Minimum entropy production rate for macroscopic systems

Sosuke Ito

NSPCS 2024, Korea Institute for advanced study, Korea

23rd, Jul. 2024

K. Yoshimura and SI, Phys. Rev. Res. 6, L022057 (2024).
R. Nagayama, K. Yoshimura, A. Kolchinsky and SI. arXiv: 2311.16569.

UTokyo

Universal Biology Institute

Reference and collaborators

K. Yoshimura (UTokyo) R. Nagayama (UTokyo) A. Kolchinsky (Pompeu Fabra U)

Main topic (Minimum entropy production rate for the macroscopic systems)

K. Yoshimura and SI, Phys. Rev. Res. 6, L022057 (2024).
R. Nagayama, K. Yoshimura, A. Kolchinsky and SI. arXiv: 2311.16569.

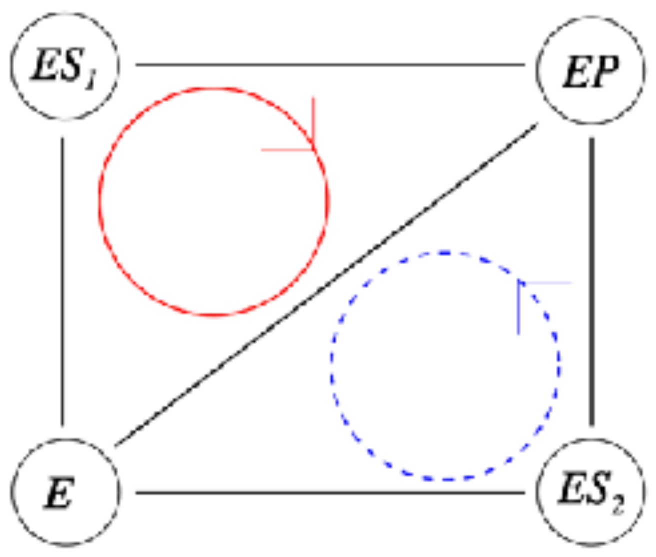
Related topic (Thermodynamics and optimal transport)

SI, information geometry, *Information* Geometry 7.Suppl 1, 441-483 (2024).

M. Nakazato and SI. Phys. Rev. Res. 3, 043093 (2021).
A. Dechant, S-I Sasa and SI. Phys. Rev. Res. 4, L012034 (2022).
A. Dechant, S-I Sasa and SI, Phys. Rev. E. 106, 024125 (2022).
K. Yoshimura, A. Kolchinsky, A. Dechant and SI. Phys. Rev. Res. 5, 013017 (2023).
Y. Fujimoto and SI, Phys. Rev. Res. 6, 013023 (2024).
K. Yoshimura and SI, Phys. Rev. Res. 6, L022057 (2024).
A. Kolchinsky, A. Dechant, K. Yoshimura and SI, arXiv:2206.14599.
R. Nagayama, K. Yoshimura, A. Kolchinsky and SI. arXiv: 2311.16569.
D. Sekizawa, SI, M. Oizumi, arXiv:2312.03489.
K. Ikeda, T. Uda, D. Okanohara and SI, arXiv:2407.04495.

Collaborators:
Lab members (+alumni): Muka Nakazato, Yuma Fujimoto,
Andreas Dechant (KyotoU), Shin-ichi Sasa (KyotoU), Daiki Sekizawa (UTokyo), Masafumi Oizumi (UTokyo), K. Ikeda (UTokyo), T. Uda (UTokyo),
D. Okanohara (Preferred Networks Inc.)

Motivation



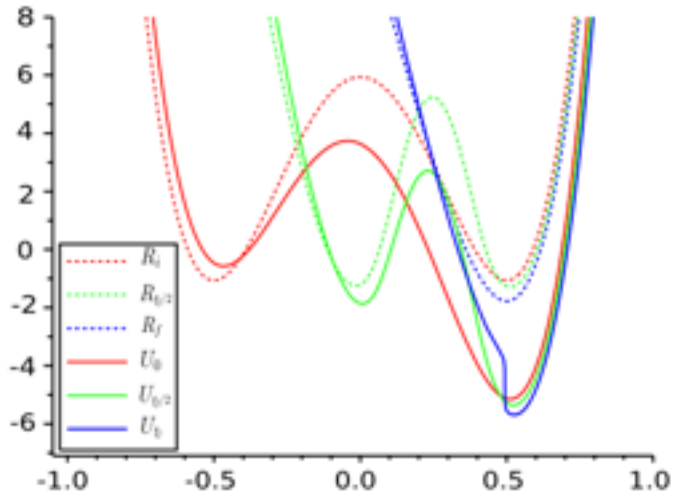
Thermodynamic trade-off relations
[Lower bounds on the entropy production (rate)]

e.g., thermodynamic uncertainty relations, speed limits…

$$\sigma_t \geq \text{(quantity corresponding to speed)}$$

$$\int_0^\tau dt\sigma_t \geq \text{(quantity corresponding to speed)}$$

Dissipation vs Speed



A. C. Barato & U. Seifert,
Physical review letters, *114*, 158101 (2015).

E. Aurell, K. Gawędzki, C. Mejía-Monasterio,
R. Mohayaee, & P. Muratore-Ginanneschi,
Journal of statistical physics, *147*, 487-505 (2012).

The derivation of these relations are based on stochastic techniques.
(e.g., Cramér–Rao bound, large deviation and optimal transport…etc.)

Q. Are these trade-offs also available even for the macroscopic (deterministic and nonlinear) systems?

e.g., Reaction-diffusion systems and hydrodynamic systems

Outline

- Introduction:
  Minimum entropy production rate for the microscopic systems

- Minimum entropy production rate for the reaction-diffusion systems

  R. Nagayama, K. Yoshimura, A. Kolchinsky and SI. arXiv: 2311.16569.

- Minimum entropy production rate for the hydrodynamic systems

  K. Yoshimura and SI, Phys. Rev. Res. 6, L022057 (2024).

Stochastic thermodynamics for the Fokker-Planck equation

Review: U. Seifert, Reports on progress in physics, 75, 126001 (2012).

Fokker-Planck equation

$$\partial_t P_t(\boldsymbol{x}) = -\nabla \cdot \boldsymbol{j}_t(\boldsymbol{x}) = -\nabla \cdot (\boldsymbol{\nu}_t(\boldsymbol{x}) P_t(\boldsymbol{x}))$$

$$\boldsymbol{\nu}_t(\boldsymbol{x}) = \mu \boldsymbol{F}_t(\boldsymbol{x}) - \mu T \nabla \ln P_t(\boldsymbol{x})$$

Entropy production rate

$$\sigma_t = \frac{1}{\mu T} \int d\boldsymbol{x} \|\boldsymbol{\nu}_t(\boldsymbol{x})\|^2 P_t(\boldsymbol{x}) \; (\geq 0)$$

Excess entropy production rate for the Fokker-Planck equation

A. Dechant, S-I Sasa and SI. Phys. Rev. Res. 4, L012034 (2022).

$$\partial_t P_t(\boldsymbol{x}) = -\nabla\cdot(\boldsymbol{\nu}_t(\boldsymbol{x})P_t(\boldsymbol{x})) = -\nabla\cdot(\boldsymbol{\nu}_t^{\mathrm{ex}}(\boldsymbol{x})P_t(\boldsymbol{x}))$$

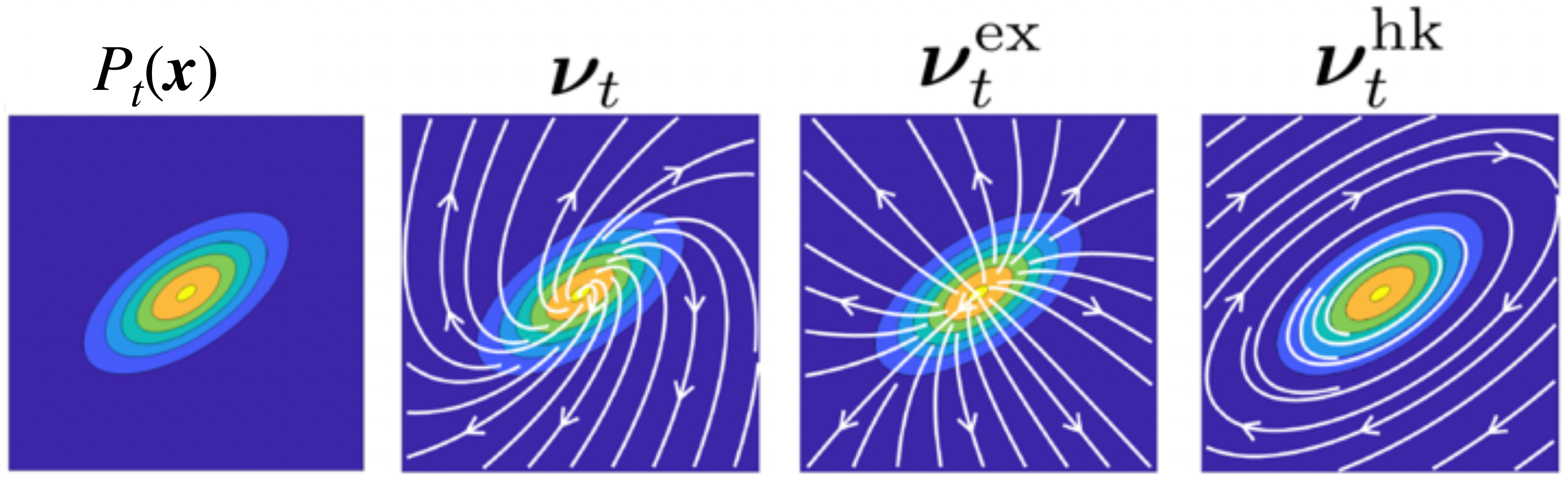
$$\boldsymbol{\nu}_t^{\mathrm{ex}}(\boldsymbol{x}) = \nabla\phi_t(\boldsymbol{x})$$

$\phi_t(\boldsymbol{x})$: Solution of

$$\nabla\cdot([\boldsymbol{\nu}_t(\boldsymbol{x}) - \nabla\phi_t(\boldsymbol{x})]P_t(\boldsymbol{x})) = 0$$

Excess entropy production rate

$$\sigma_t^{\mathrm{ex}} = \frac{1}{\mu T}\int d\boldsymbol{x}\|\boldsymbol{\nu}_t^{\mathrm{ex}}(\boldsymbol{x})\|^2 P_t(\boldsymbol{x}) \ (\geq 0)$$



(Figure from) D. Sekizawa, SI and M. Oizumi, arXiv:2312.03489.

