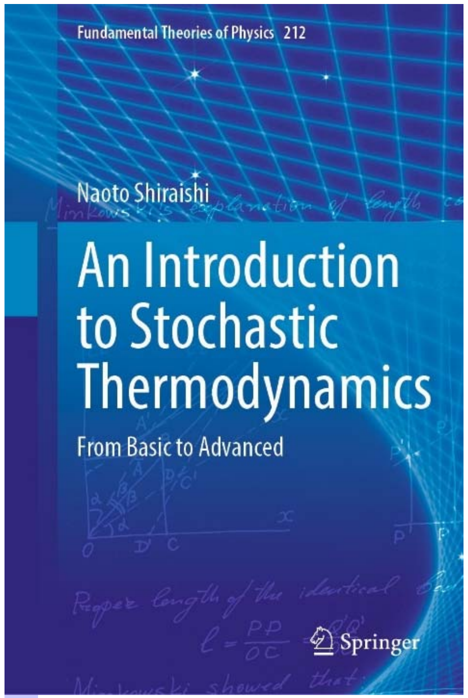
Fluctuation and response of time-symmetric current around nonequilibrium stationary states



Naoto Shiraishi (Univ. of Tokyo)

N. Shiraishi, Phys. Rev. Lett. 129, 020602 (2022)
N. Shiraishi, J. Stat. Mech. 033207 (2023)
N. Shiraishi, “An introduction to stochastic thermodynamics” Springer (2023)

Outline

Background and settings

Fluctuation-response relation of time-symmetric current for stall states

Fluctuation-response relation of time-symmetric current for general NESS

Another application of time-symmetric current

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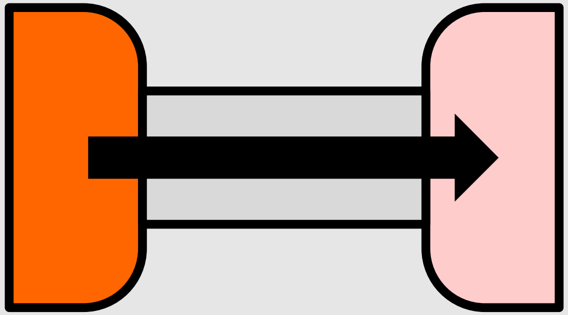
Fluctuation-response relation of time-symmetric current for stall states

Fluctuation-response relation of time-symmetric current for general NESS

Another application of time-symmetric current

Subject: Fluctuation and response

Ex) heat current between two baths with small temperature diff..



$h = \Delta\beta$ is small.

Fluctuation-response relation: Around eq. state,

$$\frac{1}{2}\langle \mathcal{J}^2 \rangle_0 = \left. \frac{\partial \langle \mathcal{J} \rangle_h}{\partial h} \right|_{h=0}$$

$\mathcal{J}$: Time-integrated current

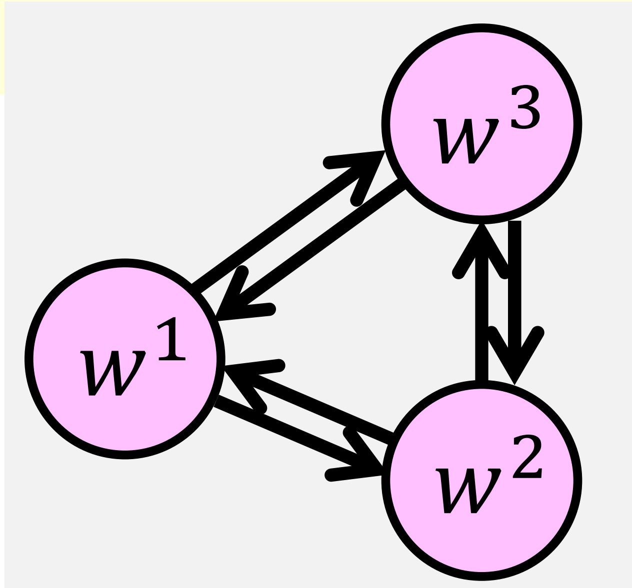
h : Conjugated external field

Stage: Stochastic thermodynamics

Time evolution of **probability distribution $\boldsymbol{p}$** is given by **master equation**.

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

transition matrix



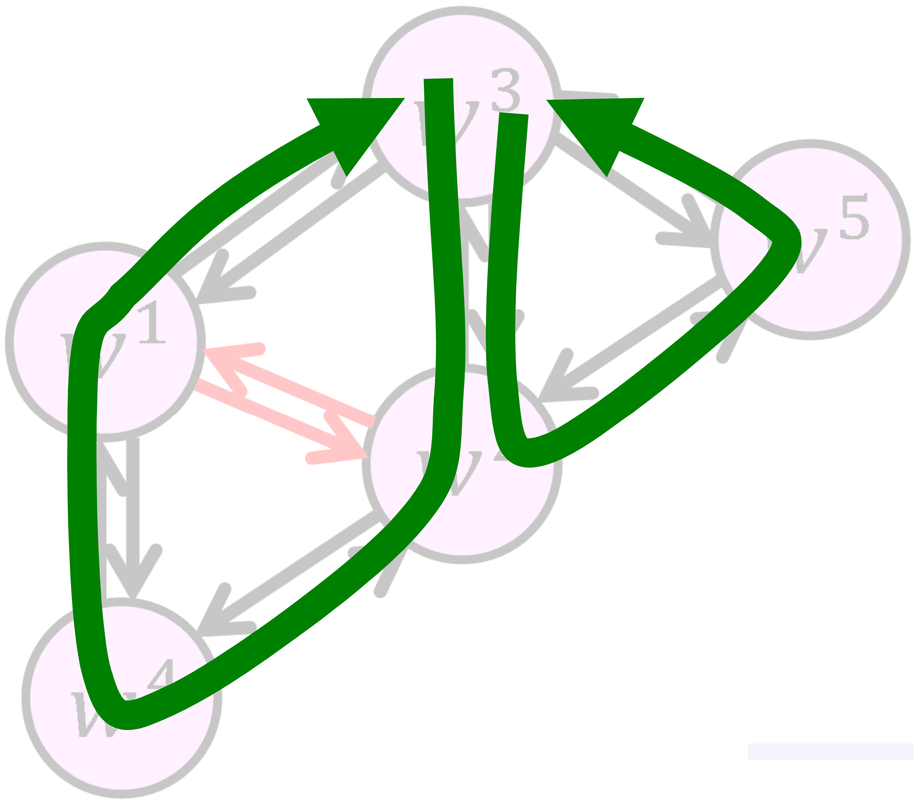
We assume the **local detailed-balance condition**.

