficiency $\eta$ satisfies

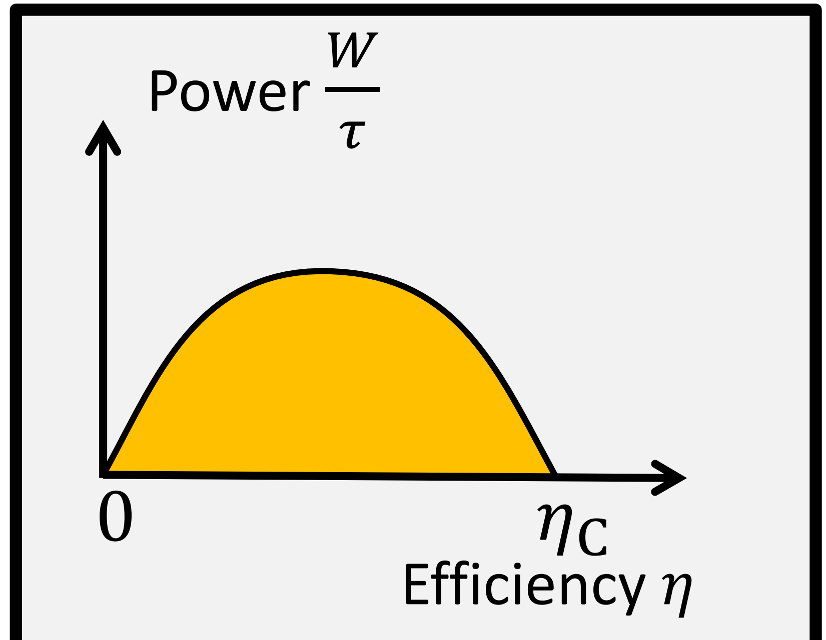
$$\frac{W}{\tau} \leq \bar{\Theta}\beta_L \eta(\eta_C - \eta)$$

$\tau$ : cyclic time interval

$\bar{\Theta}$ : average of $\Theta$ (defined later)

$\beta_L$ : inverse temperature of cold bath

$\eta_C$ : Carnot efficiency




(N. Shiraishi, K. Saito, and H. Tasaki, PRL 117, 190601 (2016))

# Definition of Θ dependent on the conditions

$$|\boldsymbol{J}| \leq \sqrt{\boldsymbol{\Theta}\dot{\boldsymbol{\sigma}}}$$

$\Theta = \Theta^{(1)}$ : General case, but weak a little

(e.g., systems with thermal wall)

$\Theta = \Theta^{(2)}$ : Case with DB, but strong

(e.g., linear Langevin systems, discrete systems without magnetic field)

# Key idea: dual transition rate

<u>Def: dual transition rate</u>

$$\tilde{R}_{ww'} := \frac{R_{w'w} e^{-\beta E_w}}{e^{-\beta E_{w'}}}$$

Invariance of canonical dist. ($\sum_w R_{w'w} e^{-\beta E_w} = 0$)
→normalization condition $\sum_w \tilde{R}_{ww'} = 0$

$$\dot{\sigma} := \sum_{w,w'} R_{w'w} p_w \ln \frac{R_{w'w} p_w}{\tilde{R}_{ww'} p_{w'}}$$

# Definitions of key quantities

Heat flux $$J = -\sum_{w'} E_{w'} \frac{dP_{w'}}{dt}$$

$$= -\sum_{w,w'} E_{w'} R_{w'w} P_w$$

$$= -\sum_{w,w'} \Delta E_{w'} (R_{w'w} P_w - \tilde{R}_{ww'} P_{w'})$$

（Energy fluctuation：$\Delta E_{w'} := E_{w'} - \langle E \rangle$）

# Lemma: Inequality for KL divergence

For $\sum_x p_x = \sum_x q_x$, Kullback-Leibler divergence satisfies

$$D(p_x||q_x) := \sum_x p_x \ln \frac{p_x}{q_x}$$

$$= \sum_x p_x \ln \frac{p_x}{q_x} + q_x - p_x$$

$$\geq \sum_x \frac{c_0 (p_x - q_x)^2}{p_x + q_x} \qquad (c_0 = 0.896 \dots)$$

# Derivation of main result

$$|J|^2$$

$$= \left| \sum_{w \neq w'} \Delta E_{w'} \left( R_{w'w} P_w - \tilde{R}_{ww'} P_{w'} \right) \right|^2$$

$$= \left| \sum_{w \neq w'} \Delta E_{w'} \sqrt{R_{w'w} P_w + \tilde{R}_{ww'} P_{w'}} \frac{R_{w'w} P_w - \tilde{R}_{ww'} P_{w'}}{\sqrt{R_{w'w} P_w + \tilde{R}_{ww'} P_{w'}}} \right|^2$$

$$\leq \sum_{w \neq w'} \Delta E_{w'}^2 \left( R_{w'w} P_w + \tilde{R}_{ww'} P_{w'} \right) \cdot \sum_{w \neq w'} \frac{\left( R_{w'w} P_w - \tilde{R}_{ww'} P_{w'} \right)^2}{R_{w'w} P_w + \tilde{R}_{ww'} P_{w'}}$$

Schwarz inequality $\left|\sum_i a_i b_i\right|^2 \leq \left(\sum_i a_i^2\right)\left(\sum_i b_i^2\right)$ is used.

# Derivation of main result

$$|J|^2$$

$$= \left| \sum_{w \neq w'} \Delta E_{w'} \left( R_{w'w} P_w - \tilde{R}_{ww'} P_{w'} \right) \right|^2$$

$$= \left| \sum_{w \neq w'} \Delta E_{w'} \sqrt{R_{w'w} P_w + \tilde{R}_{ww'} P_{w'}} \, \frac{R_{w'w} P_w - \tilde{R}_{ww'} P_{w'}}{\sqrt{R_{w'w} P_w + \tilde{R}_{ww'} P_{w'}}} \right|^2$$

$$\leq \sum_{w \neq w'} \Delta E_{w'}^2 \left( R_{w'w} P_w + \tilde{R}_{ww'} P_{w'} \right) \cdot \sum_{w \neq w'} \frac{\left( R_{w'w} P_w - \tilde{R}_{ww'} P_{w'} \right)^2}{R_{w'w} P_w + \tilde{R}_{ww'} P_{w'}}$$

$$\leq \frac{1}{c_0} \sum_{w \neq w'} \Delta E_{w'}^2 \left( R_{w'w} P_w + \tilde{R}_{ww'} P_{w'} \right) \sum_{w \neq w'} R_{w'w} P(w) \ln \frac{R_{w'w} P(w)}{\tilde{R}_{ww'} P(w')}$$

$$= \Theta \dot{\sigma}$$

# Inequality between heat flux and entropy production rate

$$\boxed{|J| \leq \sqrt{\Theta^{(1)} \dot{\sigma}}}$$

$$\Theta^{(1)} := \frac{1}{c_0} \sum_{w \neq w'} \Delta E_{w'}^2 \left( R_{w'w} P_w + R_{ww'} P_{w'} \right)$$

$\Theta^{(1)}$ is a quantity similar to dynamical activity.

(We used

$$\sum_{w(\neq w')} \tilde{R}_{ww'} = -\tilde{R}_{w'\,w'} = -R_{w'\,w'} = \sum_{w(\neq w')} R_{ww'})$$

# Case with detailed balance

Detailed balance

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

# Rewrite $J$ and $\sigma$

In this case, $\boldsymbol{\tilde{R}_{ww'}} := e^{-\beta(E_w - E_{w'})} R_{w'w} \boldsymbol{= R_{ww'}}$

$$J = -\sum_{w,w'} E_{w'} (R_{w'w} P_w - R_{ww'} P_{w'})$$

$$= -\frac{1}{2} \sum_{w,w'} (E_{w'} - E_w)(R_{w'w} P_w - R_{ww'} P_{w'})$$

(cf : $J = -\sum_{w,w'} \underline{\Delta E_{w'}} (R_{w'w} P_w - \tilde{R}_{ww'} P_{w'})$)

# Rewrite $J$ and $\sigma$

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

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

$$\geq \frac{1}{2} \sum_{w \neq w'} \frac{2(R_{w'w} P_w - R_{ww'} P_{w'})^2}{R_{w'w} P_w + R_{ww'} P_{w'}}$$

(cf: $\dot{\sigma} \geq \sum_{w \neq w'} \frac{c_0 \left(R_{w'w} P_w - \tilde{R}_{ww'} P_{w'}\right)^2}{R_{w'w} P_w + \tilde{R}_{ww'} P_{w'}}$)

# Inequality between heat flux and entropy production rate (strong)

$$\boxed{|\boldsymbol{J}| \leq \sqrt{\boldsymbol{\Theta}^{(2)}\dot{\boldsymbol{\sigma}}}}$$

$$\boldsymbol{\Theta}^{(2)} := \frac{1}{2}\sum_{w\neq w'}\left(\boldsymbol{E}_{w'} - \boldsymbol{E}_{w}\right)^{2}\boldsymbol{R}_{w'w}\boldsymbol{P}_{w}$$

(cf: $\Theta^{(1)} := \frac{1}{c_0}\sum_{w\neq w'} \Delta E_{w'}^{2} \left(R_{w'w}P_w + R_{ww'}P_{w'}\right)$)

# General properties of $\Theta$

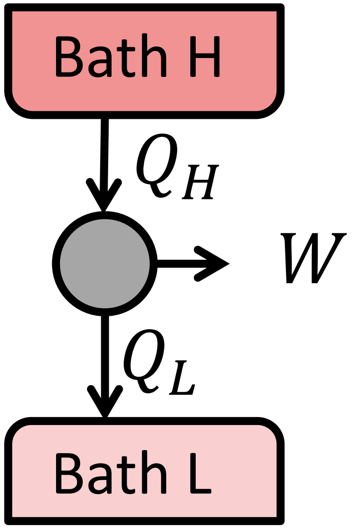
- Both $\Theta^{(1)}$ and $\Theta^{(2)}$ are proportional to system size
$\rightarrow$ The inequality $|J| \leq \sqrt{\Theta\dot{\sigma}}$ is **meaningful bound even in macroscopic case** ( $J, \dot{\sigma} \propto V$ ).

- $\Theta^{(2)} = \langle \frac{\gamma |p|^2}{\beta m^2} \rangle$ for underdamped Langevin systems.

- In linear regime, $\Theta^{(2)} = \kappa$ (thermal conductivity) and equality holds ($|J| = \sqrt{\Theta\dot{\sigma}}$).

