Stochastic thermodynamics of discrete optimal transport

Tan Van Vu (RIKEN)

in collaboration with K. Saito (Keio Universtiy)
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Workshop OT 2023
最適輸送とその周辺– 機械学習から熱力学的最適化まで

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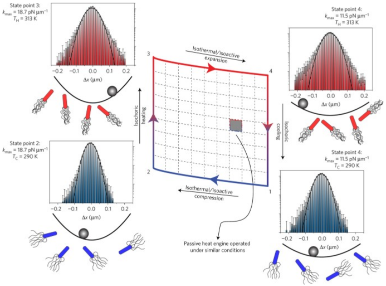
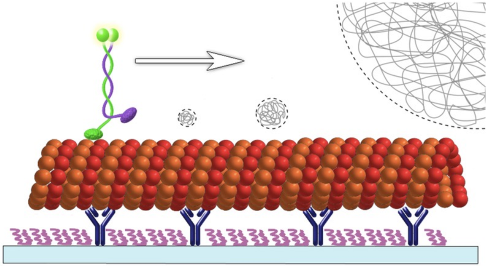
Stochastic thermodynamics

- Extension of traditional thermodynamics for small systems (e.g., nanoscale heat engines, molecular motors, etc.)



Nat. Phys. 12, 1134 (2016)



Physics 8, 114 (2015)

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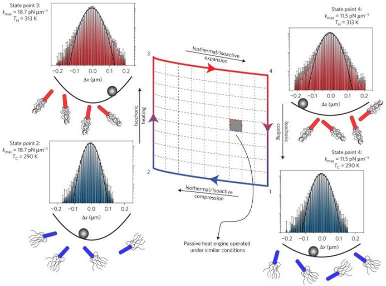

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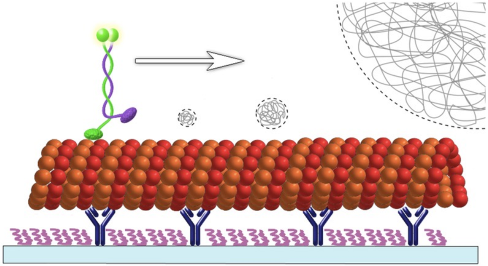

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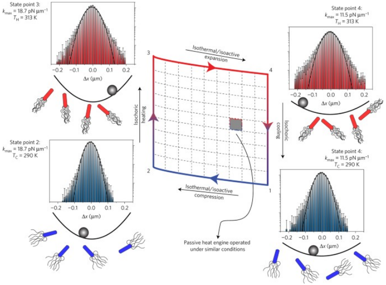
Stochastic thermodynamics

- Extension of traditional thermodynamics for small systems (e.g., nanoscale heat engines, molecular motors, etc.)
  - Thermodynamic quantities (e.g., energy, heat, and work) become stochastic
  - Incorporating other scientific fields (e.g., information theory, differential geometry, resource theory, optimal transport theory)



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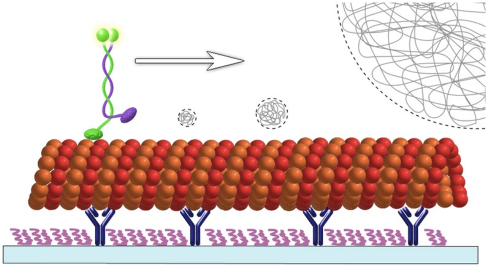

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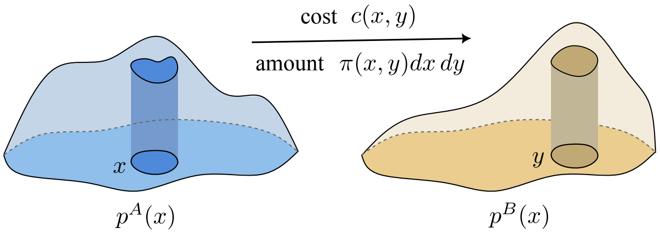
Optimal transport

Kantorovich formulation

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

$$K(p^A, p^B) \coloneqq \min_{\pi} \int c(x, y)\pi(x, y)\, dx\, dy$$

$\pi : \mathbb{R}^d \times \mathbb{R}^d \mapsto \mathbb{R}_{\geq 0}$: joint probability distribution function of p^A and p^B