Geometric decomposition for the Fokker-Planck equation

Housekeeping entropy production rate

Maes, C., & Netočný, K. *Journal of Statistical Physics*, *154*, 188-203 (2014).

A. Dechant, S-I Sasa and SI. Phys. Rev. Res. 4, L012034 (2022).

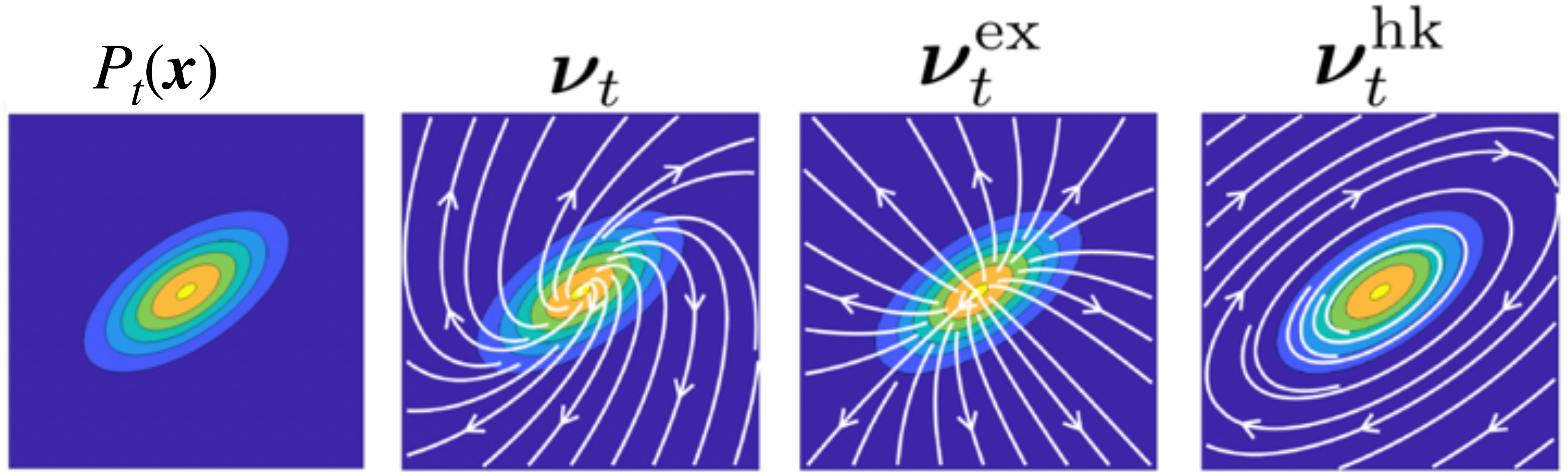
$$\sigma_t^{\rm hk} = \frac{1}{\mu T}\int d\boldsymbol{x} \|\boldsymbol{\nu}_t^{\rm hk}(\boldsymbol{x})\|^2 P_t(\boldsymbol{x}) \ (\geq 0)$$

$$\boldsymbol{\nu}_t^{\rm hk}(\boldsymbol{x}) = \boldsymbol{\nu}_t(\boldsymbol{x}) - \boldsymbol{\nu}_t^{\rm ex}(\boldsymbol{x})$$

Geometric decomposition

$$\sigma_t = \sigma_t^{\rm ex} + \sigma_t^{\rm hk}$$

$$\sigma_t \geq \sigma_t^{\rm ex}$$



(Figure from) D. Sekizawa, SI and M. Oizumi, arXiv:2312.03489.

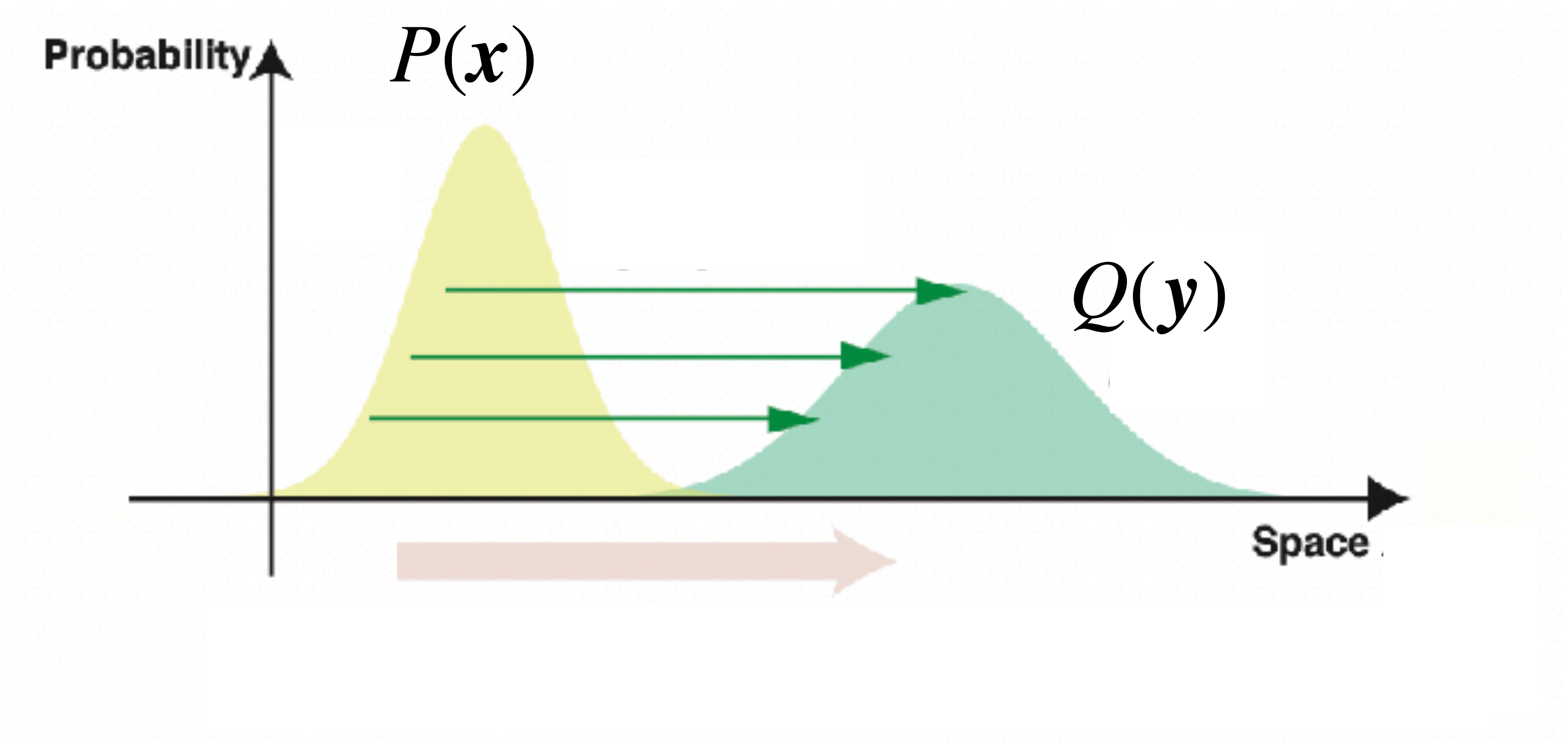
Optimal transport

The 2-Wasserstein distance

J-D. Benamou & Y. Brenier. *Numerische Mathematik* 84, 375-393 (2000).

$$\mathscr{W}_2(P,Q) = \sqrt{\inf_{\{\boldsymbol{u}_t, Q_t\}_{0\le t\le \tau}} \tau \int_0^\tau dt \int d\boldsymbol{x} \|\boldsymbol{u}_t(\boldsymbol{x})\|^2 Q_t(\boldsymbol{x})}$$

$$\partial_t Q_t(\boldsymbol{x}) = -\nabla \cdot (\boldsymbol{u}_t(\boldsymbol{x}) Q_t(\boldsymbol{x})) \quad Q_0(\boldsymbol{x}) = P(\boldsymbol{x}) \quad Q_\tau(\boldsymbol{x}) = Q(\boldsymbol{x})$$