# Derivation of power-efficiency trade-off

<u>Cyclic process with two baths</u>




Thermodynamics leads to

$$\Delta S = -\beta_H Q_H + \beta_L Q_L$$

$$\eta(\eta_C - \eta) = \frac{W}{Q_H} \frac{\beta_L Q_L - \beta_H Q_H}{\beta_L Q_H}$$

$$= \frac{W \Delta S}{\beta_L Q_H^2}$$

# Time integration of inequality

General inequality $\sum_\nu |J_\nu| \leq \sqrt{\Theta\sigma}$

By integrating with time, and using Schwarz inequality

$$\left(\int_0^\tau dt \sum_\nu |J_\nu|\right)^2 \leq \left(\int_0^\tau dt\sqrt{\Theta\sigma}\right)^2$$

$$\leq \left(\int_0^\tau dt\Theta\right)\left(\int_0^\tau dt\sigma\right) = \tau\overline{\Theta}\Delta S$$

$$\left(\overline{\Theta} := \frac{1}{\tau}\int_0^\tau dt\Theta\right)$$

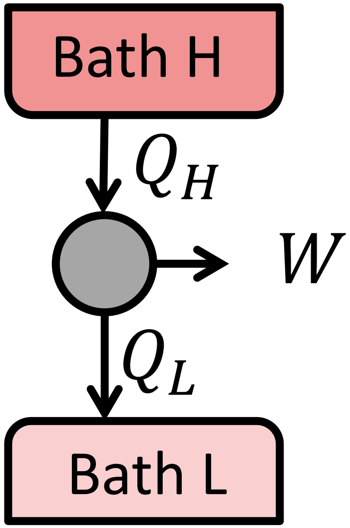
$Q_H = \int dt J_H$ etc. leads to $\boldsymbol{(Q_H + Q_L)^2 \leq \tau\overline{\Theta}\Delta S}$

# Derivation of power-efficiency trade-off

$$\eta(\eta_C - \eta) = \frac{W \Delta S}{\beta_L Q_H^2}$$

$$\geq \frac{W}{\beta_L Q_H^2} \frac{(Q_H + Q_L)^2}{\tau \bar{\Theta}}$$

$$\geq \frac{W}{\beta_L} \frac{1}{\tau \bar{\Theta}}$$

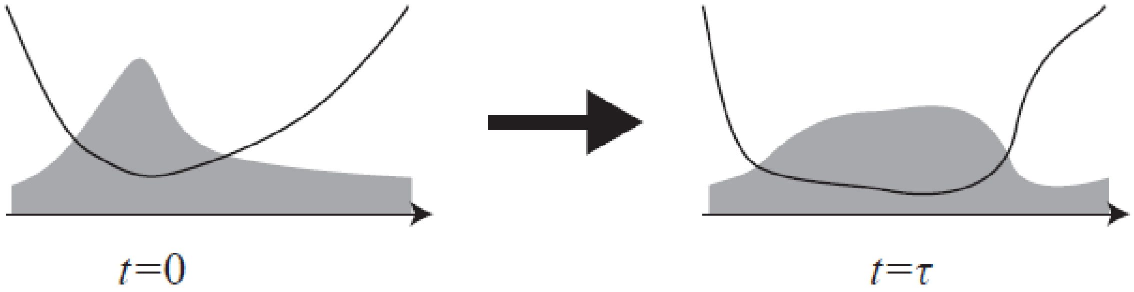



$$\boxed{\frac{\boldsymbol{W}}{\boldsymbol{\tau}} \leq \bar{\boldsymbol{\Theta}} \boldsymbol{\beta}_L \boldsymbol{\eta}(\boldsymbol{\eta}_C - \boldsymbol{\eta})}$$

# Related result: classical speed limit

Problem setting (speed limit):
Given initial and final distributions $p$ and $p'$.
We want to transform $p$ to $p'$ quickly.

**What is the cost of quick state transformation?**



# Classical speed limit inequality

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

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

$\sigma$ : total entropy production

$\langle A\rangle$: averaged dynamical activity $\frac{1}{\tau}\int_0^\tau dt A(t)$

(N. Shiraishi, K. Funo, and K. Saito, Phys. Rev. Lett. 121, 070601 (2018))

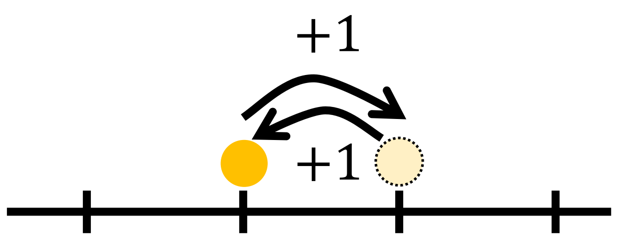
# What is dynamical activity?

Dynamical activity: How frequently jumps occur.

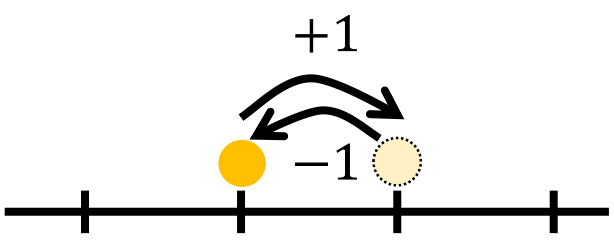
$$A(t) := \sum_{w,w'} R_{w'w} p_w(t)$$

Activity characterizes **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 our inequality

Length between initial and final states

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

Entropy production: **Cost of quick state transformation**

Time-scale of dynamics

# Derivation (instantaneous quantities)

$$\sum_{w} \left| \frac{d}{dt} p_w \right|$$

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

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

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

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

# Derivation (time integration)

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

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

This is the desired result!

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

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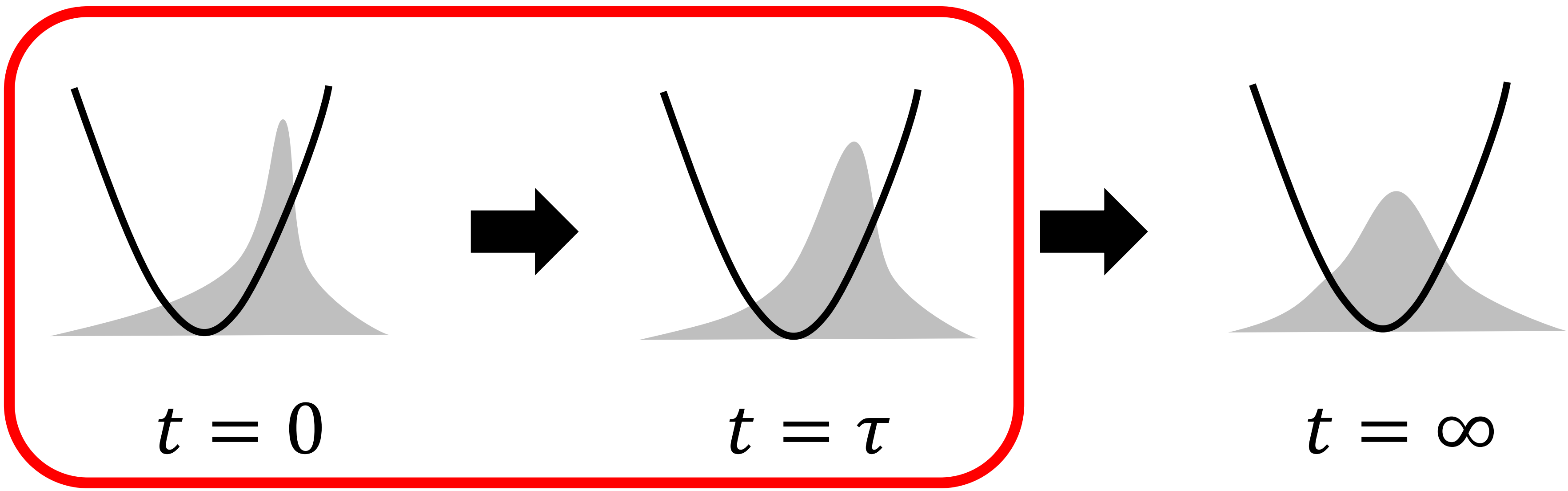
Finite-speed processes

**Relaxation processes**

# Problem: entropy production in thermal relaxation process

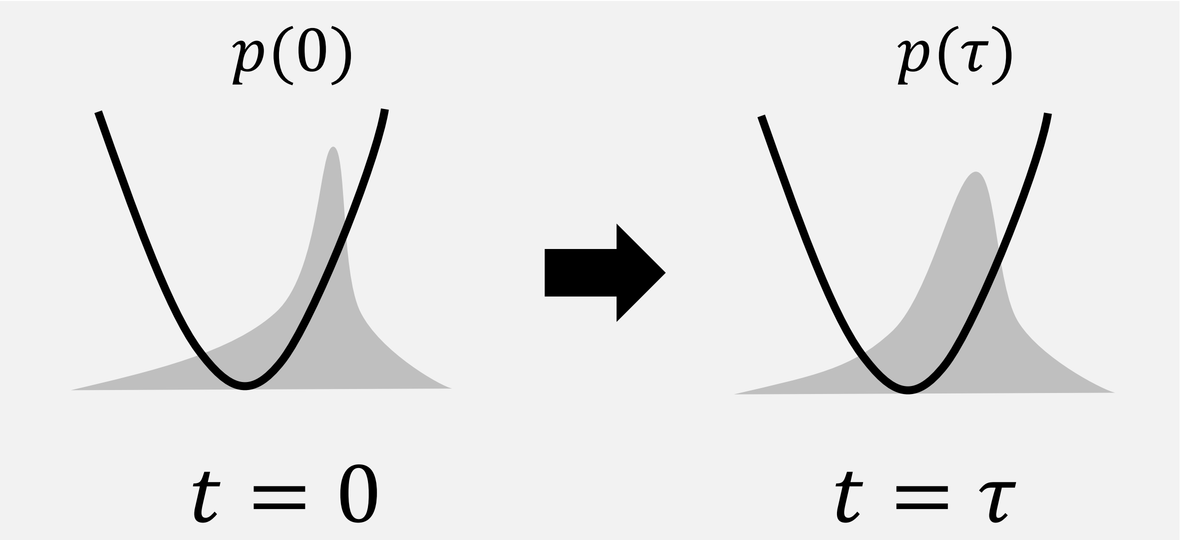
<u>Situation</u>：relaxation process with a single heat bath in continuous time. Suppose detailed balance.




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

# Main resut

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




Entropy production is bounded by the distance between the initial and final distributions!

