

# Optimal transport: From stochastic thermodynamics to quantum many-body systems

最適輸送：ゆらぎ熱力学から量子多体系まで

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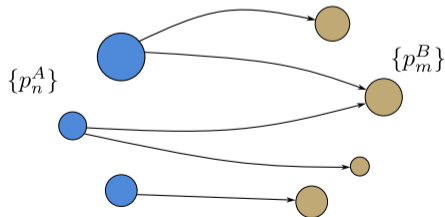
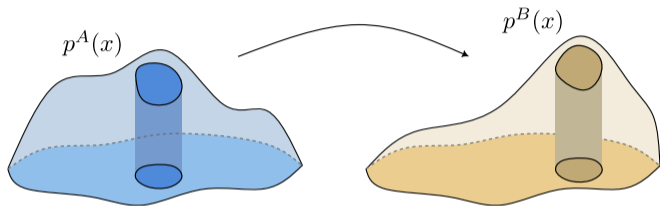
1. Optimal transport theory
2. Optimal transport and stochastic thermodynamics
3. Optimal transport and speed limits

# Optimal transport theory

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# Optimal transport

About the optimal planning and optimal cost of transporting distributions



## Monge formulation

Optimal transport cost with respect to a cost function  $c(x, y) : \mathbb{R}^d \times \mathbb{R}^d \mapsto \mathbb{R}_{\geq 0}$ :

$$M(p^A, p^B) := \min_{\varphi} \int c(x, \varphi(x)) p^A(x) dx$$

$\varphi : \mathbb{R}^d \mapsto \mathbb{R}^d$ : one-to-one map satisfying  $p^A(x) = p^B(\varphi(x)) |\nabla \varphi(x)|$

$\varphi^*$ : optimal transport map

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- ▶ Resolved by the relaxation of Kantorovich

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$\pi : \mathbb{R}^d \times \mathbb{R}^d \mapsto \mathbb{R}_{> 0}$ : coupling of  $p^A$  and  $p^B$  (a joint probability distribution function of  $x$  and  $y$ )

$$\int_{\mathbb{R}^d} \pi(x, y) dy = p^A(x) \text{ and } \int_{\mathbb{R}^d} \pi(x, y) dx = p^B(y)$$

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- ▶ Two formulations are equivalent when distributions are absolutely continuous

## $L^\alpha$ -Wasserstein distance

Optimal transport cost with respect to a cost function  $c(x, y) = \|x - y\|^\alpha$ :

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- ▶  $W_1$  and  $W_2$  are of interest

- ▶ Transport a  $N$ -dimensional distribution  $p^A = [p_x^A]$  to distribution  $p^B = [p_x^B]$  with respect to a cost matrix  $C = [c_{xy}]$



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$$W_\alpha(p^A, p^B)^\alpha := \min_{\pi \in \Pi(p^A, p^B)} \sum_{x,y} c_{xy}^\alpha \pi_{xy}$$

- $c_{xy} \geq 0$ : cost of transporting a unit probability from  $p_y^A$  to  $p_x^B$
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  - ▶ Number of choices for the cost matrix  $C$  is infinite

# Generalized Wasserstein distances

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$$\mathcal{W}_{1,\lambda}(\mathbf{x}^a, \mathbf{x}^b) := \min \left\{ \lambda(\|\mathbf{x}^a - \tilde{\mathbf{x}}^a\|_1 + \|\mathbf{x}^b - \tilde{\mathbf{x}}^b\|_1) + \mathcal{W}_1(\tilde{\mathbf{x}}^a, \tilde{\mathbf{x}}^b) \right\}$$

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- $\mathcal{W}_{1,\lambda}$  satisfies the triangle inequality

# Optimal transport and stochastic thermodynamics

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**Benamou–Brenier formula [Numer. Math. (2000)]**

$$W_2(p^A, p^B)^2 = \min_{v_t} \tau \int_0^\tau \int_{\mathbb{R}^d} \|v_t(x)\|^2 p_t(x) dx dt$$

the minimum is over all smooth paths  $\{v_t\}_{0 \leq t \leq \tau}$  subject to the continuity equation

$$\dot{p}_t(x) + \nabla \cdot [v_t(x)p_t(x)] = 0$$

with the initial and final conditions  $p_0(x) = p^A(x)$  and  $p_\tau(x) = p^B(x)$