Metric:

① $\mathscr{W}_2(P,Q) \ge 0$ ② $\mathscr{W}_2(P,Q) = 0 \Leftrightarrow P = Q$ ③ $\mathscr{W}_2(P,Q) = \mathscr{W}_2(Q,P)$

④ $\mathscr{W}_2(P,R) + \mathscr{W}_2(R,Q) \ge \mathscr{W}_2(P,Q)$

Minimum entropy production rate

Speed in the space of the 2-Wasserstein distance

M. Nakazato and SI. Phys. Rev. Res. 3, 043093 (2021).
A. Dechant, S-I Sasa and SI. Phys. Rev. Res. 4, L012034 (2022).

$$v_2(t) = \lim_{\Delta t \to +0} \frac{\mathcal{W}_2(P_t, P_{t+\Delta t})}{\Delta t} = \sqrt{\int d\boldsymbol{x} \|\boldsymbol{\nu}_t^{\mathrm{ex}}(\boldsymbol{x})\|^2 P_t(\boldsymbol{x})}$$

Excess entropy production rate = Minimum entropy production rate

$$\sigma_t^{\mathrm{ex}} = \frac{[v_2(t)]^2}{\mu T} = \inf_{\boldsymbol{\nu}_t} \frac{1}{\mu T} \int d\boldsymbol{x} \|\boldsymbol{\nu}_t(\boldsymbol{x})\|^2 P_t(\boldsymbol{x})$$

$$\partial_t P_t(\boldsymbol{x}) = -\nabla \cdot (\boldsymbol{\nu}_t(\boldsymbol{x}) P_t(\boldsymbol{x}))$$

$\partial_t P_t(\boldsymbol{x})$ is fixed.

Thermodynamic speed limits

Thermodynamic speed limits

$$\Sigma^{\mathrm{ex}}(\tau) := \int_0^\tau dt \sigma_t^{\mathrm{ex}} \geq \frac{[l_2(\tau)]^2}{\mu T \tau} \geq \frac{[\mathscr{W}_2(P_0, P_\tau)]^2}{\mu T \tau}$$

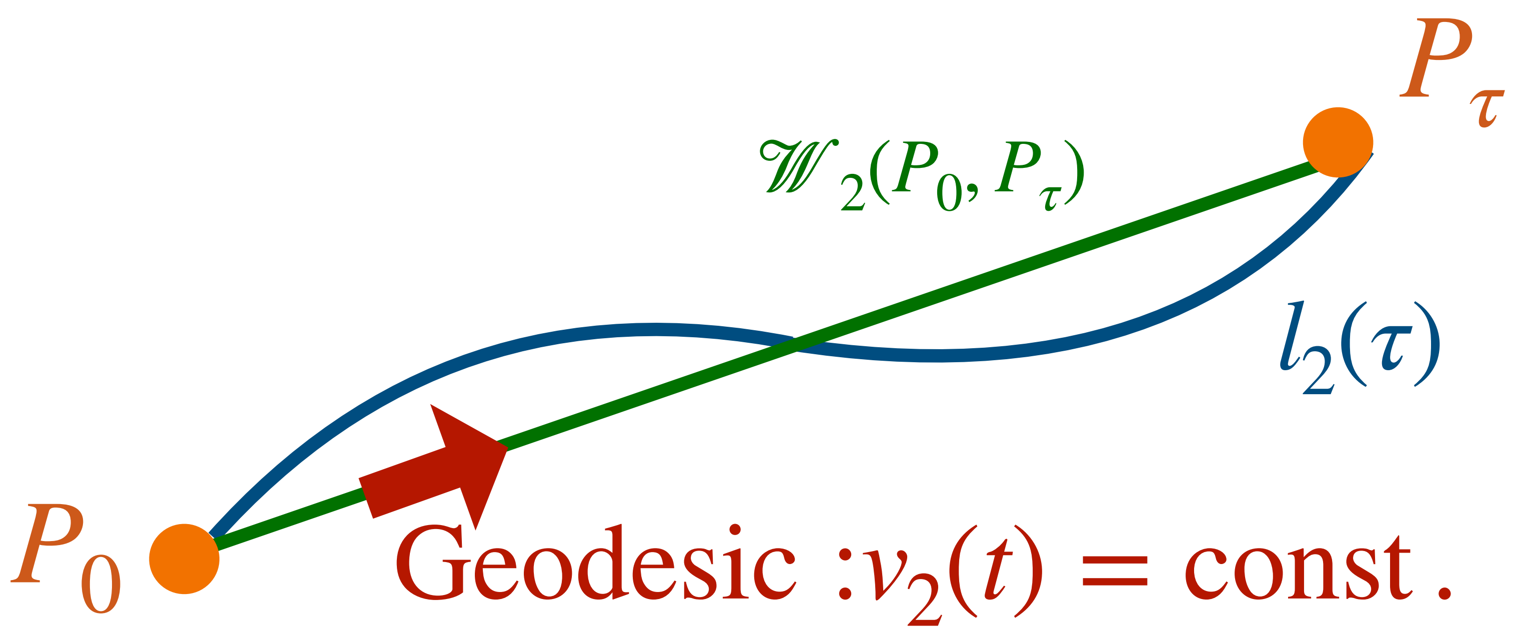
$$l_2(\tau) = \int_0^\tau dt v_2(t)$$:Path length

E. Aurell, K. Gawędzki, C. Mejía-Monasterio, R. Mohayaee, & P. Muratore-Ginanneschi, *Journal of statistical physics*, *147*, 487-505 (2012).
M. Nakazato and SI. Phys. Rev. Res. 3, 043093 (2021).
SI, information geometry, *Information* Geometry 7.Suppl 1, 441-483 (2024).

Minimum excess entropy production

$$\Sigma^{\mathrm{ex}}(\tau) = \frac{[\mathscr{W}_2(P_0, P_\tau)]^2}{\mu T \tau}$$

$$v_2(t) = \frac{\mathscr{W}_2(P_0, P_\tau)}{\tau} = \mathrm{const.}$$:Geodesic (optimal transport)



Thermodynamic uncertainty relations

Thermodynamic uncertainty relation

A. Dechant, S-I Sasa and SI. Phys. Rev. Res. 4, L012034 (2022).
A. Dechant, S-I Sasa and SI, Phys. Rev. E. 106, 024125 (2022).

cf.) Cramér–Rao bound: SI and A. Dechant, *Physical Review X*, *10*, 021056 (2020).

$$\sigma_t^{\mathrm{ex}} \geq \frac{|\partial_t \langle a \rangle_{P_t}|^2}{\mu T \langle \|\nabla a\|^2 \rangle_{P_t}}$$

$a(\boldsymbol{x})$: time-independent observable

$$\langle a \rangle_{P_t} = \int d\boldsymbol{x} a(\boldsymbol{x}) P_t(\boldsymbol{x})$$

⬇

$$v_2(t) \geq v_a(t)$$

(Normalized) speed of observable $a(\boldsymbol{x})$

$$v_a(t) = \frac{|\partial_t \langle a \rangle_{P_t}|}{\sqrt{\langle \|\nabla a\|^2 \rangle_{P_t}}}$$

Speed in the space of the 2-Wasserstein distance
is the upper bound on the speed of any observable.

General framework:
The minimum entropy production rate in this talk

Dynamics

$$\partial_t X = -\nabla \cdot J = -\nabla \cdot (MF)$$

Entropy production rate

$$\sigma(F) = JF = FMF = \langle F, F \rangle_M$$

Minimum entropy production rate
(excess entropy production rate)

$$\min_{F'} \sigma(F') = \min_{F'} \langle F', F' \rangle_M := \sigma^{\mathrm{ex}}$$

subject to $$\partial_t X = -\nabla \cdot (MF')$$ (The same time evolution)

X: State

J: Flow

F: Force

M: Onsager coefficient

Force and flow for the Fokker-Planck equation

Fokker-Planck equation:

$$\partial_t P_t(\boldsymbol{x}) = -\nabla \cdot \boldsymbol{j}_t(\boldsymbol{x}) = -\nabla \cdot (\boldsymbol{\nu}_t(\boldsymbol{x}) P_t(\boldsymbol{x}))$$

Flow:

$$\boldsymbol{j}_t(\boldsymbol{x}) = \boldsymbol{\nu}_t(\boldsymbol{x}) P_t(\boldsymbol{x})$$

Force:

$$\boldsymbol{f}_t(\boldsymbol{x}) = \frac{\boldsymbol{j}_t(\boldsymbol{x})}{\mu T P_t(\boldsymbol{x})} = \frac{\boldsymbol{\nu}_t(\boldsymbol{x})}{\mu T}$$

Onsager coefficient:

$$M_t(\boldsymbol{x}) = \frac{\boldsymbol{j}_t(\boldsymbol{x})}{\boldsymbol{f}_t(\boldsymbol{x})} = \mu T P_t(\boldsymbol{x})$$