Wasserstein distances

L^α-Wasserstein distance

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

$$W_\alpha(p^A, p^B)^\alpha \coloneqq \min_\pi \int \|x - y\|^\alpha \pi(x, y)\, dx\, dy$$

$\|\cdot\|$: Euclidean norm

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- $W_{\alpha'} \geq W_\alpha$ for any $\alpha' \geq \alpha \geq 1$
- W_1 and W_2 are of interest

Thermodynamics of continuous-variable optimal transport

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

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

velocity field $\{v_t\}_{0 \le t \le \tau}$ satisfies the continuity equation

$$\dot{p}_t(x) + \nabla \cdot [v_t(x) p_t(x)] = 0, \;\; p_0(x) = p^A(x), \;\; p_\tau(x) = p^B(x)$$

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

$$\Sigma_\tau = \frac{1}{D} \int_0^\tau \int_{\mathbb{R}^d} \|v_t(x)\|^2 p_t(x)\, dx\, dt$$

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- L^2-Wasserstein distance in terms of entropy production

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

Essential implications of Benamou–Brenier formula

- Thermodynamic speed limit for overdamped Langevin dynamics [Aurell et al., JSP (2012)]

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

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

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

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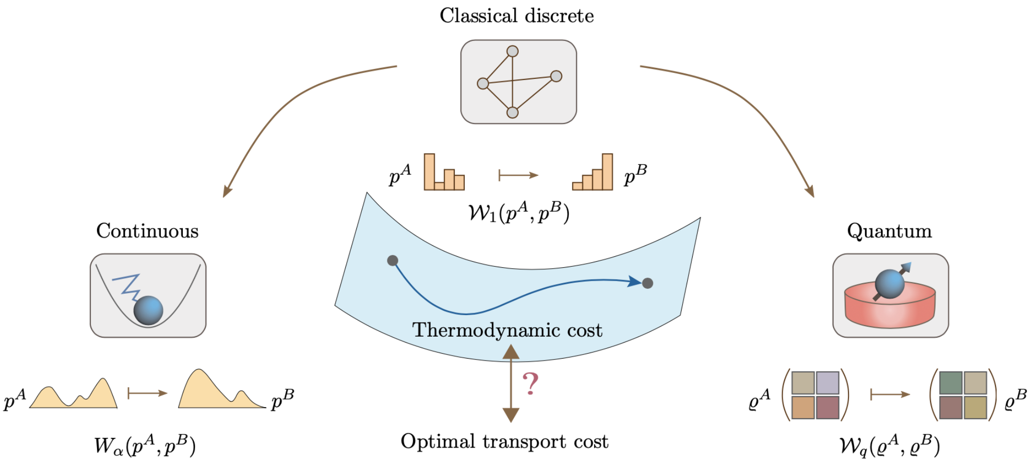
  - For 1D overdamped systems with double-well potentials and proper initial and final distributions, $W_2(p_0, p_\tau)^2 \geq \mathrm{Var}(x)/2$. Thus, we obtain [Proesman et al., PRL (2020)]

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

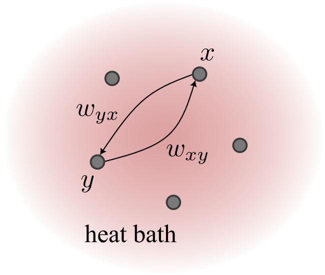
Generalizations of Benamou-Brenier formula for discrete-state systems?



Discrete-state Markovian dynamics

Markov jump processes

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



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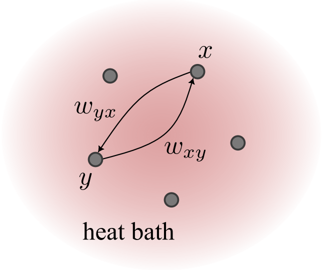

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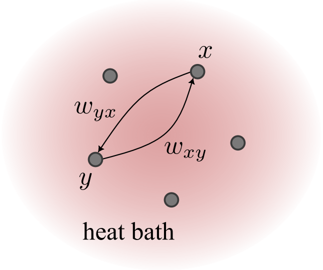
- Local detailed balance