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- For overdamped Fokker–Planck dynamics,  $v_t(x) = F_t(x) - D \nabla \ln p_t(x)$  and

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- ▶ Wasserstein distance in terms of dissipation

$$W_2(p^A, p^B) = \min_{F_t} \sqrt{D \tau \Sigma_\tau}$$

- ▶ Mandelstam-Tamm (MT) and Margolus-Levitin (ML) speed limits inspired by Heisenberg uncertainty principle  $\Delta t \times \Delta E \gtrsim \hbar$ :

$$\tau \geq \frac{\pi}{2} \max \left\{ \frac{\hbar}{\Delta H}, \frac{\hbar}{\langle H \rangle - E_g} \right\}$$

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# Essential applications of Benamou–Brenier formula

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- Quantum speed limits (QSLs): universal limitation on the operational time of quantum processes
- ▶ Thermodynamic speed limit for overdamped Langevin dynamics [Aurell et al., JSP (2012)]

$$\tau \geq \frac{W_2(p_0, p_\tau)}{\sqrt{D \langle \sigma \rangle_\tau}}$$

$\langle \sigma \rangle_\tau := \tau^{-1} \Sigma_\tau$ : time-average entropy production



## Landauer principle

Minimum heat dissipation required for erasing of one bit of information

$$Q \geq k_B T \ln 2$$

$T$ : the temperature of the environment

... | 0 | 1 | 1 | 0 | 1 | 0 | ...

↓  $\Lambda(\text{input})$

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- ▶ Finite-time Landauer principle

$$\beta Q \geq \ln 2 + \frac{W_2(p_0, p_\tau)^2}{D\tau}$$

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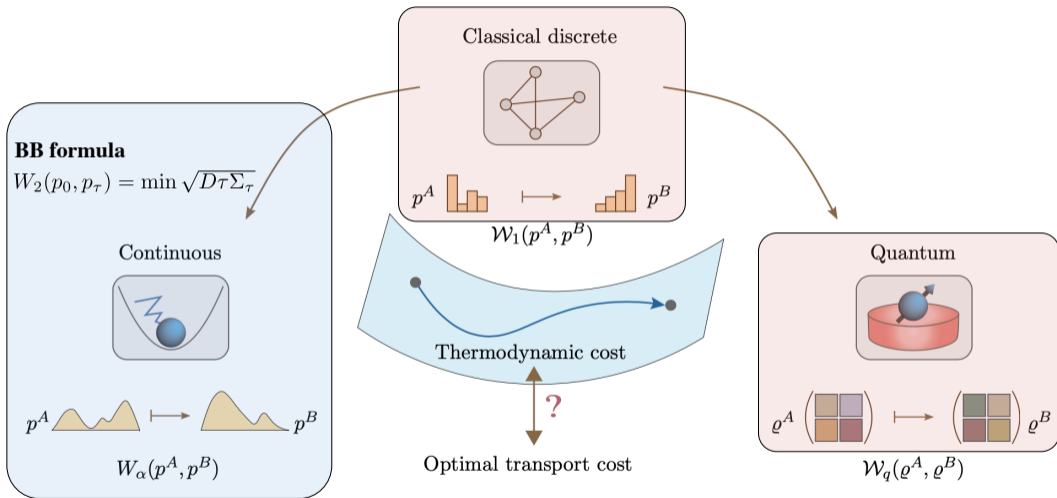
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- For 1D overdamped systems with double-well potentials [Proesman et al., PRL (2020)]

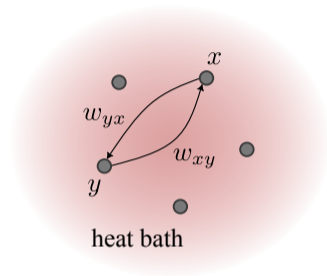
$$\beta Q \geq \ln 2 + \frac{\text{Var}(x)}{2D\tau}$$

# Motivation



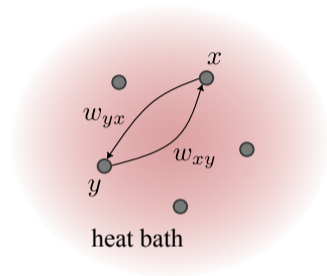
# Markov jump processes

- ▶ Discrete-state system with  $N$  states:  $\dot{p}_t = W_t p_t$ ,  $W_t = [w_{xy}(t)]$