Entropy production rate:

$$\sigma_t = \langle \boldsymbol{f}_t, \boldsymbol{f}_t \rangle_{M_t} = \int d\boldsymbol{x} \boldsymbol{f}_t(\boldsymbol{x}) \cdot M_t(\boldsymbol{x}) \boldsymbol{f}_t(\boldsymbol{x}) = \int d\boldsymbol{x} \boldsymbol{f}_t(\boldsymbol{x}) \cdot \boldsymbol{j}_t(\boldsymbol{x}) = \frac{1}{\mu T} \int d\boldsymbol{x} \|\boldsymbol{\nu}_t(\boldsymbol{x})\|^2$$

$$\partial_t X = -\nabla \cdot J = -\nabla \cdot (MF)$$

$$X \leftrightarrow P_t$$

$$J \leftrightarrow \boldsymbol{j}_t$$

$$M \leftrightarrow \mu T P_t$$

$$F \leftrightarrow \boldsymbol{\nu}_t / (\mu T)$$

Geometric structure and results

Inner product

$$\langle \boldsymbol{a}, \boldsymbol{b} \rangle_{M_t} = \int d\boldsymbol{x} \boldsymbol{a}(\boldsymbol{x}) \cdot M_t(\boldsymbol{x}) \boldsymbol{b}(\boldsymbol{x})$$

$$\boldsymbol{f}_t^{\mathrm{ex}} = \frac{\boldsymbol{\nu}_t^{\mathrm{ex}}}{\mu T} = \frac{\nabla \phi_t}{\mu T}, \quad \boldsymbol{f}_t^{\mathrm{hk}} = \frac{\boldsymbol{\nu}_t^{\mathrm{hk}}}{\mu T}$$

Orthogonality

$$\langle \boldsymbol{f}_t^{\mathrm{ex}}, \boldsymbol{f}_t^{\mathrm{hk}} \rangle_{M_t} = 0$$

Geometric decomposition

$$\underbrace{\langle \boldsymbol{f}_t^{\mathrm{ex}} + \boldsymbol{f}_t^{\mathrm{hk}}, \boldsymbol{f}_t^{\mathrm{ex}} + \boldsymbol{f}_t^{\mathrm{hk}} \rangle_{M_t}}_{\sigma_t} = \underbrace{\langle \boldsymbol{f}_t^{\mathrm{ex}}, \boldsymbol{f}_t^{\mathrm{ex}} \rangle_{M_t}}_{\sigma_t^{\mathrm{ex}}} + \underbrace{\langle \boldsymbol{f}_t^{\mathrm{hk}}, \boldsymbol{f}_t^{\mathrm{hk}} \rangle_{M_t}}_{\sigma_t^{\mathrm{hk}}}$$

Gradient flow

$$\partial_t P_t(\boldsymbol{x}) = -\nabla \cdot \left(M_t(\boldsymbol{x}) \boldsymbol{f}_t^{\mathrm{ex}} \right)$$

Thermodynamic uncertainty relation

$$\underbrace{(\langle \boldsymbol{f}_t^{\mathrm{ex}}, \nabla a \rangle_{M_t})^2}_{|d_t \langle a \rangle_{P_t}|^2} \leq \underbrace{\langle \boldsymbol{f}_t^{\mathrm{ex}}, \boldsymbol{f}_t^{\mathrm{ex}} \rangle_{M_t}}_{\sigma_t^{\mathrm{ex}}} \underbrace{\langle \nabla a, \nabla a \rangle_{M_t}}_{\mu T \langle \| \nabla a \|^2 \rangle_{P_t}}$$

Minimum entropy production rate

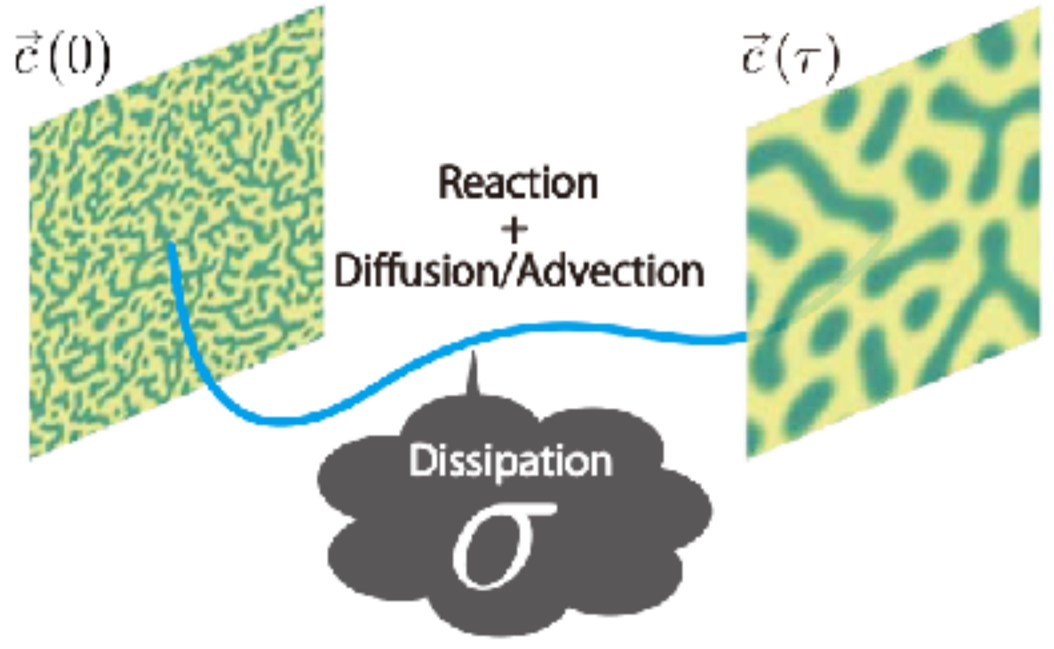
$$\sigma_t^{\mathrm{ex}} = \inf_{\boldsymbol{f}_t} \langle \boldsymbol{f}_t, \boldsymbol{f}_t \rangle_{M_t}$$

s.t. $\partial_t P_t(\boldsymbol{x}) = -\nabla \cdot (M_t(\boldsymbol{x}) \boldsymbol{f}_t(\boldsymbol{x}))$ $\quad \partial_t P_t(\boldsymbol{x})$ is fixed.

Motivation

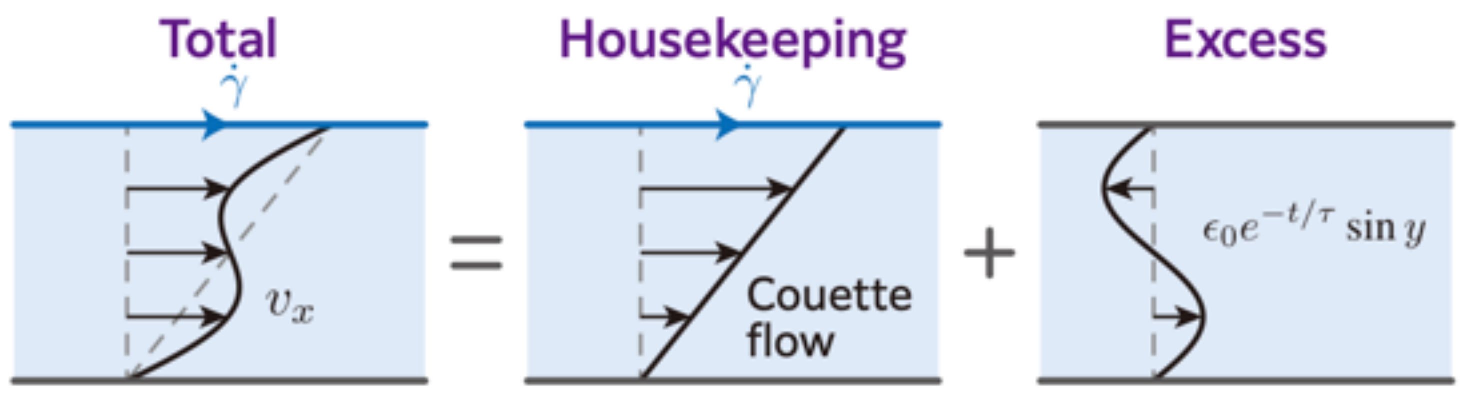
The geometric decomposition related to minimum entropy production rate and thermodynamic trade-off relations (i.e., thermodynamic speed limits and thermodynamic uncertainty relations) are based on the geometric structure.