# Significance

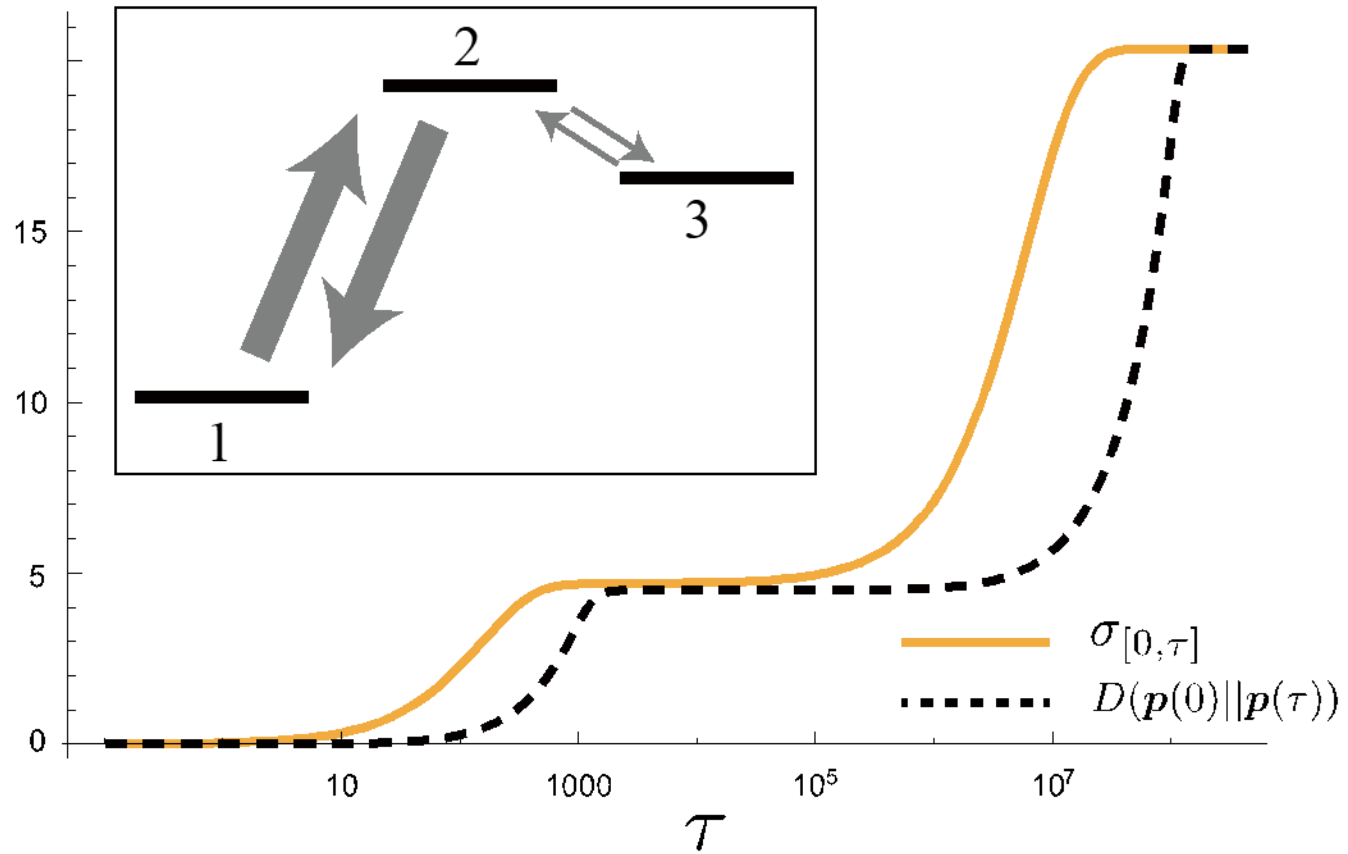
$$\boxed{\boldsymbol{\sigma}_{[\mathbf{0},\boldsymbol{\tau}]} \geq \boldsymbol{D}(\boldsymbol{p}(\mathbf{0})||\boldsymbol{p}(\boldsymbol{\tau}))}$$

- 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

Setup：three-state model

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

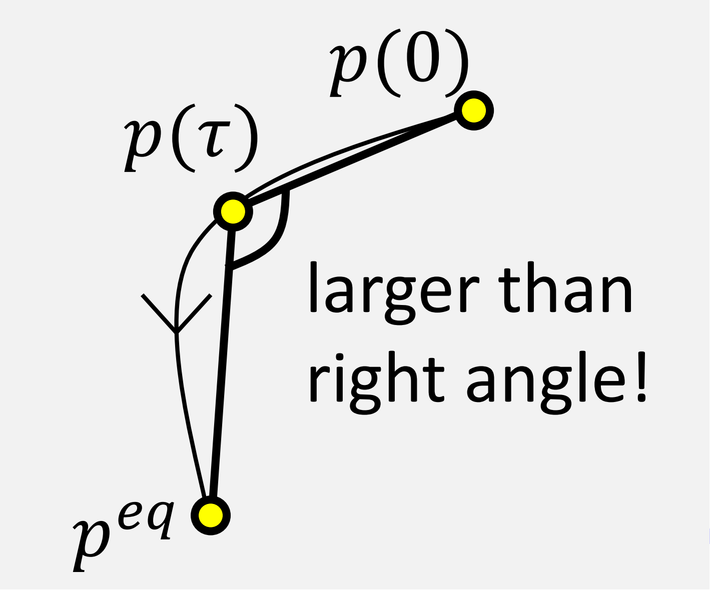


# Geometric visualization

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

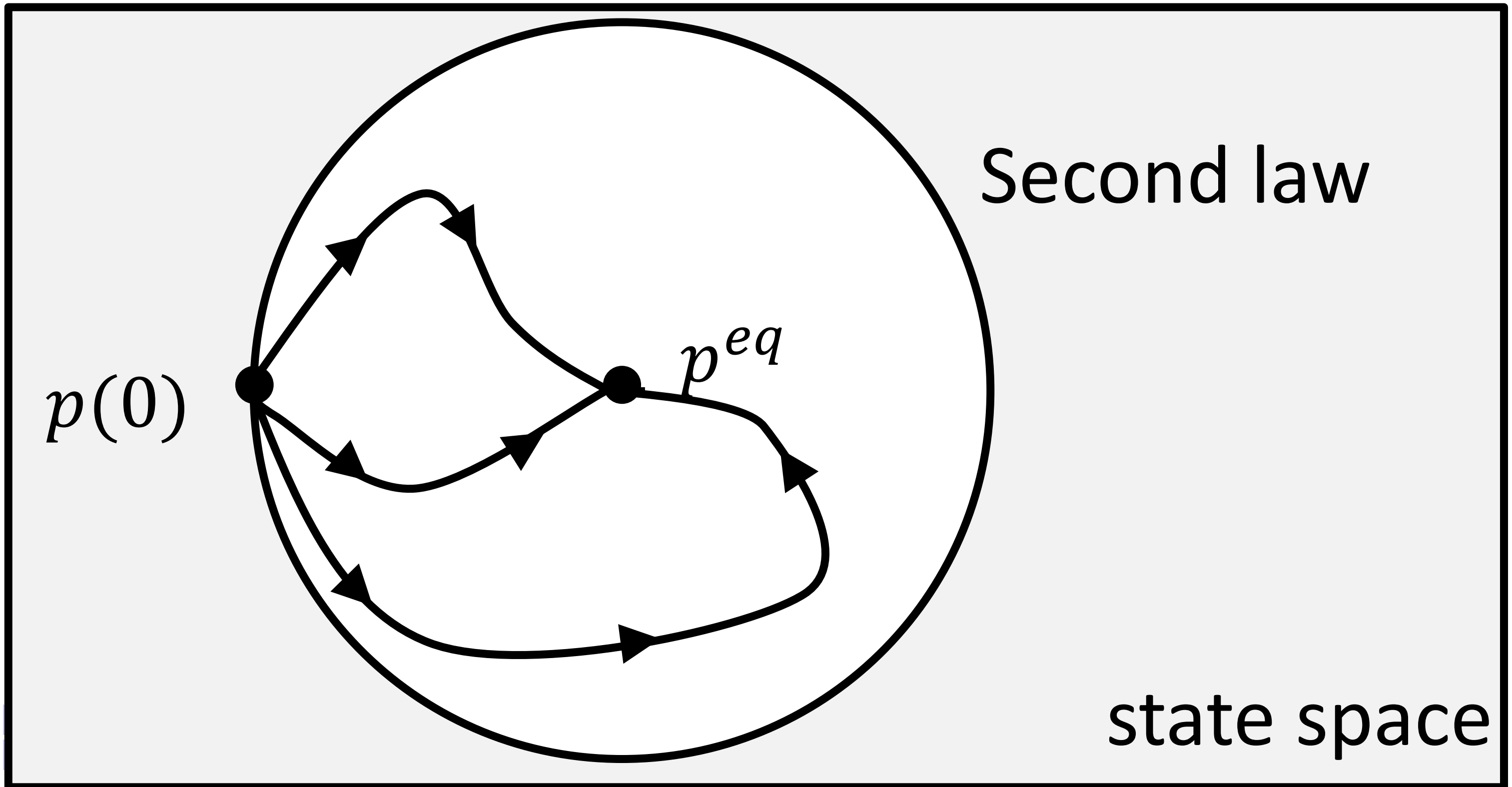
$$\boldsymbol{D(p(0)||p^{eq}) \geq D\big(p(0)\big|\big|p(\tau)\big) + D(p(\tau)||p^{eq})}$$