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

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



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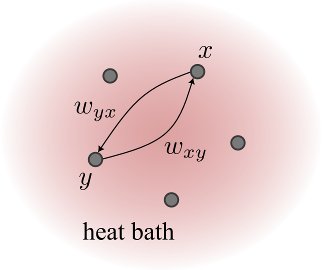

- Irreversible entropy production rate

$$\sigma_t \coloneqq \dot{\Sigma}_t = \frac{1}{2} \sum_{x \neq y} [a_{xy}(t) - a_{yx}(t)] \ln \frac{a_{xy}(t)}{a_{yx}(t)} \geq 0$$

$$a_{xy}(t) \coloneqq w_{xy}(t) p_y(t)$$

$$j_{xy}(t) \coloneqq a_{xy}(t) - a_{yx}(t)$$

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

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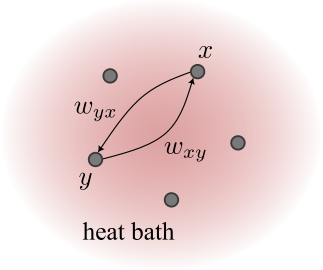

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- Dynamical activity $\mathcal{A}_\tau \coloneqq \int_0^\tau a_t \, dt$ quantifies the total number of jumps

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

$$a_{xy}(t) \coloneqq w_{xy}(t) p_y(t)$$

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Dynamical state mobility

- Onsager kinetic coefficients at the transition level

$$m_{xy}(t) \coloneqq \frac{a_{xy}(t) - a_{yx}(t)}{\ln a_{xy}(t) - \ln a_{yx}(t)} = \frac{j_{xy}(t)}{f_{xy}(t)}$$

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Linear response regime	Nonlinear regime
$J_x = \sum_y \mu_{xy} F_y$	$j_{xy}(t) = m_{xy}(t) f_{xy}(t)$
$\sigma = \sum_x J_x F_x = \sum_{x,y} \mu_{xy} F_x F_y$	$\sigma_t = \sum_{x>y} m_{xy}(t) f_{xy}(t)^2$

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- Dynamical state mobility

$$m_t := \sum_{x>y} m_{xy}(t)$$

  - Kinetic cost $\mathcal{M}_\tau := \int_0^\tau m_t \, dt = \tau \langle m \rangle_\tau$

Dynamical state mobility

- Analogy between the dynamical state mobility and macroscopic mobility

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

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- In the continuous-state limit, $m_t \to a_t/2 = D(\Delta x)^{-2}$
- Improved thermodynamic uncertainty relation [Gingrich et al., PRL (2016)]

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

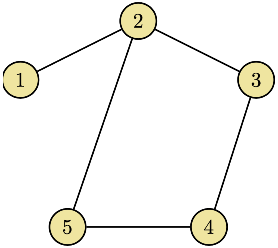
$\eta \coloneqq 2\mathcal{M}_\tau/\mathcal{A}_\tau \leq 1$

Thermodynamics of discrete optimal transport

Wasserstein distance based on connectivity of Markov jump processes

- $\mathcal{G}(V, E)$: graph characterizing topology of Markov jump process
  - V: set of states
  - $(x, y) \in E$ if jump between x and y is allowed

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



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- Shortest path distances $\{d_{yx}\}$ of graph $\mathcal{G}$

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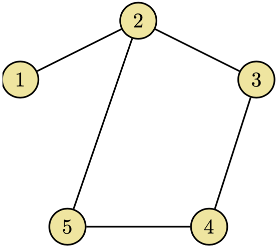

Shortest-path distances $\{d_{xy}\}$

0	1	2	3	2
1	0	1	2	1
2	1	0	1	2
3	2	1	0	1
2	1	2	1	0

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- L^1-Wasserstein distance [arXiv:1803.00567; Dechant, JPA (2022)]

$$\mathcal{W}_1(p^A,p^B) \coloneqq \min_{\pi\in\Pi(p^A,p^B)} \sum_{x,y} d_{xy}\pi_{xy}$$

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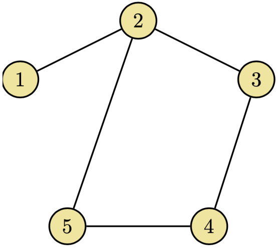

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$$\mathcal{W}_1(p^A, p^B) = \frac{1}{2} \sum_x |p_x^A - p_x^B| \eqqcolon \mathcal{T}(p^A, p^B)$$