Q. Can we generalize the results for the macroscopic deterministic systems?



Reaction-diffusion systems

R. Nagayama, K. Yoshimura, A. Kolchinsky and SI. arXiv: 2311.16569.



Hydrodynamic systems

K. Yoshimura and SI, Phys. Rev. Res. 6, L022057 (2024).

A. Yes. (Based on the geometric structure)

Outline

- Introduction:
  Minimum entropy production rate for the microscopic systems

- Minimum entropy production rate for the reaction-diffusion systems

  R. Nagayama, K. Yoshimura, A. Kolchinsky and SI. arXiv: 2311.16569.

- Minimum entropy production rate for the hydrodynamic systems

  K. Yoshimura and SI, Phys. Rev. Res. 6, L022057 (2024).

Reaction-diffusion systems

Reaction-diffusion equation

$$\partial_t c_\alpha(\boldsymbol{r};t) = -\underbrace{\nabla_{\boldsymbol{r}} \cdot \boldsymbol{J}_{(\alpha)}(\boldsymbol{r};t)}_{\text{Diffusion}} + \underbrace{\sum_\alpha S_{\alpha\rho} j_\rho(\boldsymbol{r};t)}_{\text{Reaction}}$$

$c_\alpha(\boldsymbol{r};t)$: concentration of α-th species at position $\boldsymbol{r}$ and time t

$S_{\alpha\rho}$: Stoichiometric matrix (α: species, ρ: reactions)

$j_\rho = j_\rho^+ - j_\rho^-$: Chemical flux

Example: Fisher-KPP equation

$$Z_1 + Z_2 \underset{k_1^-}{\overset{k_1^+}{\rightleftharpoons}} 2Z_1$$

$$c_1 = [Z_1] \qquad \boldsymbol{J}_{(1)} = -D_1 \nabla_{\boldsymbol{r}} c_1 \qquad S_{11} = +1 \qquad j_1^+ = k_1^+ c_1 c_2$$

$$c_2 = [Z_2] \qquad \boldsymbol{J}_{(2)} = -D_1 \nabla_{\boldsymbol{r}} c_2 \qquad S_{21} = -1 \qquad j_1^- = k_1^- c_1^2$$

$$\partial_t c_1(\boldsymbol{r};t) = D_1 \nabla_{\boldsymbol{r}}^2 c_1(\boldsymbol{r};t) + k_1^+ c_1(\boldsymbol{r};t) c_2(\boldsymbol{r};t) - k_1^- [c_1(\boldsymbol{r};t)]^2$$

$$\partial_t c_2(\boldsymbol{r};t) = D_2 \nabla_{\boldsymbol{r}}^2 c_2(\boldsymbol{r};t) - k_1^+ c_1(\boldsymbol{r};t) c_2(\boldsymbol{r};t) + k_1^- [c_1(\boldsymbol{r};t)]^2$$

Expression corresponding to the continuity equation

Reaction-diffusion equation

$$\partial_t c_\alpha(\boldsymbol{r};t) = -\underbrace{\nabla_{\boldsymbol{r}} \cdot \boldsymbol{J}_{(\alpha)}(\boldsymbol{r};t)}_{\text{Diffusion}} + \underbrace{\sum_\alpha S_{\alpha\rho} j_\rho(\boldsymbol{r};t)}_{\text{Reaction}}$$

$$\partial_t \vec{c} = -\nabla_{\boldsymbol{r}} \cdot \vec{\boldsymbol{J}} + \nabla_{\mathrm{s}}^\top \boldsymbol{j} = \underline{\nabla^\dagger} \mathscr{J}$$

Operator corresponding to $-\mathrm{div}$

$$\partial_t X = -\nabla \cdot J$$

$$X \leftrightarrow \vec{c}$$

$$-\nabla \cdot \leftrightarrow \nabla^\dagger$$

$$J \leftrightarrow \mathscr{J}$$

$$\vec{c} = (c_1, c_2, \cdots)^\top \quad \vec{\boldsymbol{J}} = (\boldsymbol{J}_{(1)}, \boldsymbol{J}_{(2)}, \cdots)^\top \quad \boldsymbol{j} = (j_1, j_2, \cdots)^\top$$

$$(\nabla_{\mathrm{s}}^\top)_{\alpha\rho} = S_{\alpha\rho} \qquad \mathscr{J} = \{\vec{\boldsymbol{J}}, \boldsymbol{j}\}$$

Forces and flows

Flow

$\vec{J} = \mathrm{M}\vec{F}$ Diffusion

$j = \mathrm{m}f$ Reaction

Force

$F_{(\alpha)} = -\nabla \ln c_\alpha$ Diffusion

$f_\rho = \ln[j_\rho^+ / j_\rho^-]$ Reaction

Onsager coefficients $(\mathrm{M})_{(\alpha\beta)} = D_\alpha c_\alpha \boldsymbol{I} \delta_{\alpha\beta}$ $\quad (\mathrm{m})_{\rho\rho'} = \dfrac{j_\rho^+ - j_\rho^-}{\ln j_\rho^+ - \ln j_\rho^-} \delta_{\rho\rho'}$

$\{\vec{J}, j\} = \mathcal{J} = \mathcal{M}\mathcal{F}$ $\quad \mathcal{F} = \{\vec{F}, f\}$

Onsager operator $\mathcal{M}$

Entropy production rate $\sigma_t = \langle \mathcal{F}, \mathcal{F} \rangle_{\mathcal{M}} = \int dr [\vec{F}^\top \mathrm{M} \vec{F} + f^\top \mathrm{m} f] \; (\geq 0)$

Geometric structure and geometric decomposition

Inner product

$$\langle \mathscr{A}, \mathscr{B} \rangle_{\mathscr{M}} = \int d\boldsymbol{r} [\vec{\boldsymbol{A}}^\top \mathsf{M} \vec{\boldsymbol{B}} + \boldsymbol{a}^\top \mathsf{m} \boldsymbol{b}]$$

Reaction diffusion equation

$$\partial_t \vec{c} = \nabla^\dagger \mathscr{J} = \nabla^\dagger \mathscr{M} \mathscr{F}$$

Operator corresponding to grad

$$\nabla \overrightarrow{\phi} = \{ \nabla_{\boldsymbol{r}} \overrightarrow{\phi}, \nabla_{\mathrm{s}} \overrightarrow{\phi} \} \qquad (\nabla_{\mathrm{s}})_{\rho\alpha} = (S^\top)_{\rho\alpha}$$

$$\partial_t \vec{c} = \nabla^\dagger \mathscr{M} \mathscr{F} = \nabla^\dagger \mathscr{M} \mathscr{F}^{\mathrm{ex}}$$

$$\mathscr{F}^{\mathrm{ex}} = \nabla \overrightarrow{\phi}$$

$\overrightarrow{\phi}$: Solution of $\nabla^\dagger \mathscr{M} (\mathscr{F} - \nabla \overrightarrow{\phi}) = 0$

Geometric decomposition

Orthogonality

$$\mathscr{F}^{\mathrm{hk}} = \mathscr{F} - \mathscr{F}^{\mathrm{ex}} \qquad \langle \mathscr{F}^{\mathrm{ex}}, \mathscr{F}^{\mathrm{hk}} \rangle_{\mathscr{M}} = 0$$

$$\underbrace{\langle \mathscr{F}^{\mathrm{ex}} + \mathscr{F}^{\mathrm{hk}}, \mathscr{F}^{\mathrm{ex}} + \mathscr{F}^{\mathrm{hk}} \rangle_{\mathscr{M}}}_{\sigma} = \underbrace{\langle \mathscr{F}^{\mathrm{ex}}, \mathscr{F}^{\mathrm{ex}} \rangle_{\mathscr{M}}}_{\sigma^{\mathrm{ex}}} + \underbrace{\langle \mathscr{F}^{\mathrm{hk}}, \mathscr{F}^{\mathrm{hk}} \rangle_{\mathscr{M}}}_{\sigma^{\mathrm{hk}}}$$

Minimum entropy production rate

Minimum entropy production rate

$$\sigma^{\mathrm{ex}} = \inf_{\mathcal{F}'} \langle \mathcal{F}', \mathcal{F}' \rangle_{\mathcal{M}}$$ s.t. $\partial_t \vec{c} = \nabla^{\dagger}(\mathcal{M}\mathcal{F}')$ $\partial_t \vec{c}$ is fixed.

The speed in the space of the (generalized) 2-Wasserstein distance $\tilde{\mathcal{W}}_2$

$$v_2(t) = \lim_{\Delta t \to +0} \frac{\tilde{\mathcal{W}}_2(P_t, P_{t+\Delta t})}{\Delta t} = \sqrt{\langle \nabla \vec{\phi}, \nabla \vec{\phi} \rangle_{\mathcal{M}}}$$