<u>Remark</u>:
KL-divergence $\leftrightarrow$ square of distance



# Restriction on possible trajectory

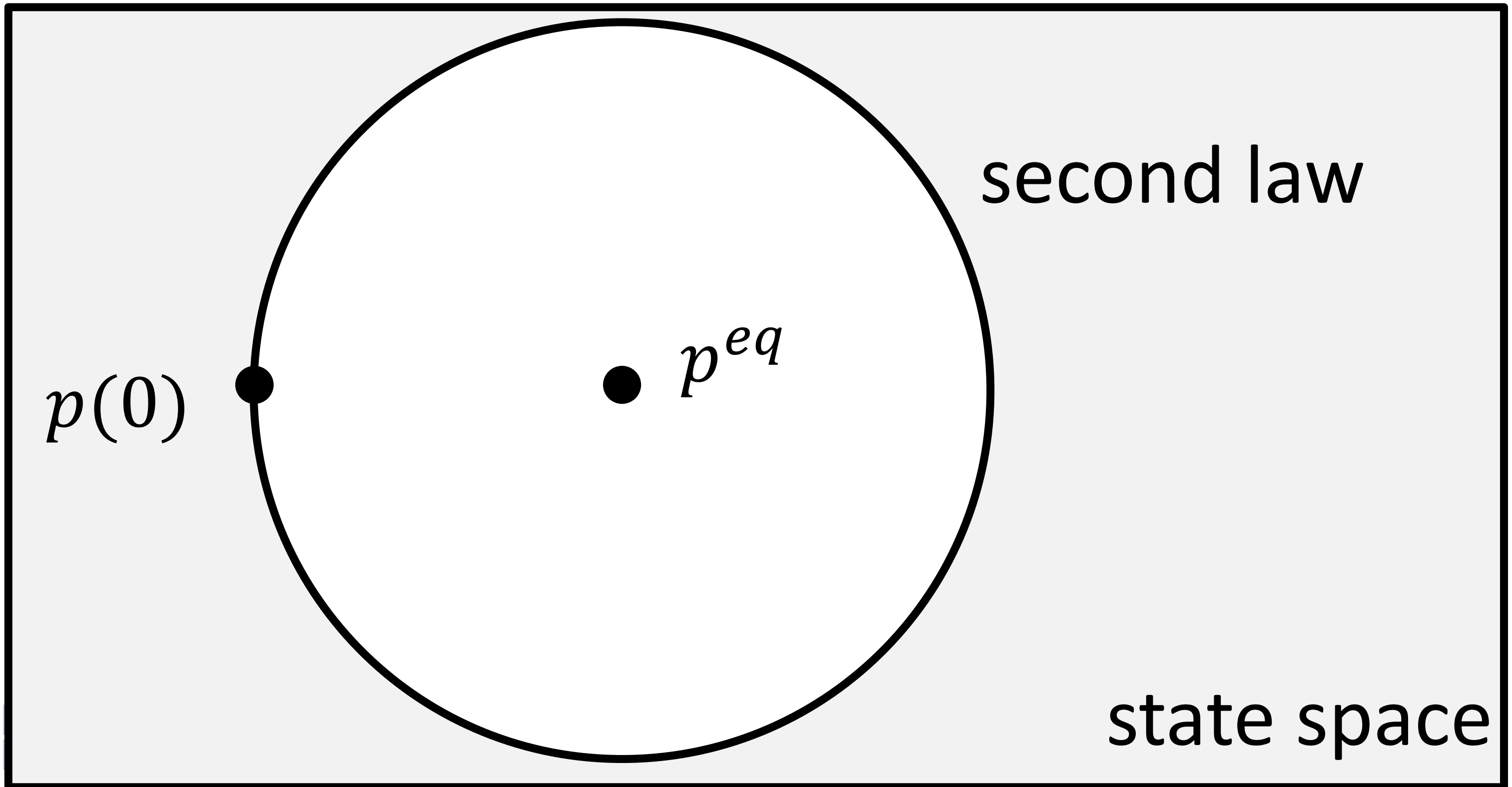
Given both initial and equilibrium distribution.
What is possible pass of relaxation processes?



# Restriction on possible trajectory

Obtained relation

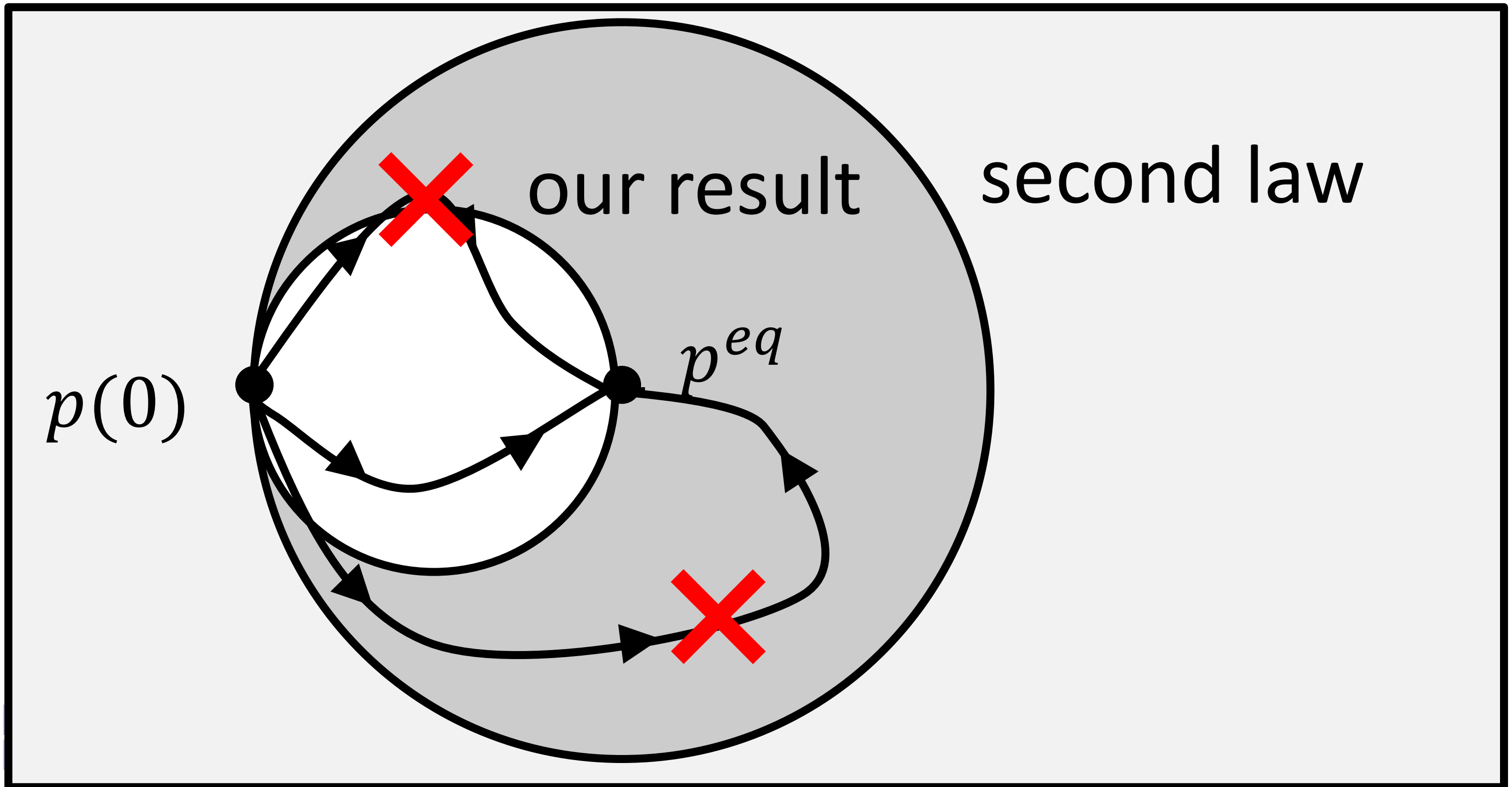
$$D(p(0)||p^{eq}) \geq D(p(0)\|p(\tau)) + D(p(\tau)||p^{eq})$$



# Restriction on possible trajectory

Obtained relation

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



# Key relation: variational expression of entropy production rate

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

Because right-hand side equals

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

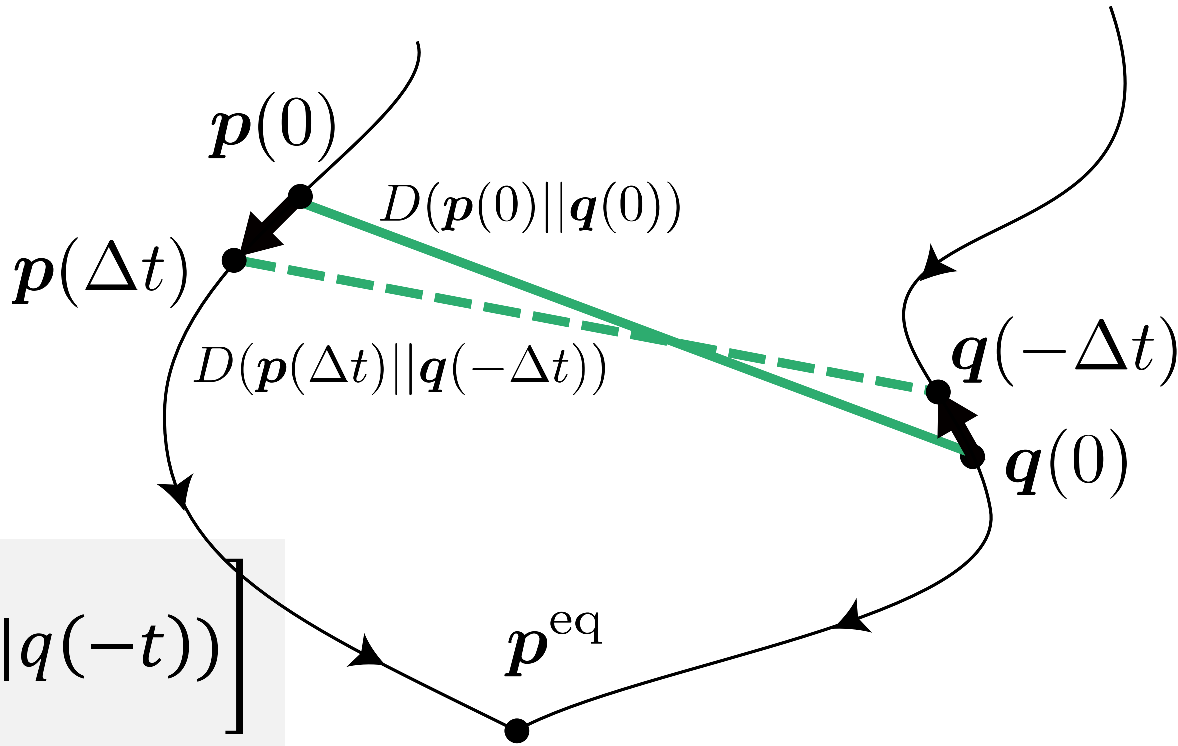
# Key relation: variational expression of entropy production rate