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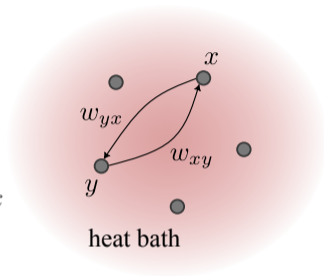


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$$\ln \frac{w_{xy}(t)}{w_{yx}(t)} = s_{xy}(t)$$

$s_{xy}(t)$ : environmental entropy change associated with jump  $y \rightarrow x$



# Markov jump processes

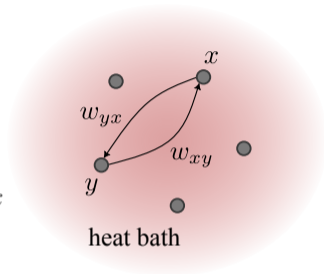
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- ▶ Irreversible entropy production rate

$$\sigma_t := \dot{s}_{\text{sys}}(t) + \dot{s}_{\text{env}}(t) = \frac{1}{2} \sum_{x \neq y} [a_{xy}(t) - a_{yx}(t)] \ln \frac{a_{xy}(t)}{a_{yx}(t)} \geq 0$$



$$a_{xy}(t) := w_{xy}(t)p_y(t)$$

$$j_{xy}(t) := a_{xy}(t) - a_{yx}(t)$$

$$f_{xy}(t) := \ln \frac{a_{xy}(t)}{a_{yx}(t)}$$



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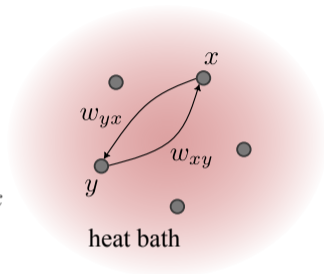
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- ▶ Dynamical activity  $\mathcal{A}_\tau := \int_0^\tau a_t dt$  quantifies the total number of jumps

$$a_t := \sum_{x \neq y} a_{xy}(t)$$



$$a_{xy}(t) := w_{xy}(t)p_y(t)$$

$$j_{xy}(t) := a_{xy}(t) - a_{yx}(t)$$

$$f_{xy}(t) := \ln \frac{a_{xy}(t)}{a_{yx}(t)}$$

- ▶ Onsager kinetic coefficients at the transition level:

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Linear response regime	Nonlinear regime
$J_x = \sum_y \mu_{xy} F_y$	$j_{xy}(t) = m_{xy}(t) f_{xy}(t)$
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- Kinetic cost  $\mathcal{M}_\tau := \int_0^\tau m_t dt = \tau \langle m \rangle_\tau$

- ▶ Analogy between the dynamical state mobility and macroscopic mobility

Macroscopic level	Microscopic level
$J = \mu F$	$j_{xy} = m_{xy} f_{xy}$
Einstein relation $ F  \ll 1$ $\mu = \beta D$	Einstein-like relation $ f_{xy}  \ll 1$ $m_{xy} = (a_{xy} + a_{yx})/2$



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- ▶ Improved thermodynamic uncertainty relation [Gingrich et al., PRL (2016)]

$$\frac{\langle J \rangle^2}{\text{Var}[J]} \leq \eta \frac{\Sigma_\tau}{2} \leq \frac{\Sigma_\tau}{2}$$

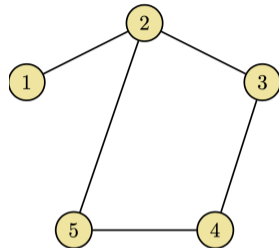
$$\eta := 2\mathcal{M}_\tau/\mathcal{A}_\tau \leq 1$$

# Wasserstein distance based on connectivity of Markov jump processes

►  $\mathcal{G}(V, E)$ : graph characterizing topology of Markov jump process

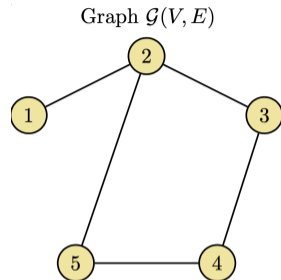
- $V$ : set of states
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Graph  $\mathcal{G}(V, E)$



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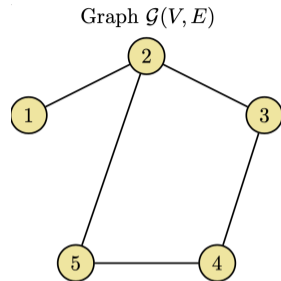
Shortest-path distances  $\{d_{xy}\}$