Thermodynamic speed limit

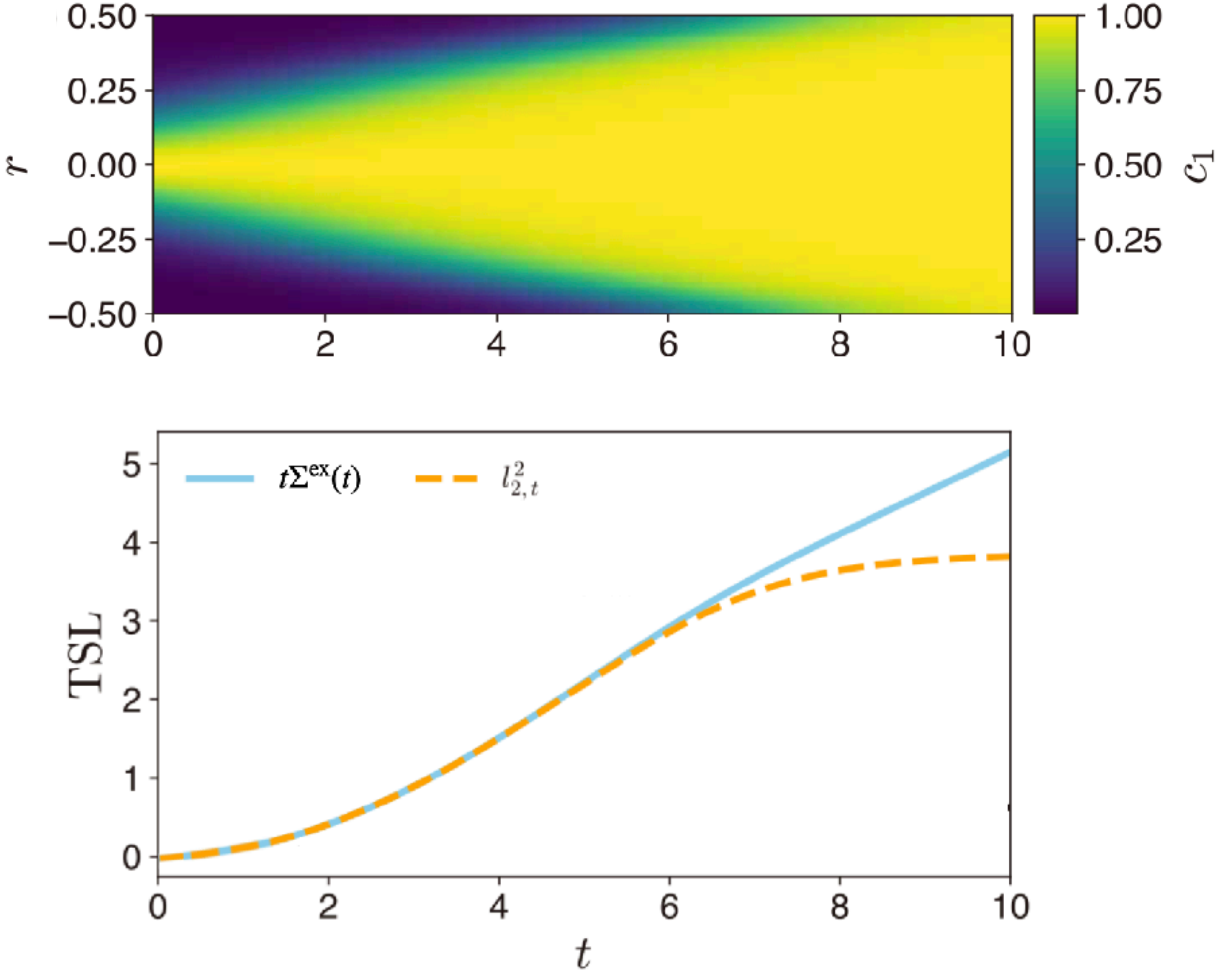
$$\Sigma^{\mathrm{ex}}(\tau) := \int_0^{\tau} dt \sigma_t^{\mathrm{ex}} \geq \frac{[l_{2,\tau}]^2}{\tau} \geq \frac{[\tilde{\mathcal{W}}_2(\vec{c}(0), \vec{c}(\tau))]^2}{\tau}$$

$l_{2,\tau} = \int_0^{\tau} dt v_2(t)$:Path length

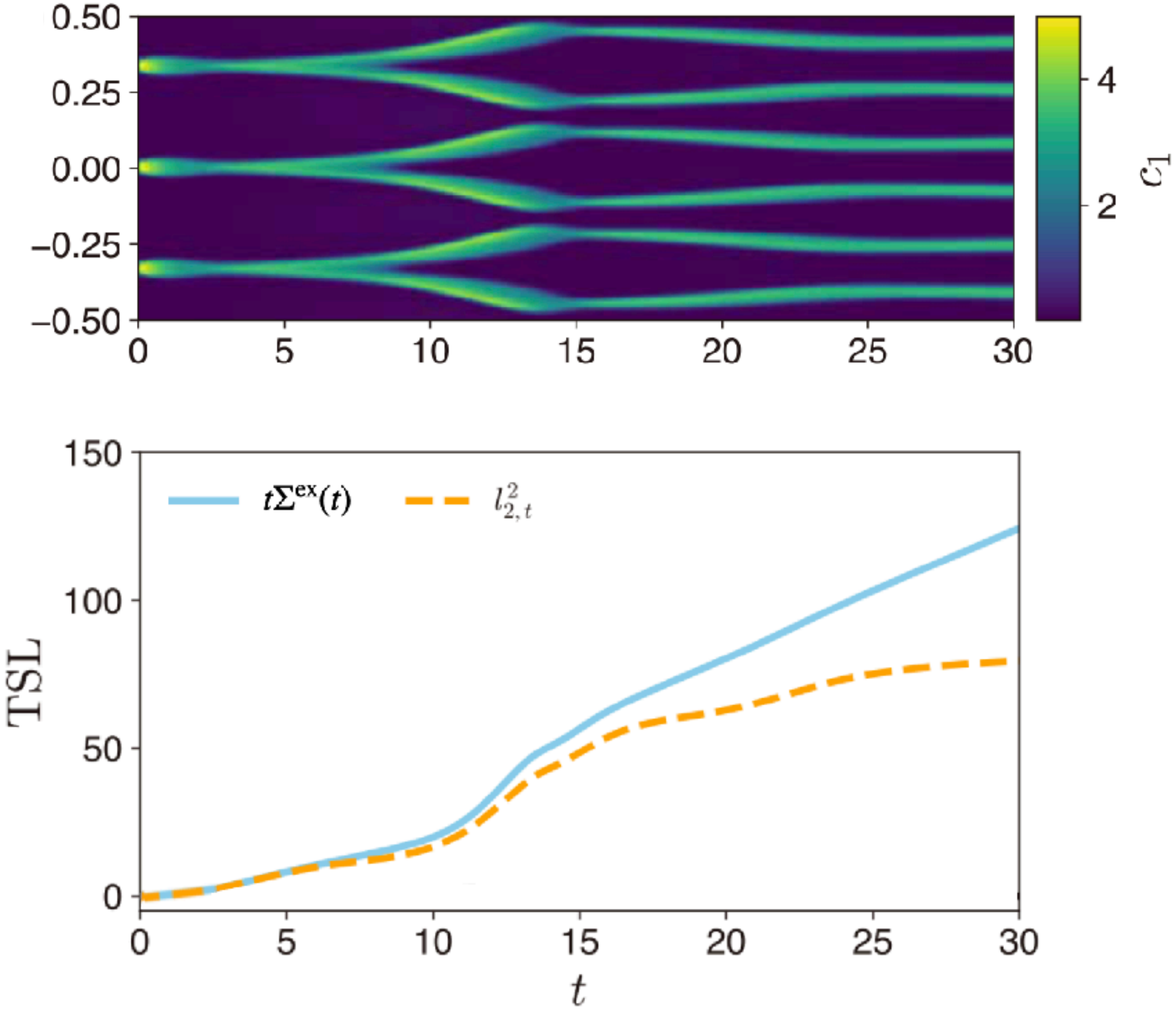
$l_{2,\tau} \geq \tilde{\mathcal{W}}_2(\vec{c}(0), \vec{c}(\tau))$ Geodesic

Numerical example:
Thermodynamic speed limit

1d-Fisher-KPP equation



1d-Brusselator



Thermodynamic uncertainty relation

Gradient flow

$$\partial_t \vec{c} = \nabla^\dagger \mathcal{M} \mathcal{F}^{\mathrm{ex}}$$

Cauchy-Schwartz inequality

$$(\langle \mathcal{F}^{\mathrm{ex}}, \nabla \vec{a} \rangle_{\mathcal{M}})^2 \leq \langle \mathcal{F}^{\mathrm{ex}}, \mathcal{F}^{\mathrm{ex}} \rangle_{\mathcal{M}} \langle \nabla \vec{a}, \nabla \vec{a} \rangle_{\mathcal{M}}$$

Thermodynamic uncertainty relations (for the reaction-diffusion systems)

$$\sigma^{\mathrm{ex}} \geq \frac{|d_t \langle \vec{a} \rangle_{\vec{c}}|^2}{\langle \nabla \vec{a}, \nabla \vec{a} \rangle_{\mathcal{M}}}$$

$$\langle \vec{a} \rangle_{\vec{c}} = \int d\boldsymbol{r} \sum_{\alpha} c_\alpha a_\alpha$$

Numerical example:
Thermodynamic uncertainty relation

Thermodynamic uncertainty relation

$$\sigma^{\mathrm{ex}} \geq \frac{|d_t\langle\vec{a}\rangle_{\vec{c}}|^2}{\langle\nabla\vec{a},\nabla\vec{a}\rangle_{\mathcal{M}}}$$

$$(\vec{a})_\beta = \delta_{\alpha\beta}\exp(-i\boldsymbol{k}\cdot\boldsymbol{r})$$