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

Our interest: Stall state

A **stall state** is a nonequilibrium stationary state where the edge in interest (12 in the figure) has zero probability current.

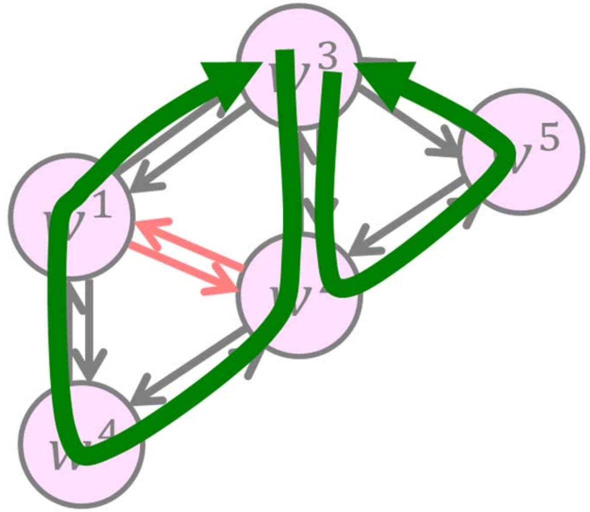
For a while, we discuss the edge in a stall state.



Fluctuation-response relation (FRR) in stall state

$\mathcal{J}_{12}$: probability current

$x_{12} := \ln \frac{R_{12}}{R_{21}}$:conjugated affinity



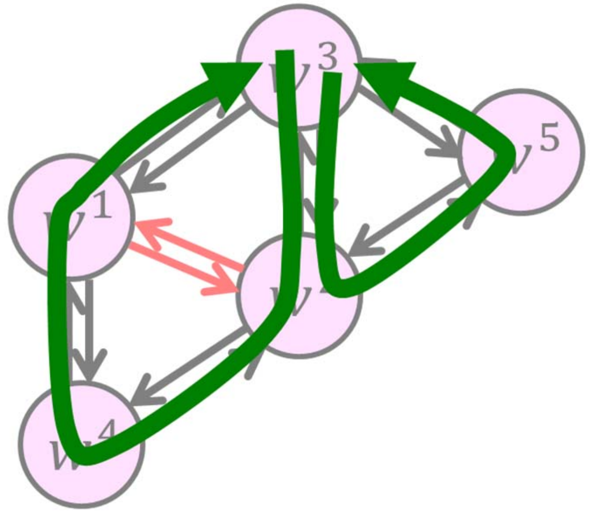
Around stalling state $x_{12} = x_{12}^{*}$, we have fluctuation response relation (FRR):

$$\frac{1}{2}\left\langle \mathcal{J}_{12}^{2} \right\rangle_{x=x^{*}} = \left.\frac{\partial \langle \mathcal{J}_{12} \rangle_{x}}{\partial x_{12}}\right|_{x=x^{*}}$$

(B. Altaner, M. Polettini and M. Esposito, PRL 117, 180601 (2016).)

Meaning of stall FRR

$$\frac{1}{2}\left\langle \mathcal{J}_{12}^2 \right\rangle_{x=x^*} = \left.\frac{\partial \langle \mathcal{J}_{12} \rangle_x}{\partial x_{12}}\right|_{x=x^*}$$



- FRR holds on the stalling edge (zero probability current), whose form is the same as the equilibrium FRR.
- Except the edge in interest, strong stationary current may flow.

Outline

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Fluctuation-response relation of time-symmetric current for stall states

Fluctuation-response relation of time-symmetric current for general NESS

Another application of time-symmetric current

Time-symmetric current

Current $\mathcal{J}$ changes its sign under time-reversal:

$$\mathcal{J}(\Gamma^{\dagger}) = -\mathcal{J}(\Gamma).$$

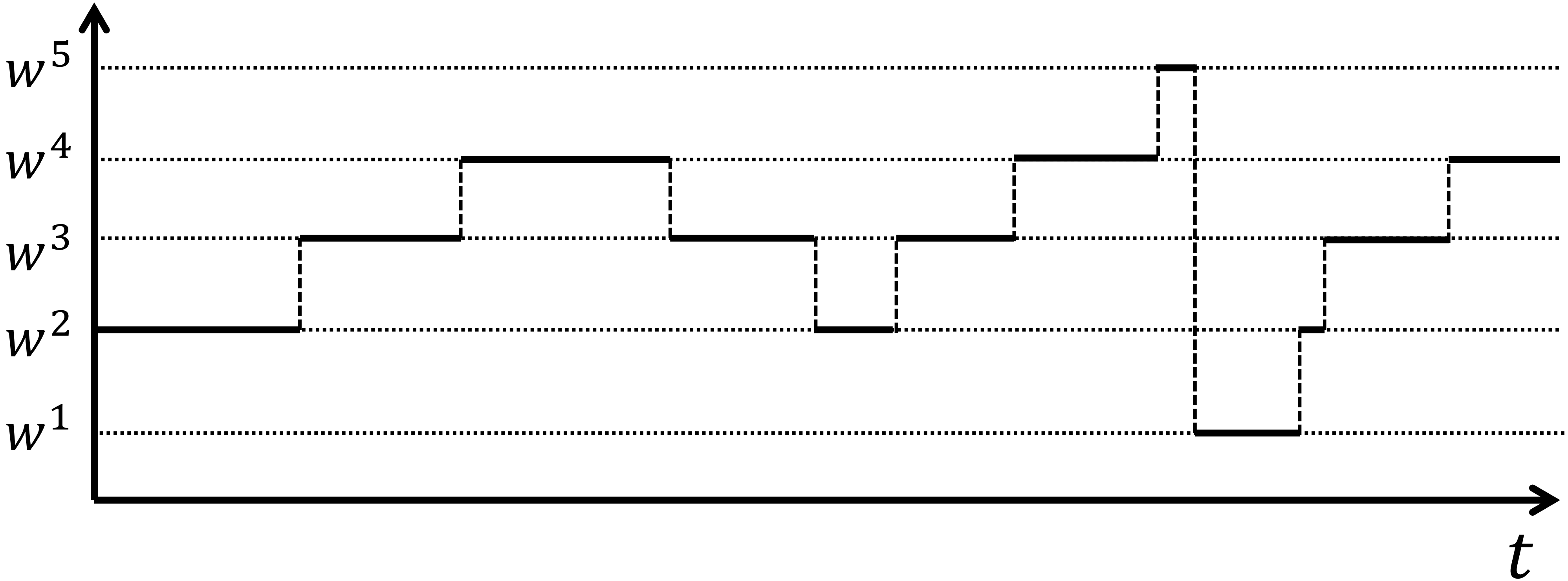
We investigate current-like but time-symmetric quantity, i.e.,

$$\boldsymbol{I}(\boldsymbol{\Gamma}^{\dagger}) = \boldsymbol{I}(\boldsymbol{\Gamma}) \ \text{ and } \ \langle \boldsymbol{\mathcal{J}} \rangle = \langle \boldsymbol{I} \rangle$$

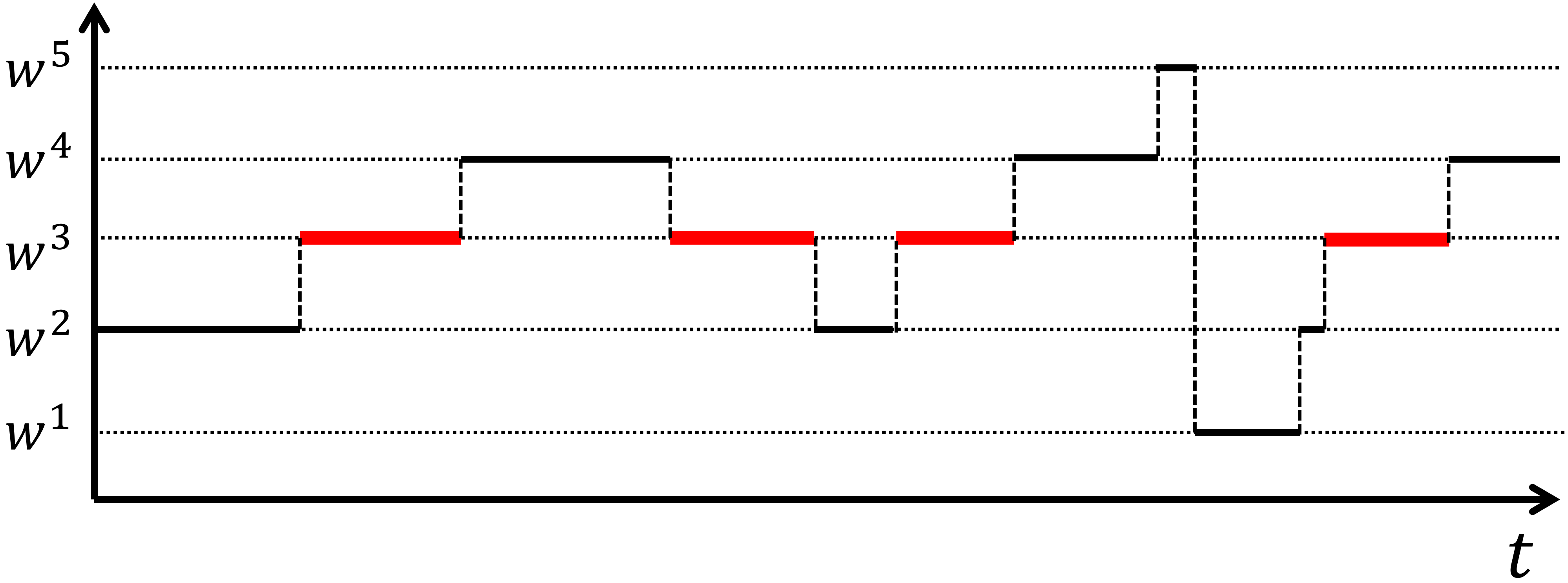
Time-symmetric quantities are considered to be important in nonequilibrium physics.