0	1	2	3	2
1	0	1	2	1
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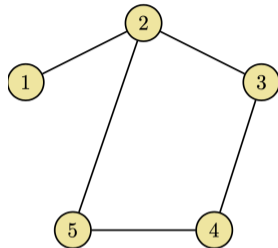
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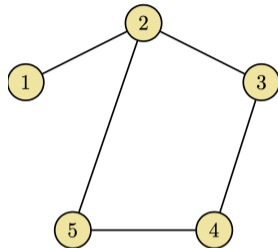
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## Theorem 1

The Wasserstein distance based on a topology  $\mathcal{G}(V, E)$  can be written in variational forms as

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the minimum is taken over all transition rate matrices  $\{\mathbb{W}_t\}_{0 \leq t \leq \tau}$  which satisfy the master equation with the boundary conditions  $p_0 = p^A$  and  $p_\tau = p^B$  and induce subgraphs of  $\mathcal{G}(V, E)$  for all times

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[step 1] Prove that  $\mathcal{W}_1(p^A, p^B) \leq \int_0^\tau \sqrt{\sigma_t m_t} dt \leq \sqrt{\Sigma_\tau \mathcal{M}_\tau}$  holds for all admissible Markovian dynamics that transform  $p^A$  into  $p^B$

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[step 2] Construct a specific process that attains the equality

## Remarks of Theorem 1

- ▶ Analogous thermodynamic properties with the continuous  $L^2$ -Wasserstein distance

$$\mathcal{W}_1(p^A, p^B) = \min_{W_t} \sqrt{\bar{D} \tau \Sigma_\tau} \quad \left[ \leftrightarrow W_2(p^A, p^B) = \min_{F_t} \sqrt{D \tau \Sigma_\tau} \right]$$

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- ▶ Tradeoff between irreversibility and state mobility:  $\Sigma_\tau \mathcal{M}_\tau \geq \mathcal{W}_1(p_0, p_\tau)^2$ 
  - Either the thermodynamic or kinetic cost must be sacrificed to achieve a feasible state transformation

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- Taking the continuum limit yields

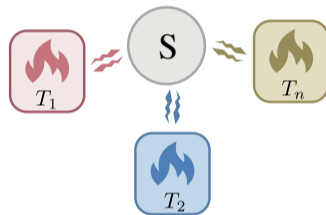
$$W_1(p^A, p^B) = \min_{j_t} \int_0^\tau \int_{\mathbb{R}} |j_t(x)| dx dt$$

Providing a unified generalization of the Benamou–Brenier formula for the  $L^1$ -Wasserstein distance

# Markovian open quantum dynamics

- ▶ Discrete-state dynamics obeying GKSL master equation

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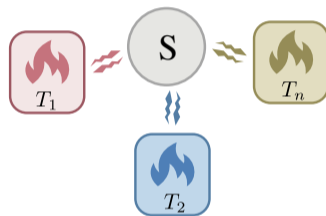
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- ▶ Local detailed balance  $L_k(t) = e^{s_k(t)/2} L_{k'}(t)^\dagger$

$s_k(t) = -s_{k'}(t)$ : entropy change in the environment



- ▶ Irreversible entropy production

$$\Sigma_\tau := \Delta S_{\text{sys}} + \Delta S_{\text{env}} \geq 0$$

$\Delta S_{\text{sys}} := S(\rho_\tau) - S(\rho_0)$ : change in the von Neumann entropy

$\Delta S_{\text{env}} := \int_0^\tau \sum_k \text{tr} \left\{ L_k(t) \rho_t L_k^\dagger(t) \right\} s_k(t) dt$ : environmental entropy production

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$$m_t := \frac{1}{2} \sum_k e^{-s_k(t)/2} \left\langle L_k(t)^\dagger, \llbracket \varrho_t \rrbracket_{s_k(t)} (\mathcal{P}_t[L_k(t)^\dagger]) \right\rangle$$

$$\langle X, Y \rangle := \text{tr} \{ X^\dagger Y \}$$

$$\mathcal{P}_t[X] := X - \sum_x \langle x_t | X | x_t \rangle | x_t \rangle \langle x_t |$$

$$\llbracket \phi \rrbracket_\theta(X) := e^{-\theta/2} \int_0^1 e^{\theta u} \phi^u X \phi^{1-u} du$$