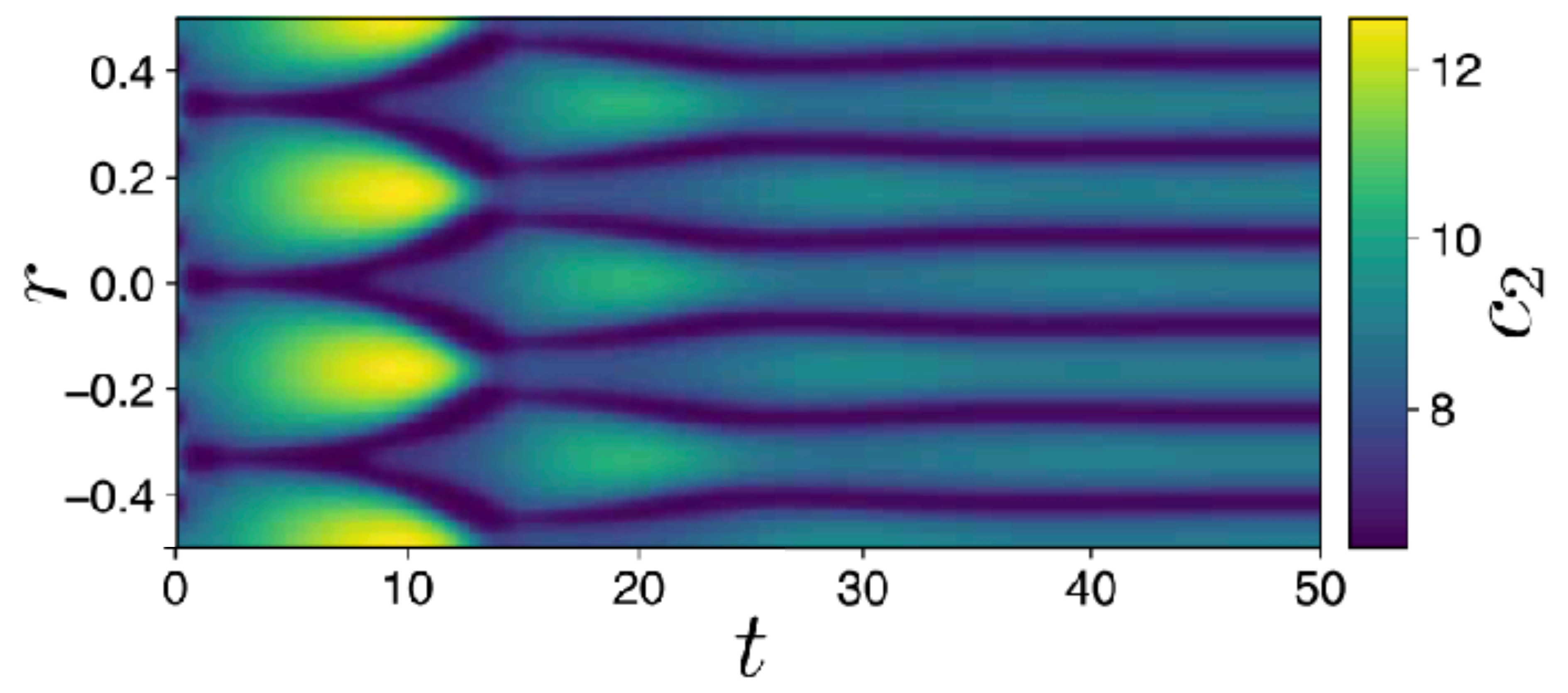
$$\langle\nabla\vec{a},\nabla\vec{a}\rangle_{\mathcal{M}} \geq \int d\boldsymbol{r}[(\nabla_{\boldsymbol{r}}\vec{a})^\dagger \mathsf{M}(\nabla_{\boldsymbol{r}}\vec{a}) + \underline{\vec{a}^\dagger D\vec{a}}]$$

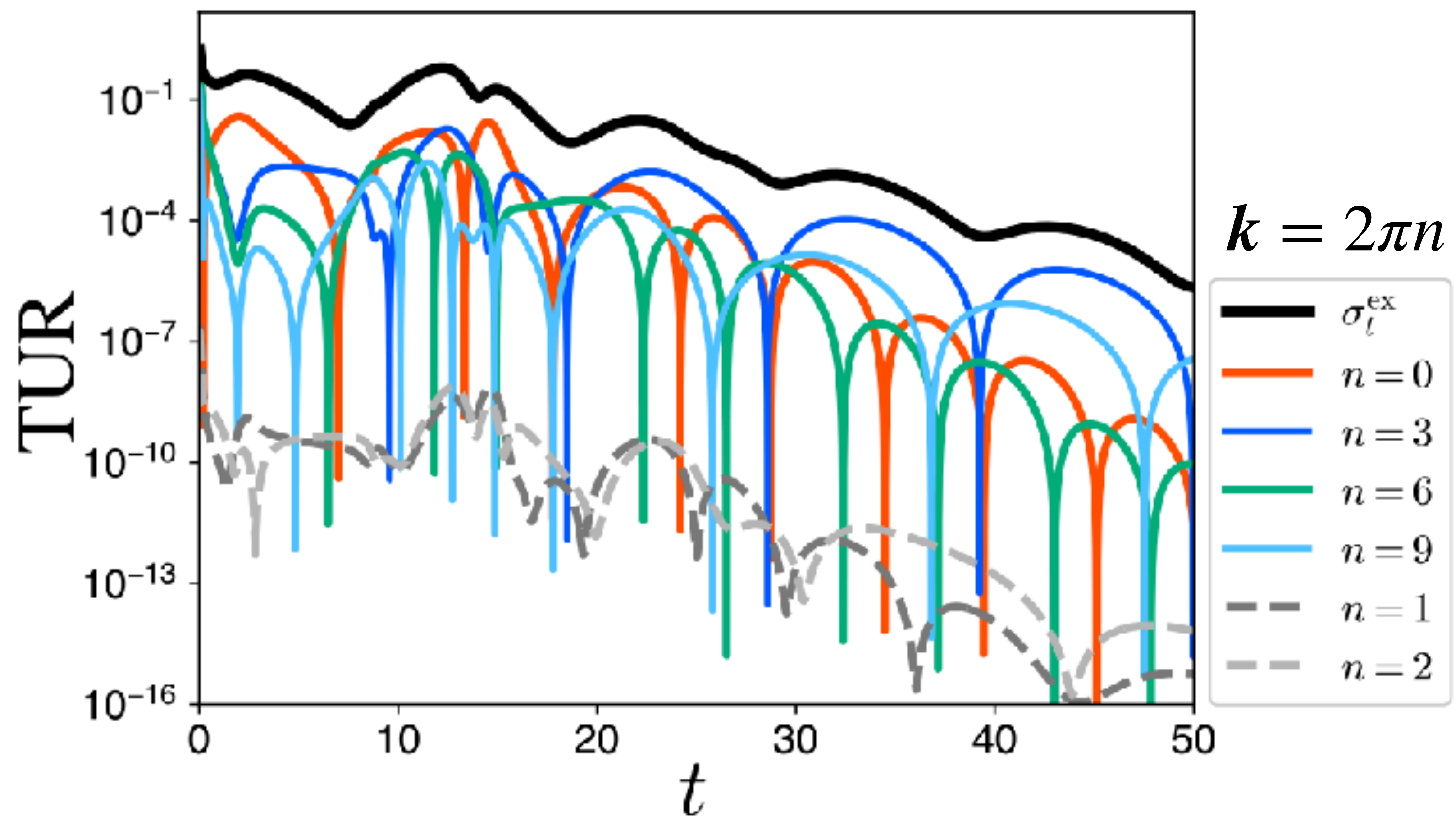
Chemical diffusion (activity)

"Wavenumber" thermodynamic uncertainty relation

$$\sigma^{\mathrm{ex}} \geq \frac{|d_t\tilde{c}_\alpha(\boldsymbol{k})|^2}{\boldsymbol{k}\cdot[\int d\boldsymbol{r}\mathsf{M}_{(\alpha\alpha)}]\boldsymbol{k} + \int d\boldsymbol{r}D_{\alpha\alpha}}$$

$$\tilde{c}_\alpha(\boldsymbol{k}) = \int d\boldsymbol{r}c_\alpha e^{-i\boldsymbol{k}\cdot\boldsymbol{r}}$$





3-fold symmetry ⇒ 6-fold symmetry

Outline

- Introduction:
  Minimum entropy production rate for the microscopic systems

- Minimum entropy production rate for the reaction-diffusion systems

  R. Nagayama, K. Yoshimura, A. Kolchinsky and SI. arXiv: 2311.16569.

- Minimum entropy production rate for the hydrodynamic systems

  K. Yoshimura and SI, Phys. Rev. Res. 6, L022057 (2024).

Hydrodynamic systems

Navier-Stokes equation

$$\rho D_t \boldsymbol{v} = \nabla \cdot \boldsymbol{\sigma}^{\mathrm{stress}}$$

$$D_t \boldsymbol{v} = \partial_t \boldsymbol{v} + \boldsymbol{v} \cdot \nabla \boldsymbol{v}$$

$$\boldsymbol{\sigma}^{\mathrm{stress}} = -p\mathsf{I} - \mathsf{J}^{\mathrm{irr}}(-\nabla^{\mathrm{S}}\boldsymbol{v})$$

Compressible Newtonian fluid

$$\mathsf{J}^{\mathrm{irr}}(-\nabla^{\mathrm{S}}\boldsymbol{v}) = \lambda \mathrm{tr}[-\nabla^{\mathrm{S}}\boldsymbol{v}]\mathsf{I} + 2\mu[-\nabla^{\mathrm{S}}\boldsymbol{v}]$$

$$\nabla^{\mathrm{S}}\boldsymbol{v} = \frac{\nabla \boldsymbol{v} + (\nabla \boldsymbol{v})^{\top}}{2}$$

Entropy production rate

S. R. de Groot and P. Mazur, Non-Equilibrium Thermodynamics (Dover, New York, 1984).

$$\sigma = \int_{\Omega} d\boldsymbol{r} \mathsf{J}^{\mathrm{irr}}(-\nabla^{\mathrm{S}}\boldsymbol{v}) : (-\nabla^{\mathrm{S}}\boldsymbol{v})$$