(J. P. Garrahan, *et al.*, PRL 98, 195702 (2007). M. Baiesi, C. Maes, and B. Wynants, PRL 103, 010602 (2009), T. Bodineau and C. Toninelli, CMP 311, 357 (2012).)

Ex) empirical measure

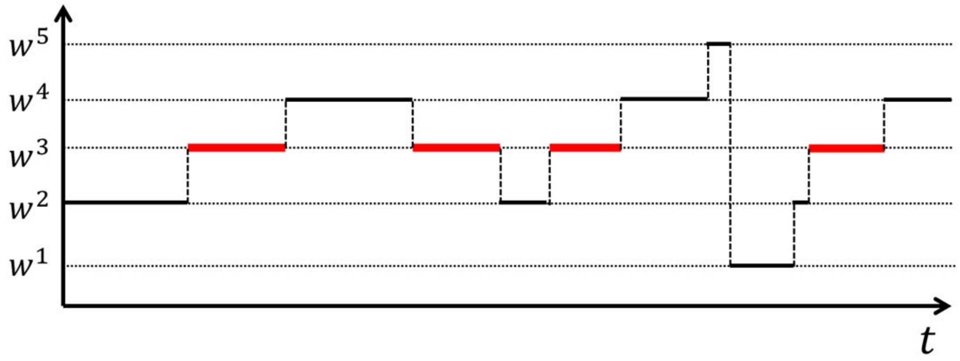


Ex) empirical measure



Empirical measure τ_3

Definition of time-symmetric current



Using empirical measure τ, time-symmetric current I_{ij} is defined as

$$\boldsymbol{I_{ij} := R_{ij}\tau_j - R_{ji}\tau_i}$$

By construction, $I_{ij}(\Gamma^\dagger) = I_{ij}(\Gamma)$ and $\langle \mathcal{J}_{ij} \rangle = \langle I_{ij} \rangle$

(Note: I_{ij} itself has x_{ij} dependence through R)

FRR for time-symmetric current

In stall states, the time-symmetric current satisfies

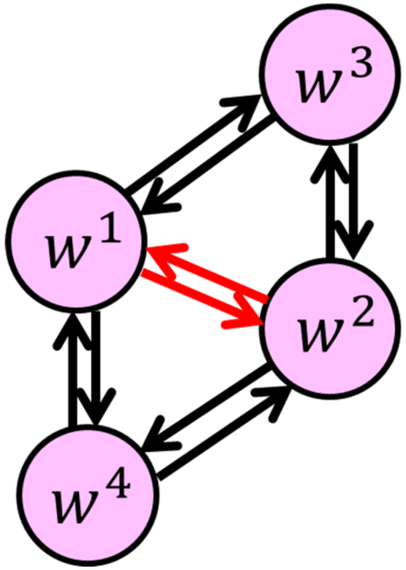
$$\frac{1}{2}\left\langle I_{ij}^{2}\right\rangle_{x=x^*} = -\left.\frac{\partial\left\langle I_{ij,x^*}\right\rangle_{x}}{\partial x_{ij}}\right|_{x=x^*}$$

(NS, Phys. Rev. Lett. 129, 020602 (2022))

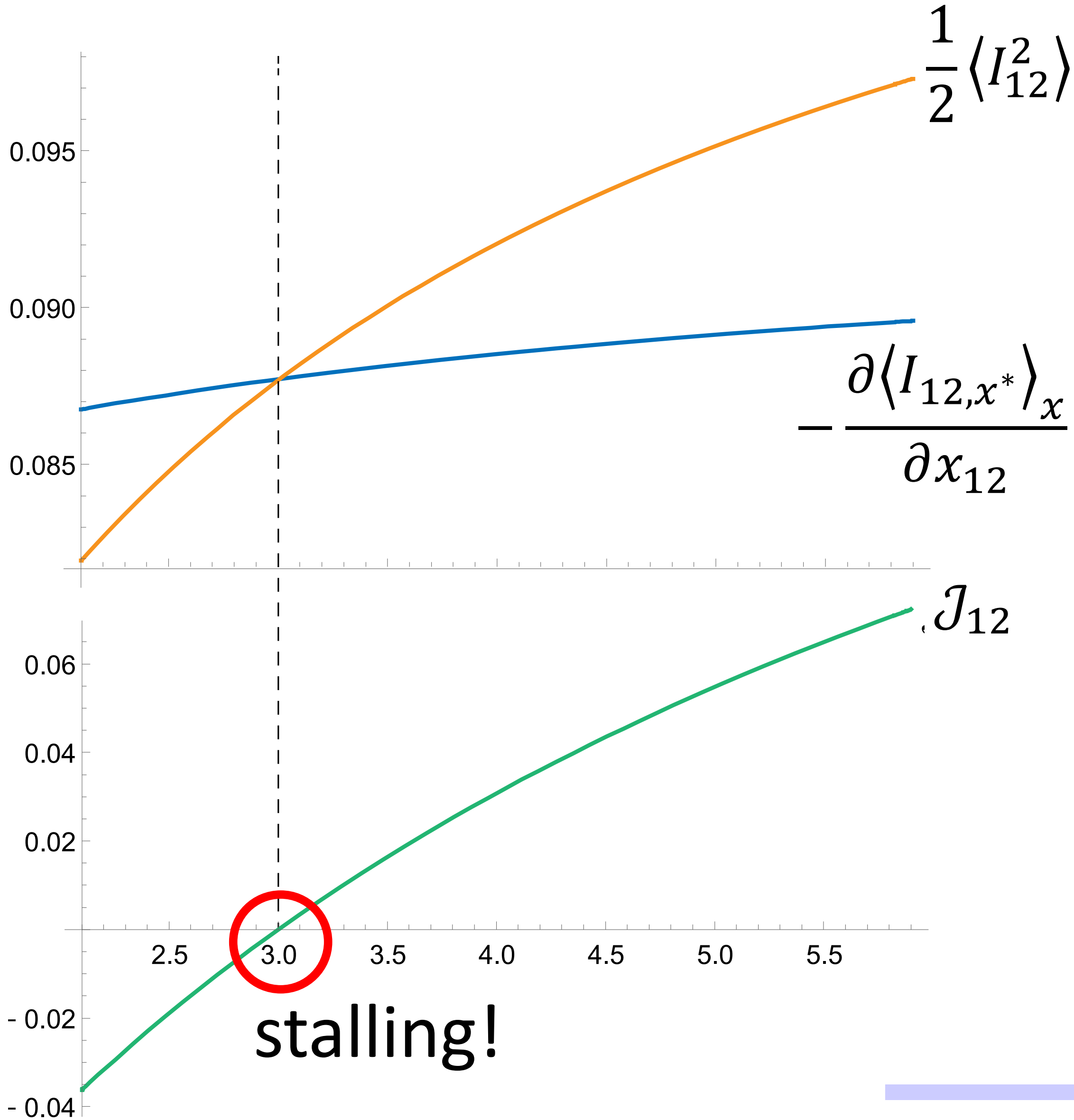
(Note: In the derivative of the r.h.s., we fix the function of I_{ij}(i.e., R in $I_{ij} \coloneqq R_{ij}\tau_j - R_{ji}\tau_i$) and perturb the path probability)