$\varrho_t = \sum_x p_x(t) |x_t\rangle \langle x_t|$ : spectral decomposition of the density matrix  $\varrho_t$

- ▶ Naive quantum extension

$$W_q(\varrho^A, \varrho^B) := \min_{\varrho^{AB} \in \Pi(\varrho^A, \varrho^B)} \text{tr}\{C \varrho^{AB}\}$$

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- ▶  $W_q(\varrho_0, \varrho_\tau) > 0$  even for unitary dynamics  $\varrho_\tau = U \varrho_0 U^\dagger$  with zero entropy production
  - Relating dissipation to the optimal transport distances defined in the naive form is impossible

- ▶ Considering dissipative structure of Lindblad dynamics, we define

$$\mathcal{W}_q(\varrho^A, \varrho^B) := \frac{1}{2} \min_{V^\dagger V = \mathbb{1}} \|V\varrho^A V^\dagger - \varrho^B\|_1$$

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the minimum is over all possible unitaries  $V$

- Analytical expression

$$\mathcal{W}_q(\varrho^A, \varrho^B) = \frac{1}{2} \sum_x |p_x^A - p_x^B| = \mathcal{T}(p^A, p^B)$$

$\{p_x^A\}$  and  $\{p_x^B\}$ : increasing eigenvalues of  $\varrho^A$  and  $\varrho^B$ , respectively

## Theorem 2

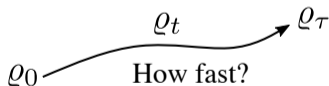
The quantum Wasserstein distance can be written in the following variational form:

$$\begin{aligned}\mathcal{W}_q(\varrho^A, \varrho^B) &= \min_{\mathcal{L}_t} \int_0^\tau \sqrt{\sigma_t m_t} dt \\ &= \min_{\mathcal{L}_t} \sqrt{\Sigma_\tau \mathcal{M}_\tau}\end{aligned}$$

the minimum is taken over all super-operators  $\{\mathcal{L}_t\}_{0 \leq t \leq \tau}$  that satisfy the Lindblad master equation with boundary conditions  $\varrho_0 = \varrho^A$  and  $\varrho_\tau = \varrho^B$

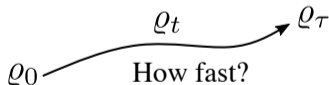
- ▶ **Thermodynamic speed limit:** lower bound on the operational time required for state transformations

$$\tau \geq \frac{\mathcal{W}_1(p_0, p_\tau)}{\langle \sqrt{\sigma m} \rangle_\tau} \geq \frac{\mathcal{W}_1(p_0, p_\tau)}{\sqrt{\langle \sigma \rangle_\tau \langle m \rangle_\tau}}$$



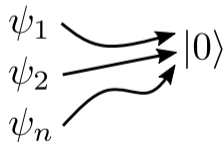
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- ▶ **Finite-time Landauer principle:** lower bound on heat dissipation required for erasing information

$$Q \geq -T \Delta S_{\text{sys}} + \frac{\mathcal{W}_1(p_0, p_\tau)^2}{\tau \beta \langle m \rangle_\tau}$$





## Numerical demonstration

Pareto-optimal protocol in information erasure of qubit

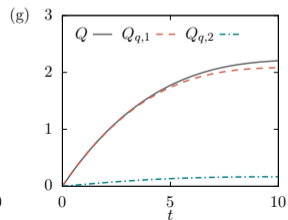
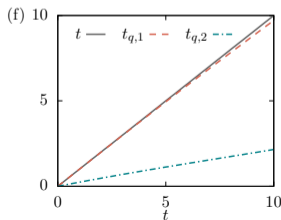
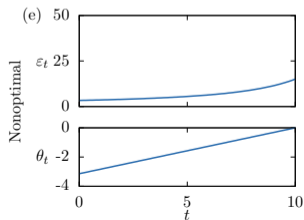
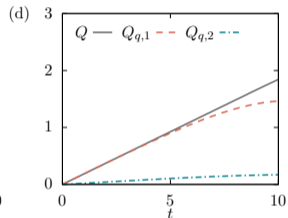
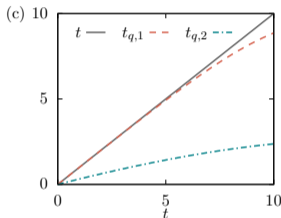
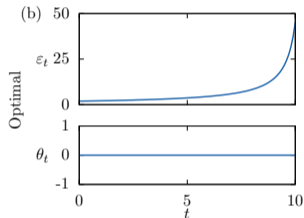
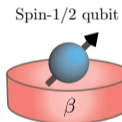
$$\mathcal{F}_q[\{\varepsilon_t, \theta_t\}] := \lambda Q - (1 - \lambda)F(\varrho_\tau, \varrho_*)$$