Ω:connected region

Hilbert-Schmidt inner product

$$\mathsf{A} : \mathsf{B} = \sum_{i,j} A_{ij} B_{ij}$$

Geometric structure

Force: $\mathsf{F} = -\nabla^{S}\boldsymbol{v}$

Flow: $\mathsf{J}^{\mathrm{irr}}(\mathsf{F})$

Entropy production rate

$$\sigma = \int_{\Omega} d\boldsymbol{r} \mathsf{J}^{\mathrm{irr}}(\mathsf{F}) : \mathsf{F} = \int_{\Omega} d\boldsymbol{r} \left[\lambda[\mathrm{tr}(\mathsf{F})]^2 + 2\mu \mathsf{F} : \mathsf{F}\right] = \langle \mathsf{F}, \mathsf{F} \rangle$$

Inner product

$$\langle \mathsf{A}, \mathsf{B} \rangle = \int_{\Omega} d\boldsymbol{r} \mathsf{J}^{\mathrm{irr}}(\mathsf{A}) : \mathsf{B} = \int_{\Omega} d\boldsymbol{r} [\lambda[\mathrm{tr}(\mathsf{A})][\mathrm{tr}(\mathsf{B})] + 2\mu \mathsf{A} : \mathsf{B}]$$

$$\partial_t X = -\nabla \cdot J$$

$$X \leftrightarrow \boldsymbol{v}$$

$$\partial_t X \leftrightarrow \rho D_t \boldsymbol{v} + \nabla p$$

$$J \leftrightarrow \mathsf{J}^{\mathrm{irr}}(\mathsf{F})$$

Geometric decomposition

$$\rho D_t \boldsymbol{v} = -\nabla p - \nabla \cdot (\mathsf{J}^{\mathrm{irr}}(\mathsf{F})) = -\nabla p - \nabla \cdot (\mathsf{J}^{\mathrm{irr}}(\mathsf{F}^{\mathrm{ex}}))$$

$$\mathsf{F}^{\mathrm{ex}} = -\nabla^{\mathrm{s}} \boldsymbol{u}^{\mathrm{ex}}$$

$\boldsymbol{u}^{\mathrm{ex}}$: Solution of

$$\nabla \cdot (\mathsf{J}^{\mathrm{irr}}(\mathsf{F}) - \mathsf{J}^{\mathrm{irr}}(-\nabla^{\mathrm{S}} \boldsymbol{u}^{\mathrm{ex}})) = \mathbf{0}$$

$$\boldsymbol{u}^{\mathrm{ex}}|_{\partial\Omega} = \mathbf{0}$$

Geometric decomposition

Orthogonality

$$\mathsf{F}^{\mathrm{hk}} = \mathsf{F} - \mathsf{F}^{\mathrm{ex}} \qquad \langle \mathsf{F}^{\mathrm{ex}}, \mathsf{F}^{\mathrm{hk}} \rangle = 0$$

→

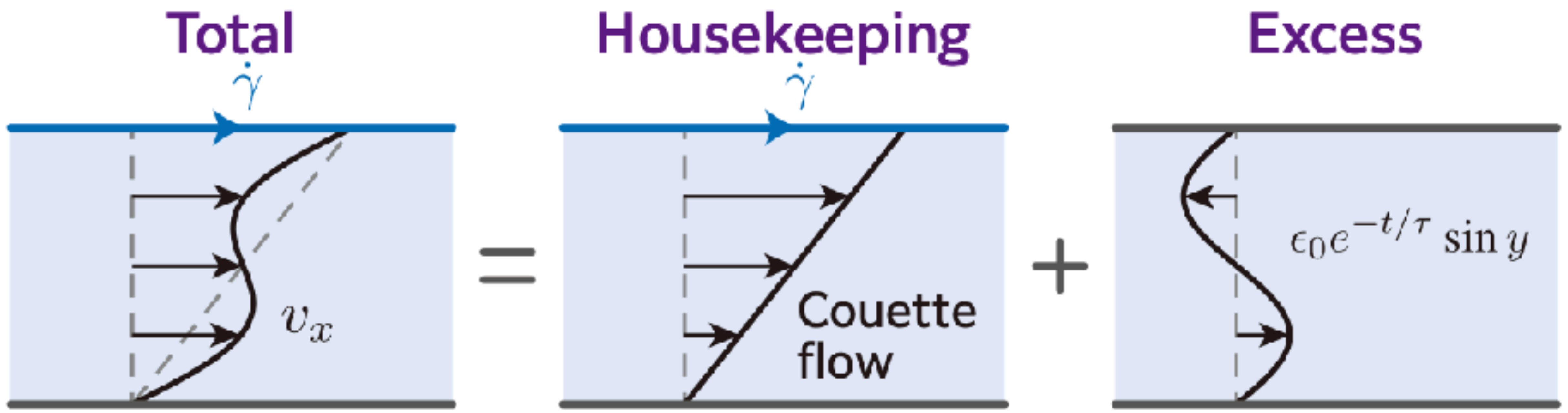
$$\underbrace{\langle \mathsf{F}^{\mathrm{ex}} + \mathsf{F}^{\mathrm{hk}}, \mathsf{F}^{\mathrm{ex}} + \mathsf{F}^{\mathrm{hk}} \rangle}_{\sigma} = \underbrace{\langle \mathsf{F}^{\mathrm{ex}}, \mathsf{F}^{\mathrm{ex}} \rangle}_{\sigma^{\mathrm{ex}}} + \underbrace{\langle \mathsf{F}^{\mathrm{hk}}, \mathsf{F}^{\mathrm{hk}} \rangle}_{\sigma^{\mathrm{hk}}}$$

Example: 2d perturbed Couette flow

$\Omega = S^1 \times [0,1]$ $\quad S^1$: 1d sphere of length 1

$\partial\Omega = S^1 \times (\{0\} \cup \{1\})$

$\boldsymbol{v}(x,0) = (0,0), \boldsymbol{v}(x,1) = (\dot{\gamma},0)$: shear rate $\dot{\gamma}$



$$\boldsymbol{v}(x,y,t) = (\gamma y + \epsilon(t)\sin(2\pi y),0) \quad \epsilon(t) = \epsilon_0 \exp\left(-\frac{4\pi^2\mu t}{\rho}\right)$$

$$\sigma^{\mathrm{ex}} = 2\pi^2\epsilon_0^2\mu \exp\left(-\frac{8\pi^2\mu t}{\rho}\right) \qquad \sigma^{\mathrm{hk}} = \mu\dot{\gamma}^2$$

Minimum entropy production rate and thermodynamic uncertainty relation

Minimum entropy production rate

$$\sigma^{\mathrm{ex}} = \inf_{\mathsf{F}'} \langle \mathsf{F}', \mathsf{F}' \rangle$$

s.t. $\rho D_t \boldsymbol{v} = -\nabla \cdot (p\mathrm{I} + \mathsf{J}^{\mathrm{irr}}(\mathsf{F}'))$ $\quad$ $\rho D_t \boldsymbol{v} + \nabla p$ is fixed.

cf.) Helmholtz minimum dissipation theorem for incompressible fluid (1868)

Cauchy-Schwartz inequality

$$(\langle \mathsf{F}^{\mathrm{ex}}, \nabla^{\mathrm{s}} \boldsymbol{a} \rangle)^2 \le \langle \mathsf{F}^{\mathrm{ex}}, \mathsf{F}^{\mathrm{ex}} \rangle \langle \nabla^{\mathrm{s}} \boldsymbol{a}, \nabla^{\mathrm{s}} \boldsymbol{a} \rangle$$

$\boldsymbol{a}$: Time-independent vector field satisfying $\nabla \cdot \boldsymbol{a} = 0$

$\langle \nabla^{\mathrm{S}} \boldsymbol{a}, \nabla^{\mathrm{S}} \boldsymbol{a} \rangle \ge \mu_{\max} \|\nabla \boldsymbol{a}\|^2$

Thermodynamic uncertainty relation

$$\sigma^{\mathrm{ex}} \ge \frac{J_{\boldsymbol{a}}^2}{\mu_{\max} \|\nabla \boldsymbol{a}\|^2}$$

$J_{\boldsymbol{a}} = \langle \mathsf{F}^{\mathrm{ex}}, \nabla^{\mathrm{s}} \boldsymbol{a} \rangle = \int_\Omega d\boldsymbol{r} \rho \boldsymbol{a} \cdot D_t \boldsymbol{v}$ $\quad$ $\mu_{\max} = \max_{\boldsymbol{r} \in \Omega} \mu$

$\|\nabla \boldsymbol{a}\|^2 = \int_\Omega d\boldsymbol{r} \nabla \boldsymbol{a} : \nabla \boldsymbol{a}$

If $\boldsymbol{a}$ is given by the vector field in the pathline, $J_{\boldsymbol{a}} = \partial_t \int_\Omega d\boldsymbol{r} \rho \boldsymbol{a} \cdot \boldsymbol{v}$

Summary

- We introduced stochastic thermodynamics based on optimal transport, and showed that the thermodynamic uncertainty relation and thermodynamic speed limit are derived from the geometric structure.

- We introduced the geometric structure for deterministic macroscopic systems (i.e., the reaction-diffusion systems and hydrodynamic systems). We derived thermodynamic uncertainty relations and minimum entropy production rate for the macroscopic system.

- Our results for the macroscopic systems are useful to understand the dissipation for the macroscopic behavior (e.g., the pattern formation and the perturbed Couette flow).

For more information and examples, see
R. Nagayama, K. Yoshimura, A. Kolchinsky and SI. arXiv: 2311.16569.
K. Yoshimura and SI, Phys. Rev. Res. 6, L022057 (2024).