Numerical demonstration

$$\frac{1}{2}\langle I_{ij}^2\rangle_{x=x^*} = -\left.\frac{\partial\langle I_{ij,x^*}\rangle_x}{\partial x_{ij}}\right|_{x=x^*}$$

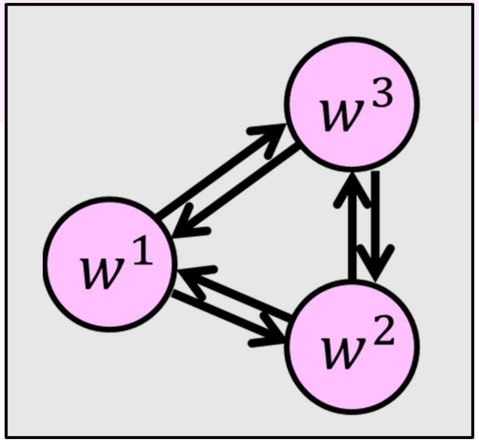


Above FRR holds only when $\mathcal{J}_{12} = 0$ (stall).



Key quantity: Partial entropy production

Partial entropy production：Assigning **entropy production** to single transitions with keeping thermodynamic properties.



second law：$\langle \sigma_{12} \rangle \geq 0$

fluctuation theorem：$\langle e^{-\sigma_{12}} \rangle = 1$

Two fashions to define partial entropy production.

-(passive) partial entropy production: σ_{12}

（NS and T. Sagawa, PRE 91. 012130 (2015)）

-informed partial entropy production: σ_{12}^{I}

(M. Polettini and M. Esposito, PRL 119, 240601 (2017))

From fluctuation theorem to FRR

$$\langle e^{-\sigma} \rangle = 1 \quad \xrightarrow{\text{expand around eq.}} \quad \frac{1}{2}\langle \mathcal{J}^2 \rangle_0 = \left.\frac{\partial \langle \mathcal{J} \rangle_h}{\partial h}\right|_{h=0}$$

$$\left\langle e^{-\sigma_{12}^I} \right\rangle = 1 \quad \xrightarrow{\text{expand around stall}} \quad \frac{1}{2}\left\langle \mathcal{J}_{ij}^2 \right\rangle_{x^*} = \left.\frac{\partial \left\langle \mathcal{J}_{ij} \right\rangle_x}{\partial x_{ij}}\right|_{x=x^*}$$

$$\langle e^{-\sigma_{12}} \rangle = 1 \quad \xrightarrow{\text{expand around stall}} \quad \boldsymbol{\frac{1}{2}\left\langle \left(\mathcal{J}_{ij} - I_{ij}\right)^2 \right\rangle_{x^*} = -\left.\frac{\partial \left\langle \mathcal{J}_{ij} \right\rangle_x}{\partial a_{ij}}\right|_{a=0}}$$

Proof: two technical relations

$$\frac{1}{2}\left\langle \left(\mathcal{J}_{ij} - I_{ij}\right)^2 \right\rangle_{x=x^*} = \left.\frac{\partial \langle \mathcal{J}_{ij} \rangle_x}{\partial a_{ij}}\right|_{a=0}$$

($a_{ij} := \ln \frac{R_{ij} p_j}{R_{ji} p_i}$:total thermodynamic force)

We use the following two relations

$$\langle \mathcal{J}_{ij} I_{ij} \rangle = 0$$

(This relation is trivial for equilibrium. For nonequilibrium stall states, we need the method with counting field.)

$$\left.\frac{\partial \langle \mathcal{J}_{ij} \rangle_x}{\partial a_{ij}}\right|_{a=0} = \left.\frac{\partial \langle \mathcal{J}_{ij} \rangle_x}{\partial x_{ij}}\right|_{x=x^*} - \left.\frac{\partial \left\langle I_{ij,x^*} \right\rangle_x}{\partial x_{ij}}\right|_{x=x^*}$$