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Pareto-optimal protocol in information erasure of qubit

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(a)



# Take-home message

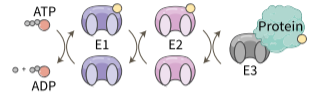
	Continuous	Classical discrete	Quantum
Wasserstein distance	$W_\alpha$ ( $\alpha \geq 1$ )	$W_1$	$W_q$
Thermodynamic interpretation of optimal transport	Benamou–Brenier formula $W_2(p^A, p^B) = \min \sqrt{\tau D \Sigma_\tau}$ $W_1(p^A, p^B) \leq \min \sqrt{\tau D \Sigma_\tau}$	Theorem 1 $W_1(p^A, p^B) = \min \sqrt{\tau \langle m \rangle_\tau \Sigma_\tau}$	Theorem 2 $W_q(\varrho^A, \varrho^B) = \min \sqrt{\tau \langle m \rangle_\tau \Sigma_\tau}$
Minimum dissipation	$\min \Sigma_\tau = \frac{W_2(p^A, p^B)^2}{\tau D}$	$\min_{\langle m \rangle_\tau = D} \Sigma_\tau = \frac{W_1(p^A, p^B)^2}{\tau D}$	$\min_{\langle m \rangle_\tau = D} \Sigma_\tau = \frac{W_q(\varrho^A, \varrho^B)^2}{\tau D}$
Thermodynamic speed limit	$\tau \geq \frac{W_{2(1)}(p^A, p^B)}{\sqrt{D \langle \sigma \rangle_\tau}}$	$\tau \geq \frac{W_1(p^A, p^B)}{\sqrt{\langle m \rangle_\tau \langle \sigma \rangle_\tau}}$	$\tau \geq \frac{W_q(\varrho^A, \varrho^B)}{\sqrt{\langle m \rangle_\tau \langle \sigma \rangle_\tau}}$

# Optimal transport and speed limits

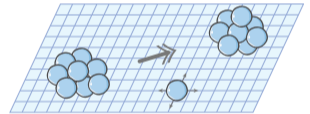
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# Motivation

- ▶ Interacting systems generally form spatial structures in their dynamics



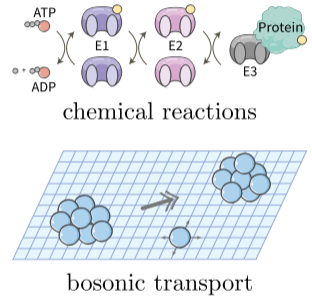
chemical reactions



bosonic transport

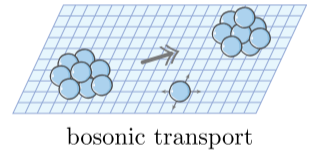
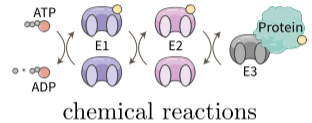
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  - Systems with long-range interactions may propagate information faster [J. Eisert et al., PRL (2013)]



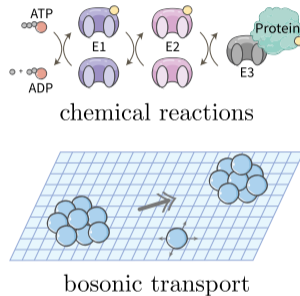
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- ▶ Conventional speed limits

$$\tau \geq \frac{\mathcal{L}(\mathbf{x}_0, \mathbf{x}_\tau)}{\bar{v}}$$

$\mathcal{L}(\mathbf{x}_0, \mathbf{x}_\tau) \leq C$  (irrelevant to system size)

$\bar{v}$ : velocity generally being order of system size





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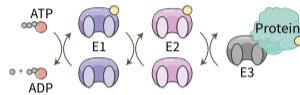
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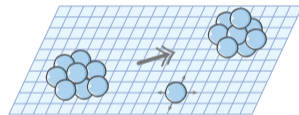
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- ▶ These speed limits generally become less tight as the system increases in terms of size