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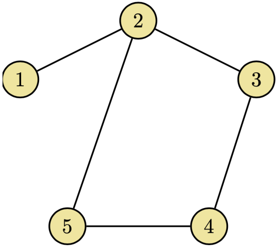

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- In general, $\mathcal{W}_1(p^A,p^B) \geq \mathcal{T}(p^A,p^B)$

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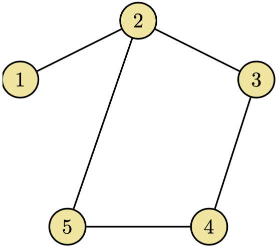

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Thermodynamic interpretation of discrete Wasserstein distances

Theorem 1

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

$$\begin{aligned} \mathcal{W}_1(p^A, p^B) &= \min_{\mathsf{W}_t} \int_0^\tau \sqrt{\sigma_t m_t}\, dt \\ &= \min_{\mathsf{W}_t} \sqrt{\Sigma_\tau \mathcal{M}_\tau} \end{aligned}$$

the minimum is taken over all transition rate matrices $\{\mathsf{W}_t\}_{0 \le t \le \tau}$ 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 $\mathcal{W}_1(p^A, p^B) \le \int_0^\tau \sqrt{\sigma_t m_t}\, dt \le \sqrt{\Sigma_\tau \mathcal{M}_\tau}$ 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

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

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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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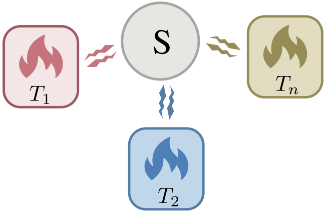
  - □ Taking the continuum limit yields

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

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

Markovian open quantum dynamics

- Discrete-state dynamics obeying Lindblad equation
  $\dot{\varrho}_t = \mathcal{L}_t(\varrho_t) \coloneqq -i[H_t, \varrho_t] + \sum_k \mathcal{D}[L_k(t)]\varrho_t$



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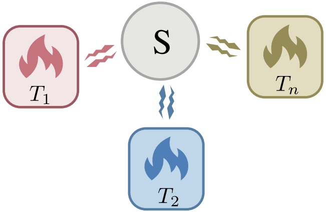
- Local detailed balance $L_k(t) = e^{s_k(t)/2} L_{k'}(t)^\dagger$
  $s_k(t) = -s_{k'}(t)$: entropy change in the environment



Entropy production, dynamical activity, and dynamical state mobility

- Irreversible entropy production

$$\Sigma_\tau \coloneqq \Delta S_{\mathrm{sys}} + \Delta S_{\mathrm{env}} \geq 0$$

$\Delta S_{\mathrm{sys}} \coloneqq S(\varrho_\tau) - S(\varrho_0)$: change in the von Neumann entropy
$\Delta S_{\mathrm{env}} \coloneqq \int_0^\tau \sum_k \mathrm{tr}\left\{L_k(t)\varrho_t L_k^\dagger(t)\right\} s_k(t)\, dt$: environmental entropy production

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- Dynamical state mobility

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

$\langle X, Y\rangle \coloneqq \mathrm{tr}\{X^\dagger Y\}$
$\mathcal{P}_t[X] \coloneqq X - \sum_x \langle x_t|X|x_t\rangle\, |x_t\rangle\!\langle x_t|$
$[\![\phi]\!]_\theta(X) \coloneqq e^{-\theta/2}\int_0^1 e^{\theta u}\phi^u X \phi^{1-u}\, du$
$\varrho_t = \sum_x p_x(t)\, |x_t\rangle\!\langle x_t|$: spectral decomposition of the density matrix ϱ_t

Quantum Wasserstein distance

- Naive quantum extension

$$W_q(\varrho^A, \varrho^B) \coloneqq \min_{\varrho^{AB} \in \Pi(\varrho^A, \varrho^B)} \operatorname{tr}\{C \varrho^{AB}\}$$

$\Pi(\varrho^A, \varrho^B)$: set of density matrices ϱ^{AB} satisfying $\operatorname{tr}_B \varrho^{AB} = \varrho^A$ and $\operatorname{tr}_A \varrho^{AB} = \varrho^B$
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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