Proof: difference between two FRR for two partial entropy production

FRR derived from σ_{ij}:

$$\frac{1}{2}\left\langle \mathcal{J}_{ij}^2 \right\rangle_{x=x^*} + \frac{1}{2}\left\langle I_{ij}^2 \right\rangle_{x=x^*} = \left.\frac{\partial \langle \mathcal{J}_{ij} \rangle_x}{\partial x_{ij}}\right|_{x=x^*} - \left.\frac{\partial \left\langle I_{ij,x^*} \right\rangle_x}{\partial x_{ij}}\right|_{x=x^*}$$

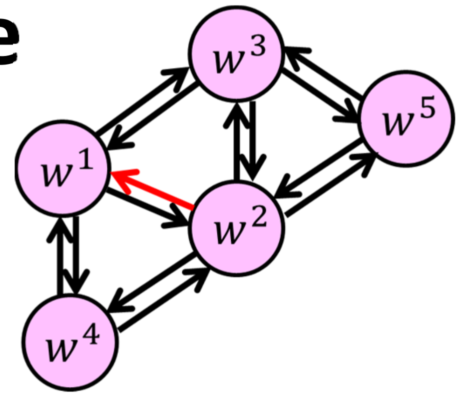
FRR derived from σ_{ij}^I:

$$\frac{1}{2}\left\langle \mathcal{J}_{ij}^2 \right\rangle_{x=x^*} = \left.\frac{\partial \langle \mathcal{J}_{ij} \rangle_x}{\partial x_{ij}}\right|_{x=x^*}$$

The difference between these two equals FRR for time-symmetric current (Proof end).

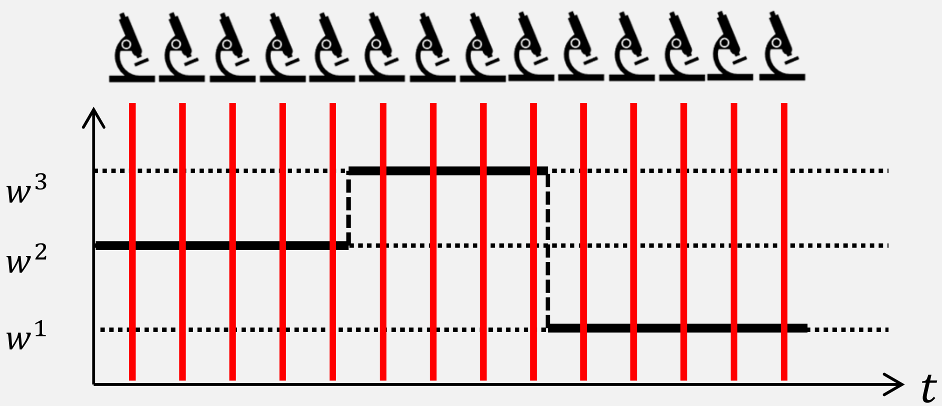
Applications for experiments

Time-symmetric current (and twisted empirical measure) are useful for estimating **a bare transition rate R_{ij}.**

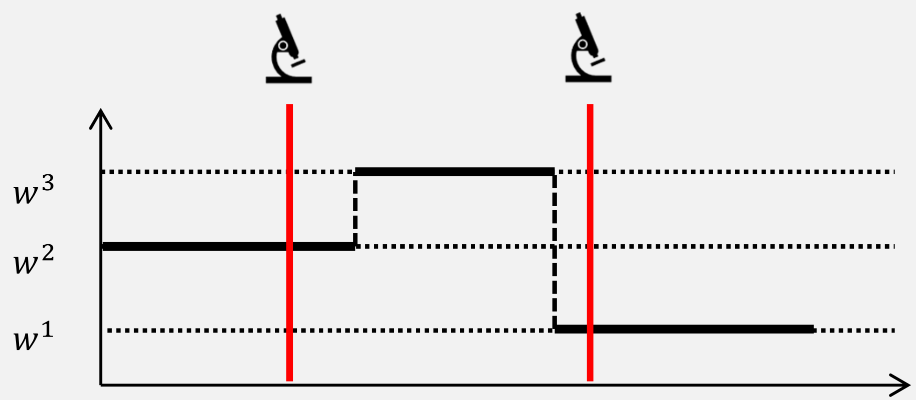


(We keep in mind the situation that **time-resolution is low** and only time-cumulative quantity is measurable)

High resolution



low resolution



Twisted empirical measure

Twisted empirical measure is defined as

$$\boldsymbol{C_{ij,x}} := \frac{\boldsymbol{\tau_j}}{\boldsymbol{p_j^{ss}(x)}} - \frac{\boldsymbol{\tau_i}}{\boldsymbol{p_i^{ss}(x)}}$$

- For any x, average is zero: $\langle C_{ij,x} \rangle_x = 0$
- In stall states, $\boldsymbol{I_{ij,x^*} = R_{ij} p_j^{ss}(x^*) C_{ij,x^*}}$
- Its derivative satisfies $\left.\frac{\partial \langle C_{ij,x^*} \rangle_x}{\partial x_{ij}}\right|_{x=x^*} = \frac{\partial}{\partial x} \ln \frac{p_j^{ss}}{p_i^{ss}}$

In application, we shall use $C_{ij,x}$ instead of I_{ij,x^*}.