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chemical reactions



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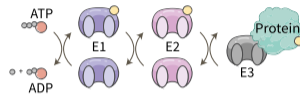
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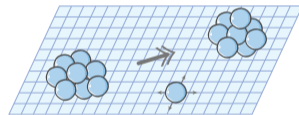
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- ▶ Metrics that are scalable to system size should be considered



chemical reactions



bosonic transport

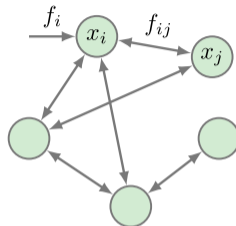
# General dynamics

- ▶ A physical state  $\mathbf{x}_t = [x_1(t), \dots, x_N(t)]$  described by

$$\dot{x}_i(t) = f_i(t) + \sum_{j \in \mathcal{B}_i} f_{ij}(t)$$

$f_{ij}(t) = -f_{ji}(t)$ : flow exchange between  $i$  and  $j$

$f_i(t)$ : arbitrary external flow



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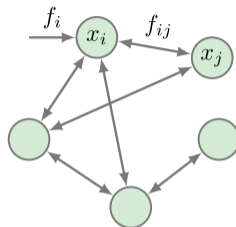
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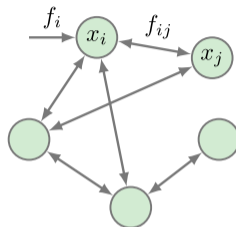
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- ▶ Time-dependent velocity

$$v_{t,\lambda} := \lambda \sum_i |f_i(t)| + \sum_{(i,j) \in \mathcal{E}} |f_{ij}(t)|$$

$\lambda \geq 0$ : weighting factor



$$\dot{x}_i(t) = f_i(t) + \sum_{j \in \mathcal{B}_i} f_{ij}(t)$$

## Speed limit using generalized Wasserstein distance

The operational time required for transform  $\mathbf{x}_0$  into  $\mathbf{x}_\tau$  is lower bounded by the Wasserstein distance divided by the average velocity:

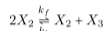
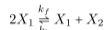
$$\tau \geq \frac{\mathcal{W}_{1,\lambda}(\mathbf{x}_0, \mathbf{x}_\tau)}{\langle v_{t,\lambda} \rangle_\tau} \quad \forall \lambda \geq 0$$

In the case that the external flows are absent [i.e.,  $f_i(t) = 0$ ]

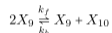
$$\tau \geq \frac{\mathcal{W}_1(\mathbf{x}_0, \mathbf{x}_\tau)}{\langle v_t \rangle_\tau}$$

## Quantitative

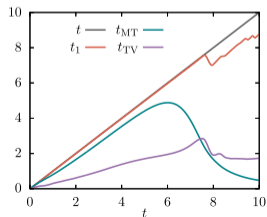
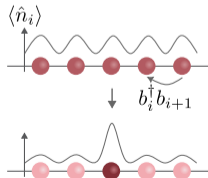
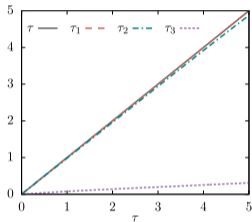
Reaction channels



⋮



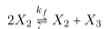
Graph  $G(\mathcal{V}, \mathcal{E})$



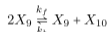
$$H_t = -\gamma \sum_{i=1}^{N-1} (b_i^\dagger b_{i+1} + b_{i+1}^\dagger b_i) + \sum_{i=1}^N U_i(t) \hat{n}_i (\hat{n}_i - 1) / 2$$

## Quantitative

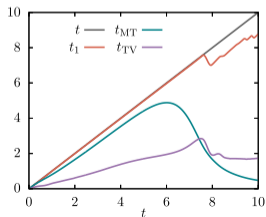
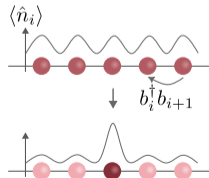
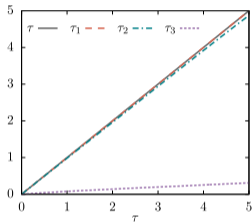
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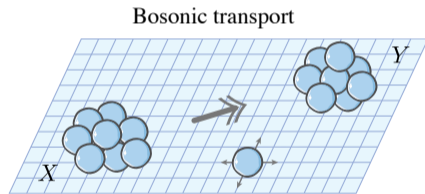
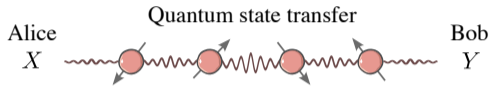