Quantum Wasserstein distance

- Considering dissipative structure of Lindblad dynamics, we define

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

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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 ϱ^A and ϱ^B, respectively

Thermodynamic interpretation of quantum Wasserstein distance

Theorem 2

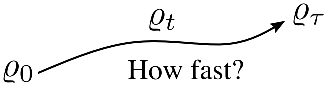
The quantum Wasserstein distance can be written in the following variational form:

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

the minimum is taken over all super-operators $\{\mathcal{L}_t\}_{0 \le t \le \tau}$ 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

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



Applications

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

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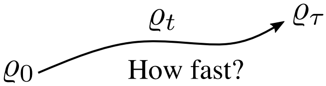
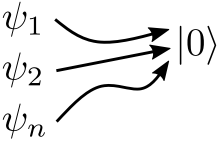


- **Finite-time Landauer principle**: lower bound on heat dissipation required for erasing information

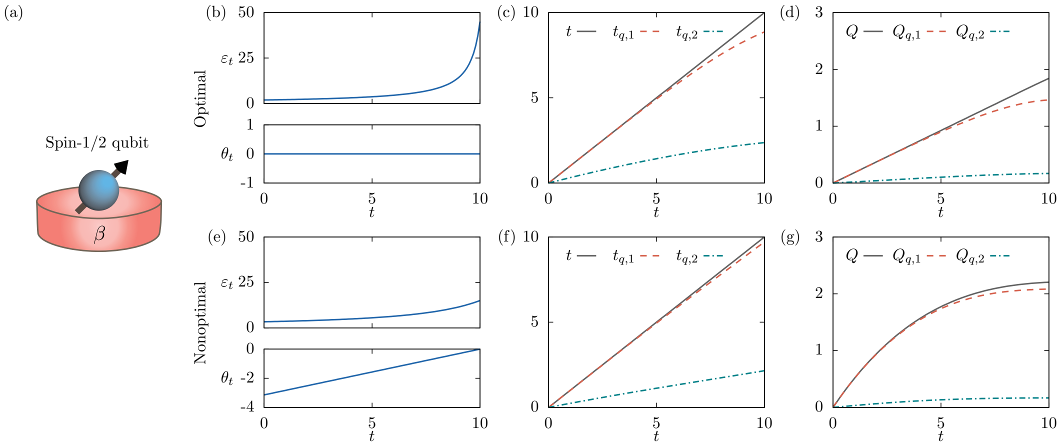
$$Q \geq -T\Delta S_{\mathrm{sys}} + \frac{\mathcal{W}_1(p_0, p_\tau)^2}{\tau \beta \langle m \rangle_\tau}$$



Numerical demonstration

Pareto-optimal protocol in information erasure of qubit

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



Summary

	Continuous	**Classical discrete**	**Quantum**
Wasserstein distance	$W_\alpha \ (\alpha \geq 1)$	$\mathcal{W}_1$	$\mathcal{W}_q$
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 $\mathcal{W}_1(p^A,p^B) = \min\sqrt{\tau \langle m \rangle_\tau \Sigma_\tau}$	Theorem 2 $\mathcal{W}_q(\varrho^A,\varrho^B) = \min\sqrt{\tau \langle m \rangle_\tau \Sigma_\tau}$
Minimum dissipation	$\min \Sigma_\tau = \dfrac{\mathcal{W}_2(p^A,p^B)^2}{\tau D}$	$\min\limits_{\langle m \rangle_\tau = D} \Sigma_\tau = \dfrac{\mathcal{W}_1(p^A,p^B)^2}{\tau D}$	$\min\limits_{\langle m \rangle_\tau = D} \Sigma_\tau = \dfrac{\mathcal{W}_q(\varrho^A,\varrho^B)^2}{\tau D}$
Thermodynamic speed limit	$\tau \geq \dfrac{W_{2(1)}(p^A,p^B)}{\sqrt{D\langle \sigma \rangle_\tau}}$	$\tau \geq \dfrac{\mathcal{W}_1(p^A,p^B)}{\sqrt{\langle m \rangle_\tau \langle \sigma \rangle_\tau}}$	$\tau \geq \dfrac{\mathcal{W}_q(\varrho^A,\varrho^B)}{\sqrt{\langle m \rangle_\tau \langle \sigma \rangle_\tau}}$