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

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

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

# Schematic of variational expression




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

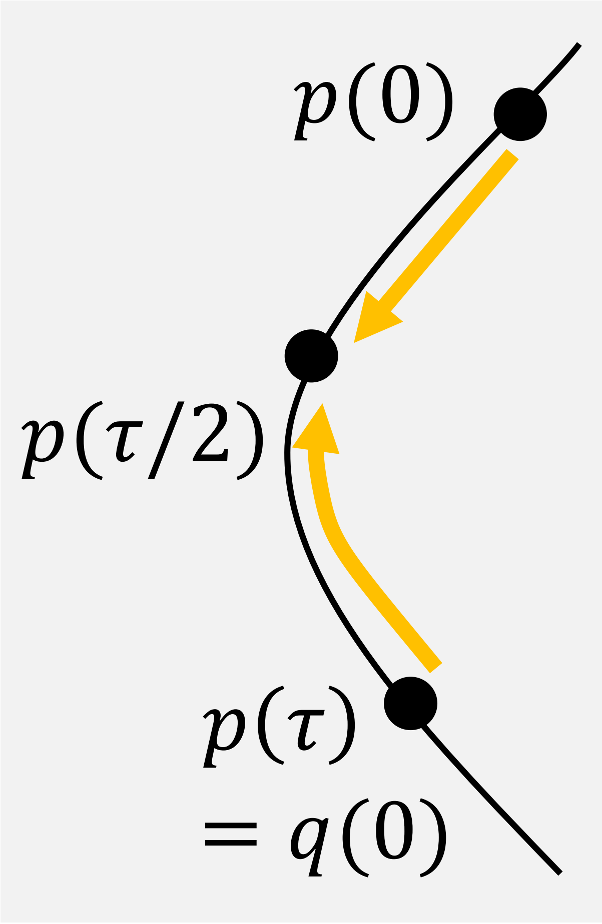
Green lines：KL divergence $D(p||q)$

Difference of solid line from 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

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

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

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

# Proof of variational expression

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

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

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

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

# Proof of variational expression

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

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

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

$$=\sum_{i\neq j}R_{ij}p_j\ln\left(\frac{R_{ij}q_j}{R_{ji}q_i}\right)+\sum_{i\neq j}R_{ij}p_j\frac{R_{ji}q_i}{R_{ij}q_j}-\sum_{i\neq j}R_{ij}p_j$$

$$=\sum_{i\neq j}R_{ij}p_j\left[\frac{R_{ji}q_i}{R_{ij}q_j}-1-\ln\left(\frac{R_{ji}q_i}{R_{ij}q_j}\right)\right]$$

$\geq 0.$ （We used $x-1-\ln x\geq 0$）

# Summary

- Trade-off relation between power (speed) and efficiency (entropy production):

$$|J| \le \sqrt{\Theta\dot{\sigma}}$$

$$\frac{W}{\tau} \le \bar{\Theta}\beta_L \eta(\eta_C - \eta)$$

- Bound on entropy production in relaxation process:

$$\sigma \ge D(p(0)||p(\tau))$$

END

# Bound for non-Markovian engine

$$\boldsymbol{\eta \leq \eta_C - \frac{(Q_L)^2}{8\beta_L Q_H j_{max}\left(\frac{2\mathrm{v}\tau}{\mu} + \mathrm{C}\right)^D}}$$

$\tau$ : time-interval of a cycle
$v, \mu, C$ : constants came from Lieb-Robinson bound
$j_{max}$ : maximum Fisher information per unit volume
$D$ : spatial dimension

- The slower process (large $\tau$) have better efficiency.
- The larger $Q_L$ implies worse efficiency.

# Second law (reviewal)

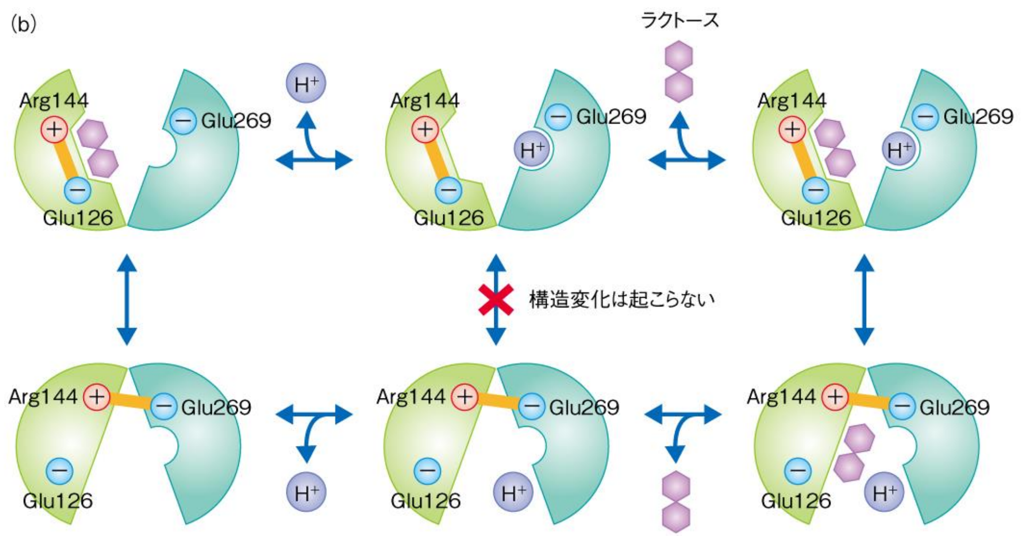
Integration of entropy production rate is entropy production (entropy increase)

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

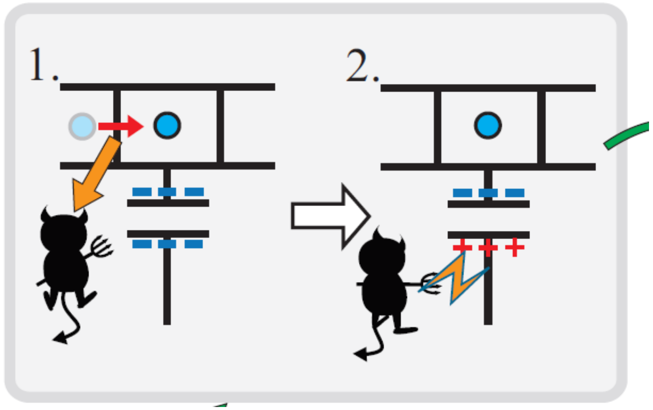
$\dot{\sigma} \geq 0$ implies $\sigma \geq 0$.

(Both inequalities are called the second law)

# Schematics (example)




(http://leading.lifesciencedb.jp/2-e009)

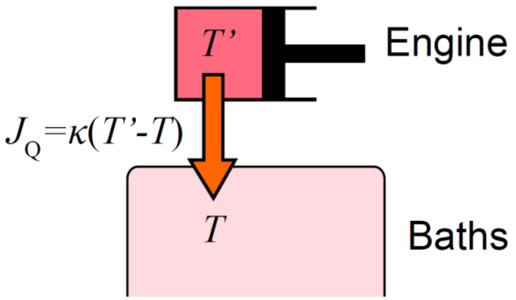



(https://phys.org/news/2016-01-maxwell-demon-self-contained-information-powered-refrigerator.html)

State space is discrete and finite.
(for continuous systems, we take proper discretization and continuum limit)

# Previous studies on power and efficiency

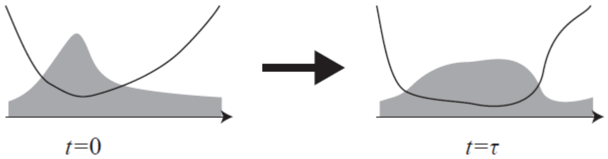
## Endoreversible thermodynamics




F. L. Curzon and B. Ahlborn, Am. J. Phys. 43, 22 (1975).
P. Salamon and R. S. Berry, PRL 51, 1127 (1983).
B. Anderson, et.al., Acc. Chem. Res. 17, 266 (1984).
M. Esposito, et.al., PRL 105, 150603 (2010).

## Overdamped Langevin system

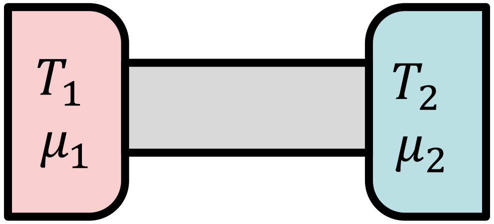
K. Sekimoto and S.-i. Sasa, J. Phys. Soc. Jpn. 66, 3326 (1997).
E. Aurell, et.al., J. Stat. Phys. 147, 487 (2012).




**Problems in these results**

- Model specific.
- Most cases are in linear response regime.

# Linear irreversible thermodynamics




<u>Ex) Thermoelectric transport</u>

$J_i$: heat flux $F_i$:temperature difference

$J_j$: particle flux $F_j$: chemical potential difference

Using Onsager matrix $L$,

$$J_i = L_{ii}F_i + L_{ij}F_j$$
$$J_j = L_{ji}F_j + L_{jj}F_j$$

$\dot{S} = J_iF_i + J_jF_j \geq 0$ (second law)

$$\rightarrow L_{ii} \geq 0, L_{jj} \geq 0, 4L_{ii}L_{jj} - \left(L_{ij} + L_{ji}\right)^2 \geq 0$$

# Difference between with and without time-reversal symmetry

$$\dot{S} = \frac{1}{L_{ii}}\left(J_i + \frac{L_{ji} - L_{ij}}{2} X_j\right)^2 + \frac{4L_{ii}L_{jj} - \left(L_{ij} + L_{ji}\right)^2}{4L_{ii}} X_j^2$$
$$\geq \frac{1}{L_{ii}}\left(J_i + \frac{L_{ji} - L_{ij}}{2} X_j\right)^2$$

Carnot efficiency⇔$\dot{S} = 0$

$L_{ij} = L_{ji}$ (Time-reversal symmetry) $\dot{S} = 0 \rightarrow J_i = 0$

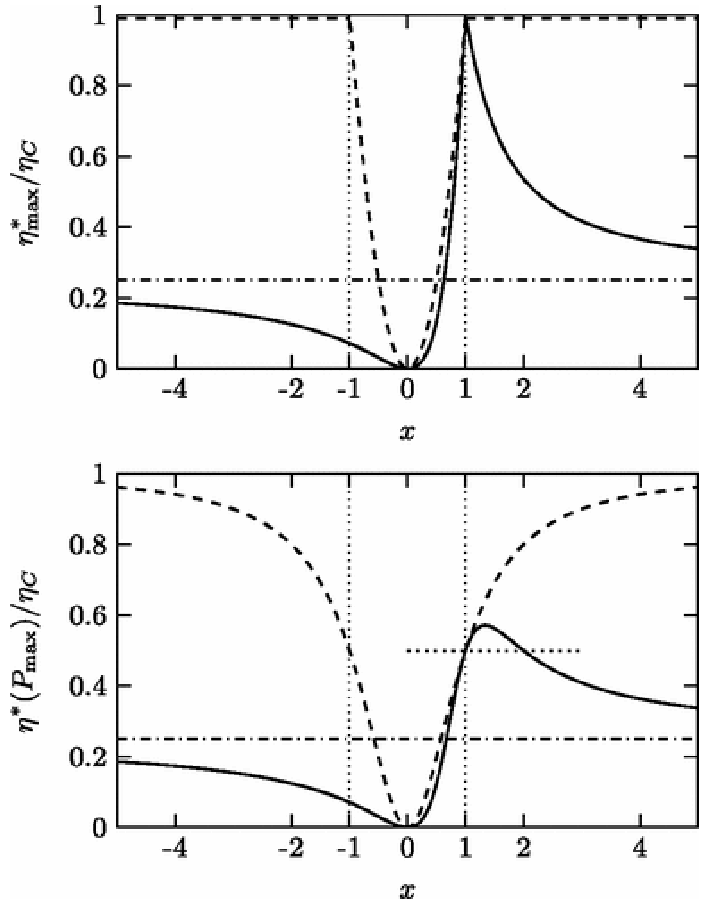
$L_{ij} \neq L_{ji}$ (broken TRS) With proper $X_j$, $\dot{S} = 0$ formally allow $\boldsymbol{J_i \neq 0}$ (**Finite power is not excluded**)