Evaluation of R_{ij} (1)

Rewriting FRR for time-symmetric current in terms of C_{ij}, we have

$$\boldsymbol{R_{ij}} = -\frac{2}{\left\langle C_{ij,x^*}^2 \right\rangle_{x^*} p_j^{ss}} \frac{\partial \langle C_{ij,x^*} \rangle_x}{\partial x_{ij}} \Bigg|_{x=x^*}$$

Only empirical measure appears.
(No current appears.)

$$C_{ij,x} := \frac{\tau_j}{p_j^{ss}(x)} - \frac{\tau_i}{p_i^{ss}(x)}$$

Evaluation of R_{ij} (2)

Calculating from the definition of time-symmetric current, we have

$$\boldsymbol{R_{ij}} = \frac{\left.\frac{\partial\langle\mathcal{J}_{ij}\rangle_x}{\partial x_{ij}}\right|_{x=x^*}}{p_j^{ss}\left(\tau + \left.\frac{\partial\langle C_{ij,x^*}\rangle_x}{\partial x_{ij}}\right|_{x=x^*}\right)}$$

(τ : measurement time length)

Fluctuation term does not appear.

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Situation beyond stall state

Two key quantities:

<u>Time-symmetric current</u>

$$I_{ij,x^*} := R_{ij}\tau_j - R_{ji}\tau_i$$

<u>Twisted empirical measure</u>

$$C_{ij,x^*} := \frac{\tau_j}{p_j^{ss}} - \frac{\tau_i}{p_i^{ss}}$$

In stall states, these two are connected via

$$R_{ij} p_j^{ss} C_{ij,x^*} = I_{ij,x^*}.$$

In general nonequilibrium stationary states (NESS), no simple connection exists.

Result: FRR for general NESS

Around general NESS with $x = x'$, current, time-symmetric current and twisted empirical measure satisfy

$$\frac{\mathbf{2}}{\langle \boldsymbol{C}_{ij,x'}^{2} \rangle_{x'}} = \frac{\dfrac{d\langle \boldsymbol{I}_{ij,x'} \rangle_{x}}{dx_{ij}} - \dfrac{d\langle \boldsymbol{\mathcal{J}}_{ij} \rangle_{x}}{dx_{ij}}}{\dfrac{d\langle \boldsymbol{C}_{ij,x'} \rangle_{x}}{dx_{ij}}}$$