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## Qualitative



time  $\propto$  dist( $X, Y$ )



- ▶ Model of bosons that hop on an arbitrary finite-dimensional lattice and interact with each other

$$H := -\gamma \sum_{(i,j)} (b_i^\dagger b_j + b_j^\dagger b_i) + \sum_{Z \subseteq \Lambda} h_Z$$

## Applications – Bosonic transport

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- ▶ Weakly coupled to a Markovian thermal reservoir and can exchange particles with the reservoir

$$\dot{\rho}_t = -i[H, \rho_t] + \sum_{i \in \Lambda} (\mathcal{D}[L_{i,+}] + \mathcal{D}[L_{i,-}])\rho_t$$

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- ▶ Time evolution of  $x_i(t)$  can be expressed using  $f_i(t) = \text{tr}\{L_{i,+} \rho_t L_{i,+}^\dagger\} - \text{tr}\{L_{i,-} \rho_t L_{i,-}^\dagger\}$  and  $f_{ij}(t) = 2\gamma \Im[\text{tr}\{b_j^\dagger b_i \rho_t\}]$

- ▶ Upper bound of velocity

$$v_{t,\lambda} \leq \gamma d_G \mathcal{N}_t + \lambda \frac{\sigma_t}{2} \Phi\left(\frac{\sigma_t}{2a_t}\right)^{-1}$$

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- ▶ Thermodynamic speed limit

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- This statement holds for *arbitrary* initial states, including the pure states considered in [Faupin et al., PRL (2022)]

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- ▶ Applicable to a wide range of dynamics, from classical to quantum, from continuous time to discrete time

## Corollary 1

The discrete Wasserstein distance can be expressed in terms of irreversible entropy production and dynamical activity as

$$\begin{aligned}\mathcal{W}_1(p^A, p^B) &= \min_{\mathcal{W}_t} \int_0^\tau \frac{\sigma_t}{2} \Phi\left(\frac{\sigma_t}{2a_t}\right)^{-1} dt \\ &= \min_{\mathcal{W}_t} \frac{\Sigma_\tau}{2} \Phi\left(\frac{\Sigma_\tau}{2\mathcal{A}_\tau}\right)^{-1}\end{aligned}$$

$\Phi(x)$ : inverse function of  $x \tanh(x)$

## Corollary 2

The discrete Wasserstein distance can be expressed in terms of pseudo entropy production and dynamical activity as

$$\begin{aligned}\mathcal{W}_1(p^A, p^B) &= \min_{W_t} \int_0^\tau \sqrt{\sigma_t^{\text{ps}} a_t} dt \\ &= \min_{W_t} \sqrt{\Sigma_\tau^{\text{ps}} \mathcal{A}_t}\end{aligned}$$

$\sigma_t^{\text{ps}} := \dot{\Sigma}_t^{\text{ps}}$ : the pseudo entropy production rate

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$\sigma_t^{\text{PS}} := \dot{\Sigma}_t^{\text{PS}}$ : the pseudo entropy production rate

- ▶ Pseudo entropy production rate

$$\sigma_t^{\text{PS}} = \sum_{m>n} \frac{(a_{mn}(t) - a_{nm}(t))^2}{a_{mn}(t) + a_{nm}(t)} \leq \sigma_t/2$$



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- ▶  $(\Sigma_\tau, \mathcal{M}_\tau)$  and  $(\Sigma_\tau^{\text{ps}}, \mathcal{A}_\tau)$  are two thermodynamic-kinetic conjugate pairs in the context of optimal transport

## Corollary 3

The quantum Wasserstein distance can be expressed in terms of irreversible entropy production and dynamical activity as

$$\begin{aligned}\mathcal{W}_q(\varrho^A, \varrho^B) &= \min_{\mathcal{L}_t} \int_0^\tau \frac{\sigma_t}{2} \Phi\left(\frac{\sigma_t}{2a_t}\right)^{-1} dt \\ &= \min_{\mathcal{L}_t} \frac{\Sigma_\tau}{2} \Phi\left(\frac{\Sigma_\tau}{2\mathcal{A}_\tau}\right)^{-1}\end{aligned}$$