(G. Benenti, K. Saito, and G. Casati, PRL 106, 230602 (2011))

# Constraint in mesoscopic transport

Unitarity of scattering matrix says

$$L_{ii}L_{jj} + L_{ij}L_{ji} - L_{ij}^2 - L_{ji}^2 \geq 0$$

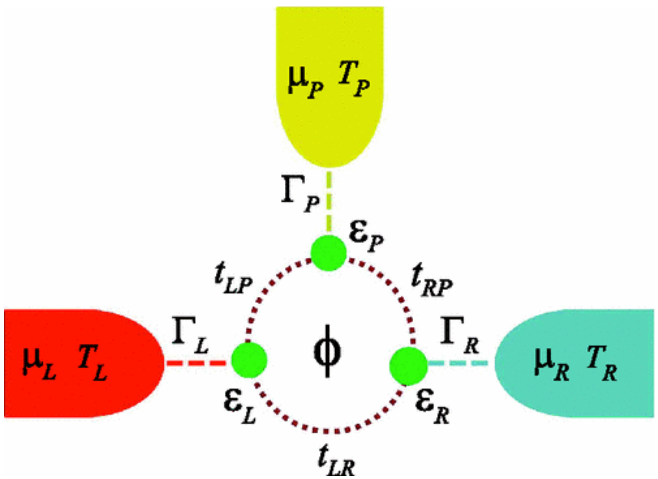


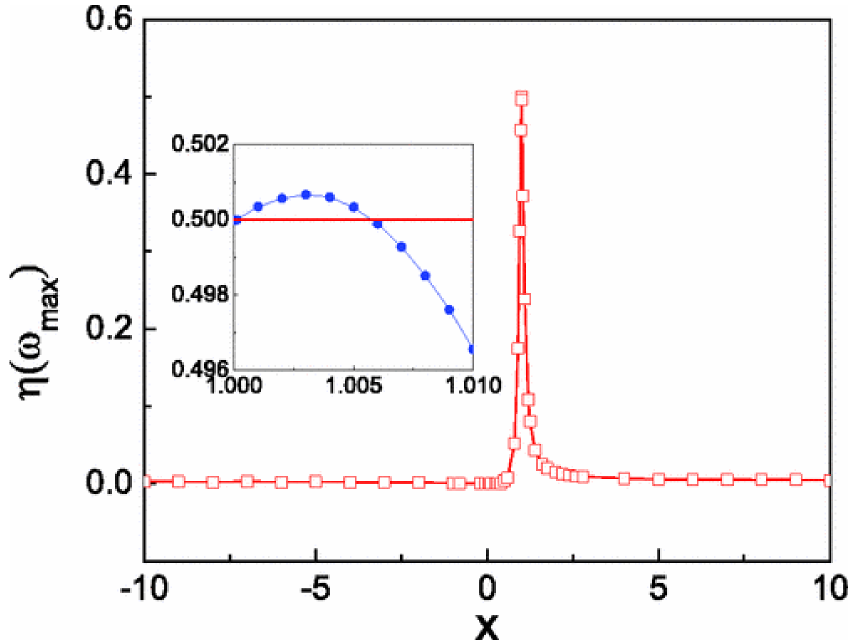

Carnot efficiency is achievable only when $x = 1$ (no magnetic field)

Efficiency at maximum power may be larger than 1/2

K. Brandner, K. Saito, and U. Seifert, PRL 110, 070603 (2013).
V. Balachandran, G. Beneti, and G. Casati, PRB 87, 165419 (2013).

# EMP is indeed larger than 1/2

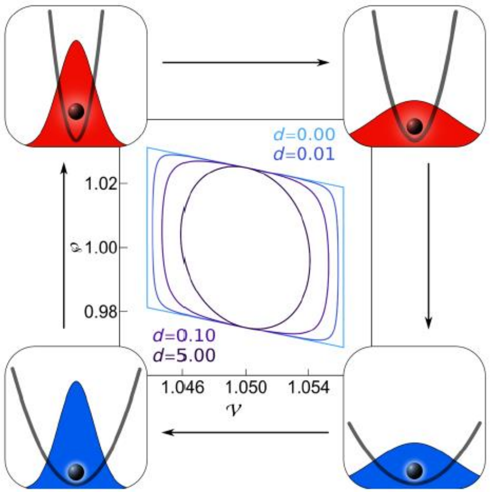



Direct numerical calculation of AB effect.

V. Balachandran, G. Beneti, and G. Casati, PRB 87, 165419 (2013).

# Onsager matrix in cyclic process



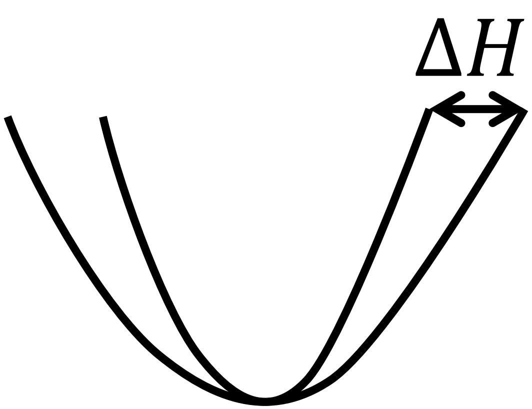

$J_q$ : heat from hot bath/time

$J_w$ : extracted work/time

$F_q := \beta_c - \beta_H$

$F_w := \Delta H / T_C$

$$\dot{S} = J_Q F_Q + J_w F_w$$




We define Onsager matrix by using them.

K. Brandner, K. Saito, and U. Seifert, PRX 5, 031019 (2015).

# Inequality for relative entropy

$$
\begin{aligned}
D(p_x||q_x) &= \sum_x p_x \ln \frac{p_x}{q_x} + q_x - p_x \\
&\geq \sum_x \frac{c_0(p_x - q_x)^2}{p_x + q_x} \qquad \left(c_0 = \frac{8}{9}\right)
\end{aligned}
$$

We used a relation: $a \ln \frac{a}{b} + b - a \geq \frac{c_0(a-b)^2}{a+b}$,

which is equivalent to $y \ln y + 1 - y \geq \frac{c_0(y-1)^2}{y+1}$.

# $J$ and $\sigma$ with detailed balance

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

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

$$\geq \frac{1}{2} \sum_{w \neq w'} \frac{2(R_{w'w} P_w - R_{ww'} P_{w'})^2}{R_{w'w} P_w + R_{ww'} P_{w'}}$$

(cf: $\sigma \geq \sum_{w \neq w'} \frac{c_0 \left(R_{w'w} P_w - \tilde{R}_{ww'} P_{w'}\right)^2}{R_{w'w} P_w + \tilde{R}_{ww'} P_{w'}}$)

# Case with detailed balance

Detailed balance

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

Remark: we do NOT take time reversal of $w$.

This is different from

$$\frac{R_{ww'}}{R^{\dagger}{}_{w'^*w^*}} = e^{-\beta(E_w - E_{w'})}$$

# Case of nonlinear Langevin equation

$$L^{1,1} := \frac{\gamma(v)}{m}\left\{\frac{\partial}{\partial v}\cdot v + \frac{1}{\beta m}\frac{\partial^2}{\partial v^2}\right\}$$

Desired relation is only $\boldsymbol{R^{1,1}_{v'v} = R^{1,1}_{-v'-v}}$ (detailed-balance: DB)

- If $\gamma(v) = \gamma(-v)$, DB is satisfied.
- For one-dimensional systems, DB is satisfied.
- For two or more dimensional systems, if rotation does not change energy, we can apply the above discussion to radial direction.

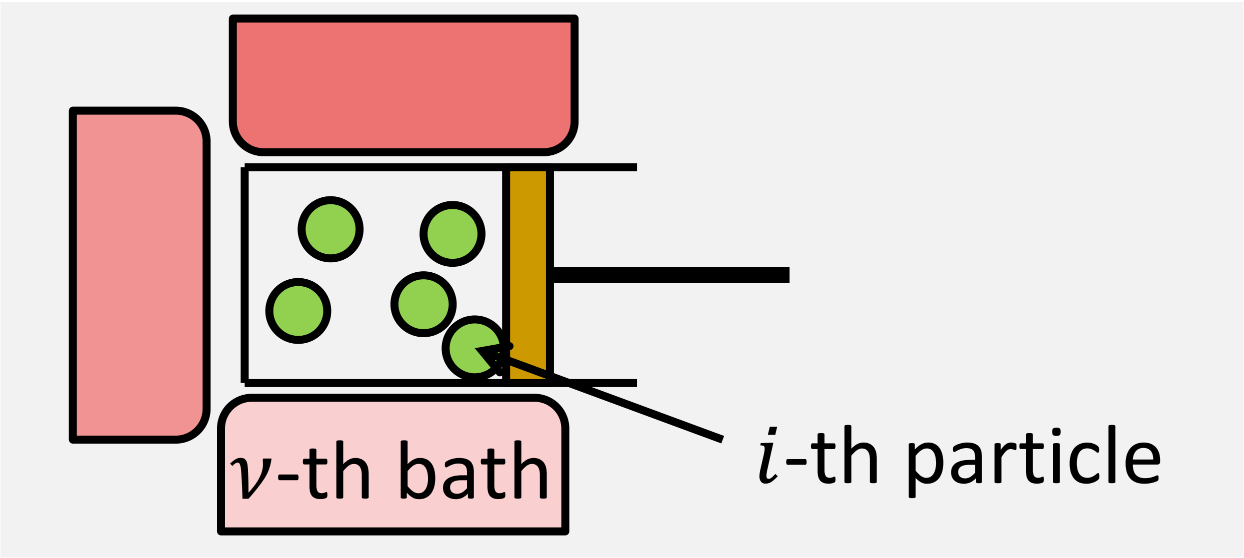
# Application to many-body and multi-bath systems with Hamilton dynamics