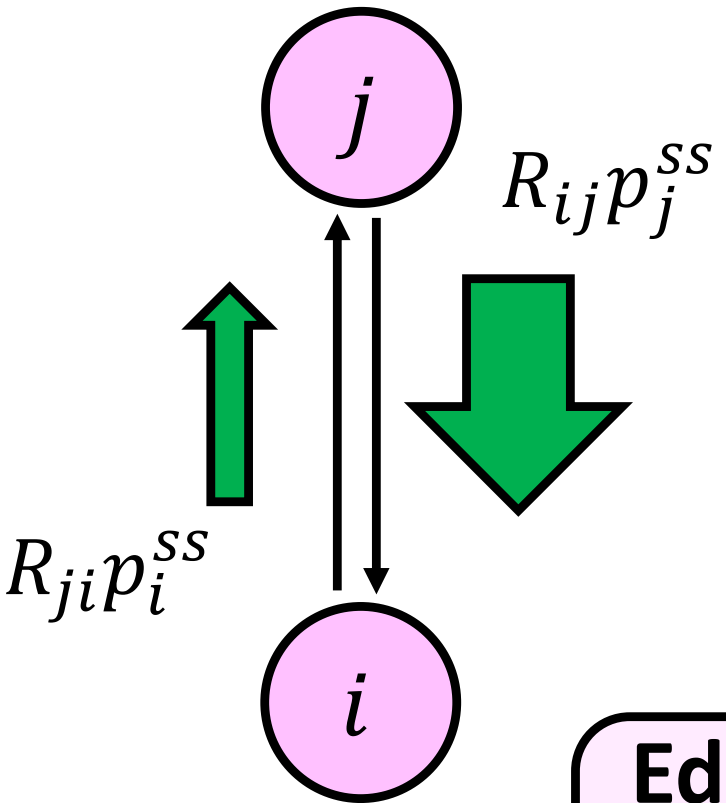
Fluctuation term

Response terms

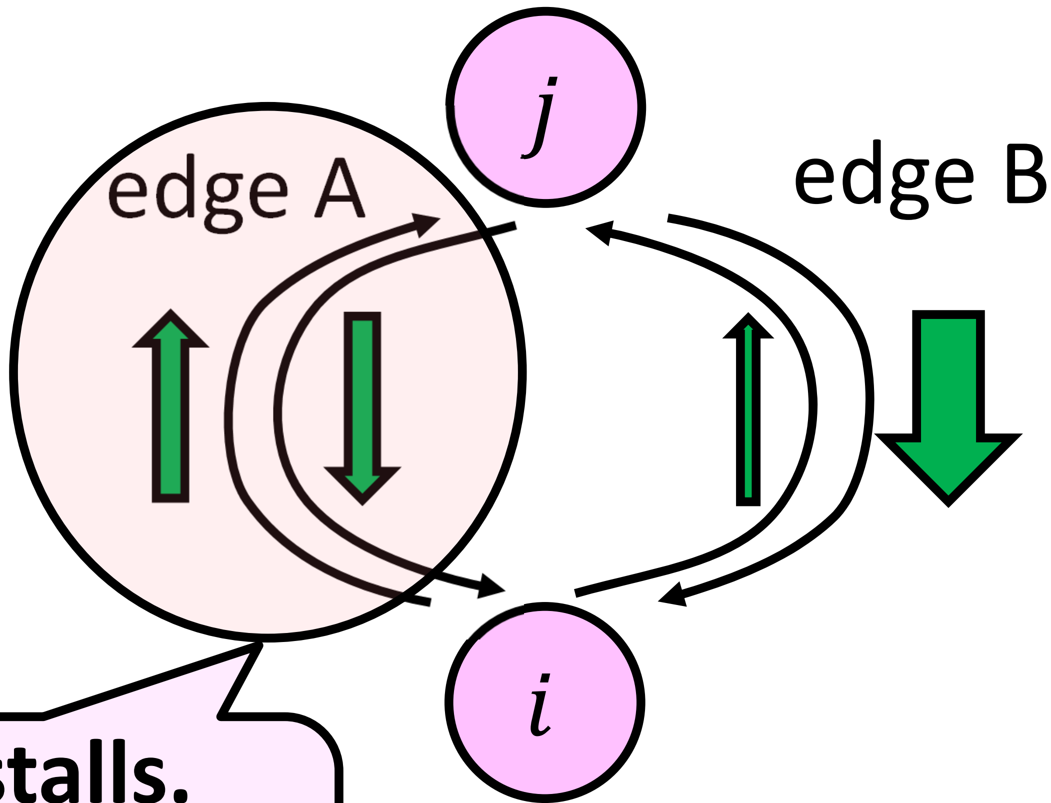
(N. Shiraishi, J. Stat. Mech. 033207 (2023))

Proof idea: decomposing transition

<u>Original</u>



<u>Edge decomposed</u>



Edge A stalls.
→We can apply previous FRR!

$$R_{ij} = R_{ij}^{A} + R_{ij}^{B}$$

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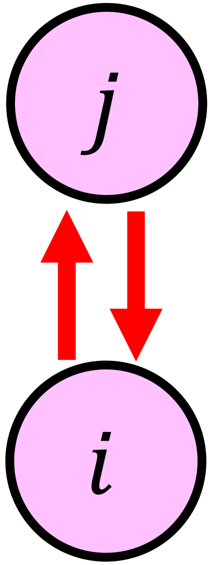
One-way current version

J_{ij}: count +1 for $j \to i$ / count -1 for $i \to j$

$$I_{ij} := R_{ij}\tau_j - R_{ji}\tau_i$$



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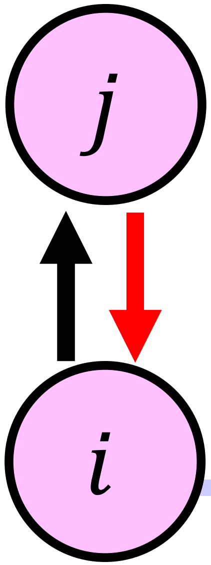
j_{ij}: count +1 for $j \to i$

$$i_{ij} := R_{ij}\tau_j$$



one-way counterpart

Further application: continuous-discrete correspondence

Langevin equation:

$$\dot{x} = F(x)dt + \sigma(x)dW \quad (D = \sigma\sigma^{\top}/2)$$

For any current $J_d = \int d(x)dx$, we decompose it as

$$J_d^{I} := \int d(x)\sigma(x)dW \qquad \text{(zero average, stochastic)}$$

$$J_d^{II} := \int [d(x)F(x) + \nabla(d(x)D(x))]dt \qquad \text{(average)}$$

Counterpart for Markov jump processes is

$$J_d^{I} := \sum\int d_{ij}(j_{ij} - i_{ij}) \qquad \text{(zero average, stochastic)}$$

$$J_d^{II} := \sum\int d_{ij}i_{ij} \qquad \text{(average)}$$

(C. Dieball and A. Godec, PRL 130, 087101 (2023))

Direct proof of TUR

Setting $J_\Pi^I := \sum\int \underline{\frac{R_{ij}p_j - R_{ji}p_i}{R_{ij}p_j + R_{ji}p_i}}(j_{ij} - i_{ij})$, we have

Π: pseudo entropy production

$$\sigma \mathrm{Var}[J_d] \geq \Pi \mathrm{Var}[J_d] \geq 2\left\langle \left(J_\Pi^I\right)^2 \right\rangle \langle (J_d - \langle J_d \rangle)^2 \rangle$$

$$\geq 2\left\langle J_\Pi^I (J_d - \langle J_d \rangle) \right\rangle^2 = 2\left(\underbrace{\left\langle J_\Pi^I J_d^I \right\rangle}_{= \langle J_d \rangle} + \underbrace{\left\langle J_\Pi^I J_d^{II} \right\rangle}_{= 0} \right)^2$$

This is thermodynamic uncertainty relation (TUR)!

(C. Dieball and A. Godec, PRL 130, 087101 (2023))

Summary

- We introduced time-symmetric current $I_{ij,x}$ and twisted empirical measure $C_{ij,x}$.
- We showed the FRR around stall states:

$$\frac{1}{2}\left\langle I_{ij}^2\right\rangle_{x=x^*} = -\left.\frac{\partial\left\langle I_{ij,x^*}\right\rangle_x}{\partial x_{ij}}\right|_{x=x^*}$$

- We showed the FRR around general NESS:

$$\frac{2}{\left\langle C_{ij,x'}^2\right\rangle_{x'}} = \frac{\frac{d\left\langle I_{ij,x'}\right\rangle_x}{dx_{ij}} - \frac{d\left\langle \mathcal{J}_{ij}\right\rangle_x}{dx_{ij}}}{\frac{d\left\langle C_{ij,x'}\right\rangle_x}{dx_{ij}}}$$

W ' V