Total transition rate is decomposed into

$$R_{ww'} = \underbrace{R^0_{ww'}}_{\text{Hamiltonian dynamics}} + \sum_{\nu} \sum_{i} R^{\nu,i}_{ww'}$$

label of bath

label of particle



# Hamilton and stochastic parts in underdamped Langevin system

$$\frac{d}{dt}P_{x,v} = LP_{x,v}$$

$$L \coloneqq -v\frac{\partial}{\partial x} + \frac{\partial}{\partial v}\cdot\left(\gamma v + \frac{1}{m}\frac{dU}{dx} + B\times v\right) + \frac{\gamma}{\beta m}\frac{\partial^2}{\partial v^2}$$

$$\Downarrow$$

$$L^0 \coloneqq -v\frac{\partial}{\partial x} + \frac{\partial}{\partial v}\cdot\left(\frac{1}{m}\frac{dU}{dx} + B\times v\right)$$

$$L^{1,1} \coloneqq \frac{\gamma}{m}\left\{\frac{\partial}{\partial v}\cdot v + \frac{1}{\beta m}\frac{\partial^2}{\partial v^2}\right\}$$

# Properties of $R^0$ $(L^0)$ and $R^{\nu,i}$ $(L^{1,1})$

$$L^0 := -v\frac{\partial}{\partial x} + \frac{\partial}{\partial v}\cdot\left(\frac{1}{m}\frac{dU}{dx} + B\times v\right)$$

- Effects of magnetic field, many-body interactions, inertia is taken in $R^0$ $(L^0)$.
- **$R^0$ $(L^0)$ conserves both energy and entropy.**

→ **$R^0$ $(L^0)$ is irrelevant to $J$ and $\sigma$!**

$$L^{1,1} := \frac{\gamma}{m}\left\{\frac{\partial}{\partial v}\cdot v + \frac{1}{\beta m}\frac{\partial^2}{\partial v^2}\right\}$$

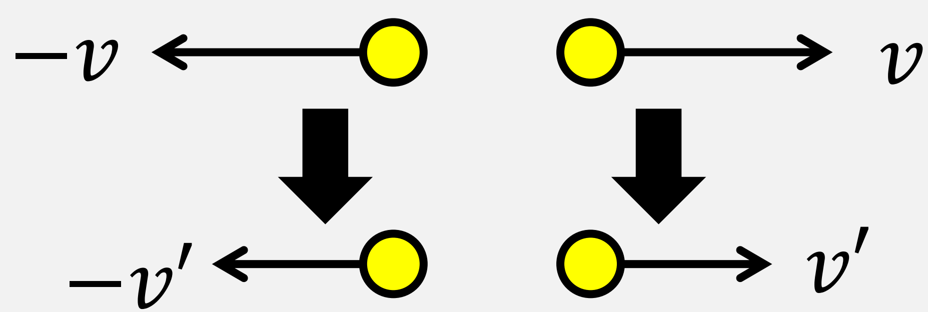
- $R^{\nu,i}$ $(L^{1,1})$ acts only on velocity $v$, not position $x$.

# Properties of $R^{\nu,i}$ ($L^{1,1}$) in linear Langevin systems

$$L^{1,1} := \frac{\gamma}{m}\left\{\frac{\partial}{\partial v}\cdot v + \frac{1}{\beta m}\frac{\partial^2}{\partial v^2}\right\}$$

For linear Langevin systems, corresponding transition rate $R^{1,1}_{v'v}$ satisfies $\boldsymbol{R^{1,1}_{v'v} = R^{1,1}_{-v',-v}}$, which implies **detailed balance**.

This reflect spatial symmetry of noise!

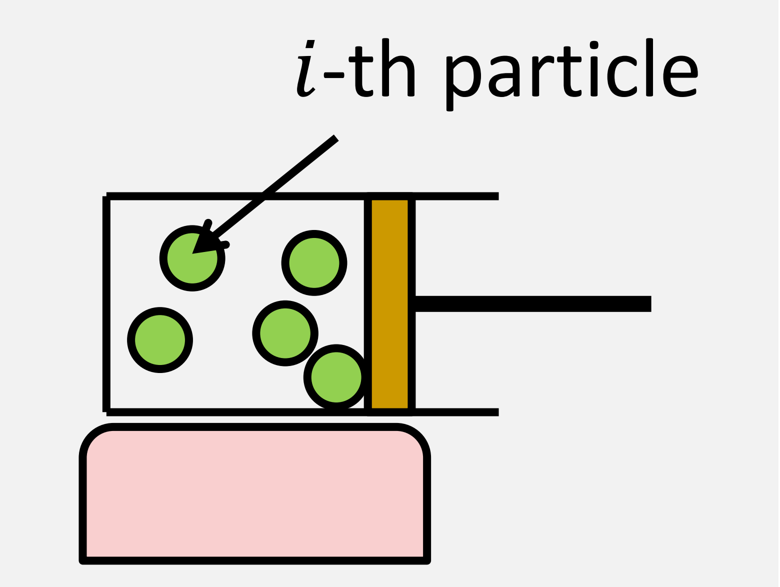


# $\Theta$ in multi-particle case and thermodynamic limit

$$|J| = \sum_i |J_i| \leq \sum_i \sqrt{\Theta_i \sigma_i}$$

$$\leq \sqrt{\left(\sum_i \Theta_i\right)\left(\sum_i \sigma_i\right)}$$

$$= \sqrt{\Theta \sigma}$$




All of $J, \sigma, \Theta := \sum_i \Theta_i$ are proportional to volume $V$

$\rightarrow |J| \leq \sqrt{\Theta\sigma}$ **is meaningful even in $V \rightarrow \infty$.**

# Upper bound of $\Theta^{(1)}$

By putting $|R_{ww}| \leq R_{max}$, we have

$$\Theta^{(1)} \leq \frac{1}{c_0}\left(\frac{d}{dt}\langle \Delta E^2 \rangle + 2R_{max}\langle \Delta E^2 \rangle\right)$$

# Discretization of transition rate

We set

$$P_{p\to p\pm\epsilon} := \frac{\gamma}{\beta\epsilon^2} e^{-\frac{\beta}{4m}\left((p\pm\epsilon)^2-p^2\right)}.$$

Then, in $\epsilon\to 0$ limit, master equation becomes

$$\frac{d}{dt}P(p) = \frac{\partial}{\partial t}\left(\frac{\gamma p}{m}P(p)\right) + \frac{\gamma}{\beta}\frac{\partial^2}{\partial p^2}P(p)$$

which is Kramers equation.

# Discretization of transition rate

We set

$$P_{(x,p)\to(x,p+\epsilon)} := \frac{1}{\epsilon} F(x,p)$$

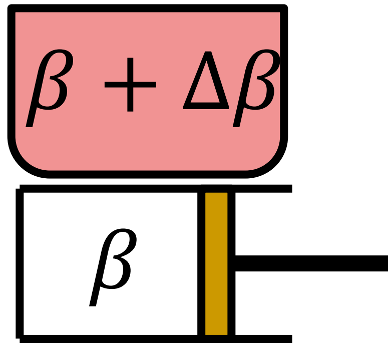
$$P_{(x,p)\to(x+\epsilon\prime,p)} := \frac{1}{\epsilon'}\frac{p}{m}$$

Then, in $\epsilon, \epsilon' \to 0$ limit, master equation becomes

$$\frac{d}{dt}P(x,p) = -\frac{p}{m}\frac{\partial}{\partial x}P(x,p) - \frac{\partial}{\partial p}\,F(x,p)P(x,p)$$

which is Liouville equation.

# The inequality is tight in linear regime




In $\Delta\beta \ll 1$, Fourier law tells

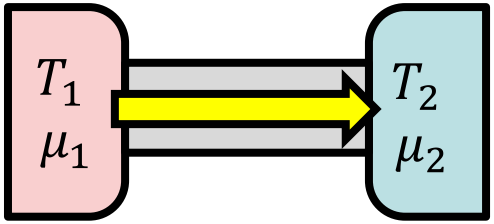
$$J = \kappa\Delta\beta \quad \Rightarrow \quad \sigma = \Delta\beta J = J^2/\kappa$$

($\kappa$ : thermal conductivity)

Fluctuation-dissipation like relation $\langle J^2 \rangle_{eq} = 2\kappa$ says $\boldsymbol{\Theta_2 = \kappa}$

Inequality $J^2 \leq \Theta_2 \sigma$ **always becomes equality in the linear regime.**

# Thermoelectricity




$T_1 > T_2, \mu_2 > \mu_1.$

Heat current $J_q$, particle current $J_n$ flow along $1 \to 2$

Efficiency is defined as $\eta_C = 1 - \frac{T_2}{T_1} \geq \eta := \frac{\Delta\mu J_n}{J_q - \mu_1 J_n}$

($\Delta\mu \coloneqq \mu_2 - \mu_1$   We assumed $J_q - \mu_1 J_n > 0$)

# Inequality for heat and particle currents

In a similar manner, we have

$$\mathbf{2}\boldsymbol{J}_{\boldsymbol{q}} \leq \sqrt{\boldsymbol{\Theta}_{\boldsymbol{q}}\boldsymbol{\sigma}}$$

$$\mathbf{2}\boldsymbol{J}_{\boldsymbol{n}} \leq \sqrt{\boldsymbol{\Theta}_{\boldsymbol{n}}\boldsymbol{\sigma}}$$

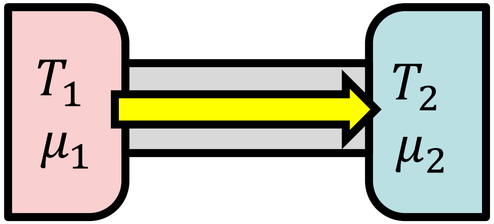
Here $\Theta_q$ takes $\Theta^1$ or $\Theta^2$, $\Theta_n$ is

$$\Theta_n := \frac{9}{8}\sum_{w\neq w'} \Delta N_{w'}^2 \left(R_{w'w}P_w + R_{ww'}P_{w'}\right)$$

# Power-efficiency trade-off in thermoelectricity

Using them, power and efficiency satisfy

$$\boldsymbol{\Delta\mu J_n \leq \frac{\Theta_q + (\mu_1)^2\Theta_n}{2}\beta_2\eta(\eta_C - \eta)}$$



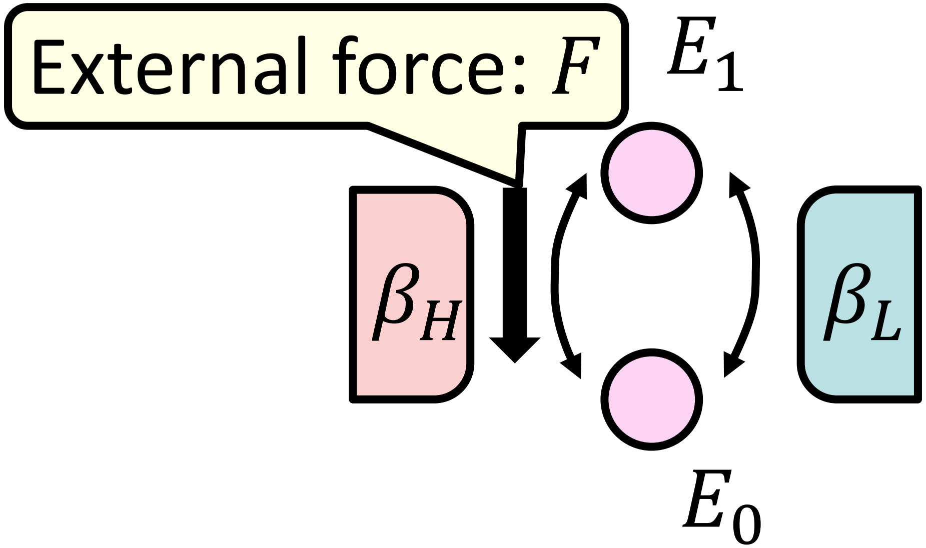
# Quantum case and non-Markovian case

- We can extend our result to quantum Markov process by considering microscopic origin of quantum Markov process.

- Trade-off inequality between speed and efficiency for quantum non-Markovian system is derived with completely different approach (employing **Lieb-Robinson bound** and **quantum information geometry**)

(N. Shiraishi and H. Tajima, PRE 96, 022138 (2017))

# “trivial” achievement of Carnot efficiency at finite power




$$R_{10}^{H} = ke^{-\frac{\beta_H(\Delta E+F)}{2}}$$

$$R_{01}^{H} = ke^{\frac{\beta_H(\Delta E+F)}{2}}$$

$$R_{10}^{L} = ke^{-\frac{\beta_L \Delta E}{2}}$$

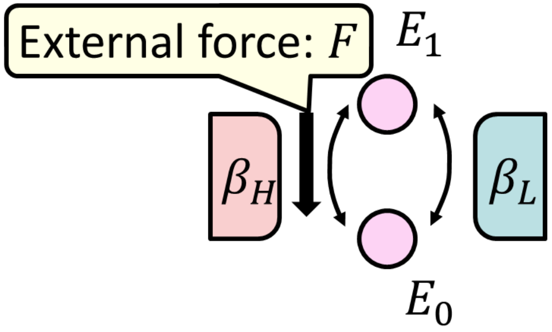
$$R_{01}^{L} = ke^{\frac{\beta_L \Delta E}{2}}$$

Taking $F \to \left(\frac{\beta_L}{\beta_H} - 1\right)\Delta \mathrm{E}$ and $k \to \infty$ **simultaneously**,

both $\eta = \eta_C$ and finite power are trivially achieved.

**But, this is physically meaningless!**

# What we indeed investigate in “finite power and Carnot efficiency”?




$$R_{10}^{H} = ke^{-\frac{\beta_H(\Delta E+F)}{2}}$$
$$R_{01}^{H} = ke^{\frac{\beta_H(\Delta E+F)}{2}}$$
$$R_{10}^{L} = ke^{-\frac{\beta_L \Delta E}{2}}$$
$$R_{01}^{L} = ke^{\frac{\beta_L \Delta E}{2}}$$

Taking $F \to \left(\frac{\beta_L}{\beta_H} - 1\right)\Delta\mathrm{E}$ and $k \to \infty$ **simultaneously**, both $\eta = \eta_C$ and finite power are trivially achieved.

Transition coefficient $k$ is **inherent time-scale** of system which cannot be changed externally.

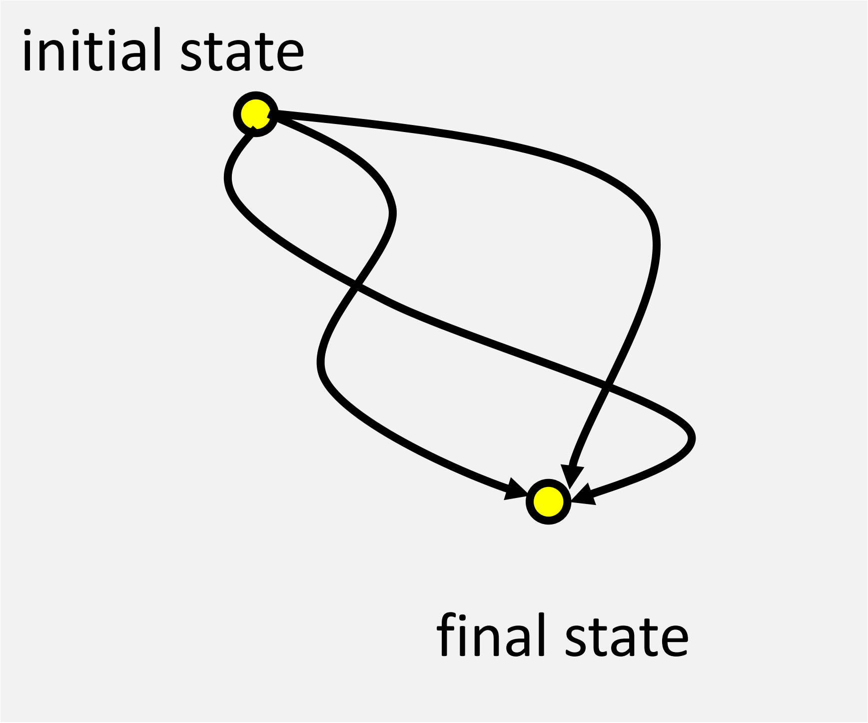
Our problem is whether finite power and CE coexist **with fixed time-scale parameter**.

# Speed limit: problem

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

**How quick can we transform this state?**

We can tune how to change the control parameters.



# Speed limit: known results

Quantum speed limit

Mandelstam-Tamm relation: $$\frac{\mathcal{L}(\rho_i, \rho_f)}{\Delta E / h} \leq \tau$$

(L. Mandelstam and I. Tamm, J. Phys. (USSR) 9, 249 (1945))

**Energy fluctuation** bounds the speed of operation.
(Background: uncertainty relation)

What about classical systems?

# Classical speed limits: some attempts

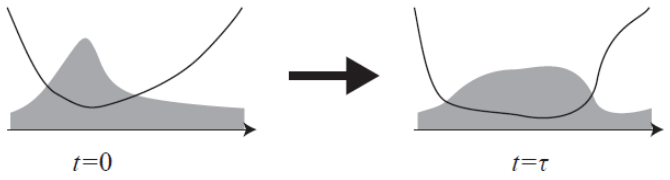
<u>Some formal extensions to classical Hamiltonian/stochastic systems</u>

S. Deffner, New J. Phys. 19, 103018 (2017), B. Shanahan, A. Chenu, N. Margolus, A. del Campo, Phys. Rev. Lett. 120, 070401 (2018), M. Okuyama and M. Ohzeki, Phys. Rev. Lett. 120, 070402 (2018), S. Ito, arXiv:1712.04311.

**Physical picture/meaning is highly unclear!**

<u>Overdamped Langevin systems</u>

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




**Physical picture is clear.**
**But system is very specific!**

# Setting and goal of this part

System: general Markov process on discrete states with detailed-balance condition.

Initial and final distributions ($p$ and $p'$) are given.

What we want to obtain is…

$$\frac{\mathcal{L}(p,p')^2}{\blacksquare \ \blacktriangle} \leq \tau$$

$\uparrow \ \uparrow$

established physical quantities

# Main result

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

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

$\Sigma$ : total entropy production

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

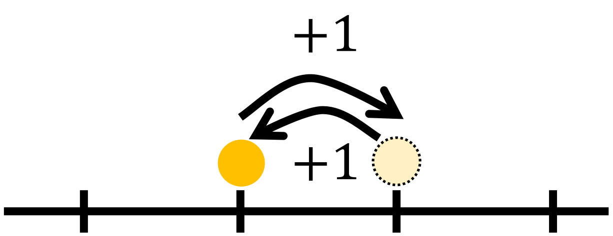
# What is dynamical activity?

Dynamical activity: How frequently jumps occur.

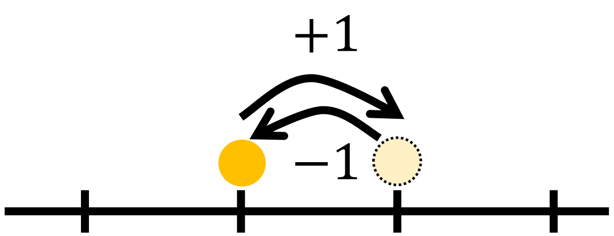
$$A(t) := \sum_{w,w'} R_{w'w} p_w(t)$$

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

<u>Activity</u>




<u>cf) Current</u>





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 our inequality

Length between initial and final states

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

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

Time-scale of dynamics (cf: Planck constant)

# Fro systems without detailed-balance condition

Case with detailed-balance condition

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

Case without detailed-balance condition

$$\frac{c_0\mathcal{L}(p,p')^2}{2\Sigma_{\mathrm{HS}}\langle A\rangle} \leq \tau$$

$\Sigma_{HS}$: Hatano-Sasa entropy production

(Heat $\beta Q_{w\to w'}$ is replaced by excess heat $\ln\frac{p_{w'}^{ss}}{p_{w}^{ss}}$)

(T. Hatano and S.-i. Sasa, Phys. Rev. Lett. **86**, 3463 (2001))

# Proof (technical part 1)

Normalization condition: $$\sum_{i(\neq j)} R_{ij} = -R_{jj}$$

$$\rightarrow \sum_{i(\neq j)} R_{ij} p_j \ln\left(\frac{q_j}{p_j^{\mathrm{eq}}}\right) = -R_{jj} p_j \ln\left(\frac{q_j}{p_j^{\mathrm{eq}}}\right) \quad \cdots \star$$

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

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

We used ☆

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

# Proof (technical part 2)

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

$$= \sum_{i\neq j} R_{ij}p_j \ln\left(\frac{R_{ij}q_j}{R_{ji}q_i}\right) + \sum_{i\neq j} R_{ij}p_j \frac{R_{ji}q_i}{R_{ij}q_j} - \sum_{i\neq j} R_{ij}p_j$$

We just exchange the dummy indexes i and j

normalization condition

# Corresponding fluctuation theorem

This relation (variational expression) is not derived from the conventional FT, but derived from a little modified FT:

$$\left\langle \exp\left[-\hat{\sigma}(\Gamma_{i\to j}) - \ln\frac{p_j(\Delta t)}{q_j(0)} + \ln\frac{p_i(0)}{q_i(\Delta t)}\right]\right\rangle = 1$$