The role of optimal transportation and geometry in stochastic thermodynamics

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Amirhossein Taghvaei[†]

Joint work with O. Movilla Miangolarra[*], R. Fu[*], Y. Chen[+], and T. T. Georgiou[*]

[†]University of Washington, Seattle

[*]University of California, Irvine

[+]Georgia Institute of Technology

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Outline

- Background on stochastic thermodynamics
- 2nd law of thermodynamics and Wasserstein geometry
- Extracting energy from anisotropic fluctuations

What is stochastic thermodynamics?

- study thermodynamics at the level of individual particle and far from equilibrium
- a branch of non-equilibrium statistical physics (developed over the last few decades)

Applications:

- biological molecular machines (e.g. kinesin and myosin)
- artificial nano devices (energy of order $k_B T$)

Questions:

- minimum dissipation over finite time transitions
- maximum power from a stochastic thermodynamic engine
- ...

Tools from optimal transport and control can be used to study these questions

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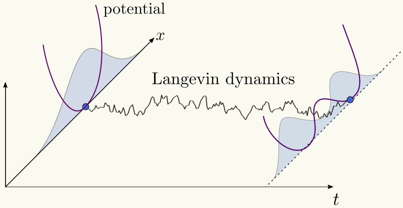
Overdamped Langevin eq.

$$\gamma \mathrm{d}X_t = -\nabla_x U(t, X_t)\mathrm{d}t + \sqrt{2\gamma k_B T}\mathrm{d}B_t$$

- particle in a medium of temperature T
- manipulated by external potential $U(t, x)$
- γ is the viscosity coefficient



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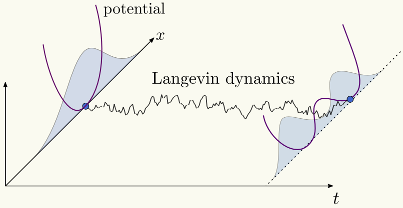

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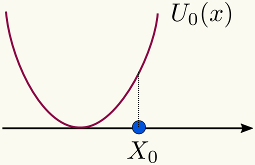
Stochastic thermodynamic
Definitions of work and heat for individual particle



Energy:

$$E = U_0(X_0)$$

Work: energy exchange by changing the potential (with external agent)

$$W = U_1(X_0) - U_0(X_0)$$

Heat: energy exchange when particle moves (with medium)

$$Q = U_1(X_1) - U_1(X_0)$$

1st law: conservation of energy

$$\Delta E = Q + W$$

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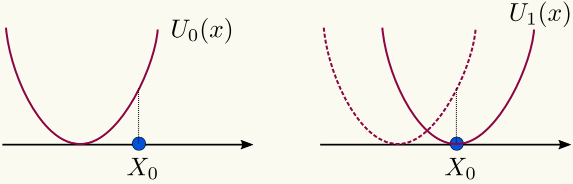

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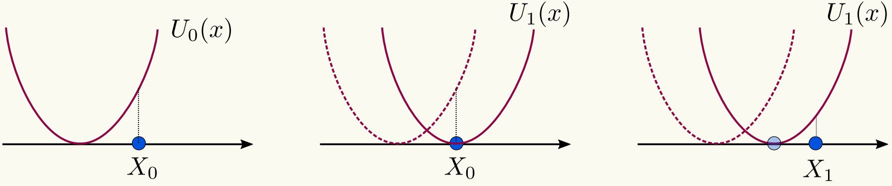

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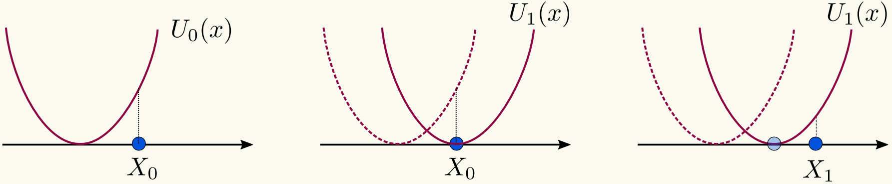

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Stochastic thermodynamic

Definitions of work and heat in continuous-time

Consider continuous-time trajectory $\{X_t; t \in [0, t_f]\}$ and $\{U(t, \cdot); t \in [0, t_f]\}$

- change in energy

$$\mathrm{d}E_t = \mathrm{d}U(t, X_t) = \frac{\partial U}{\partial t}(t, X_t)\mathrm{d}t + \nabla_x U(t, X_t) \circ \mathrm{d}X_t$$

- Work

$$W = \int_0^{t_f} \frac{\partial U}{\partial t}(t, X_t)\mathrm{d}t$$

- heat

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$$\Delta E = W + Q$$

- Average energy

$$\mathcal{E}_t = \mathbb{E}[U(t, X_t)] = \int U(t,x)p(t,x)\mathrm{d}x$$

- Average work

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$p(t,x)$ is probability dist. of X_t given by Fokker-Planck eq.

$$\frac{\partial p}{\partial t} = \frac{1}{\gamma}\nabla \cdot (p\nabla U) + \frac{k_B T}{\gamma}\Delta p$$

Stochastic thermodynamic

Definitions of work and heat for ensemble

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Outline

- Background on stochastic thermodynamics
- 2nd law of thermodynamics and Wasserstein geometry
- Extracting energy from anisotropic fluctuations and isoperimetric inequalities

Entropy:

$$\mathcal{S}(p) = -\int \log(p(x))p(x)\mathrm{d}x$$

Free energy:

$$\mathcal{F}(p, U) = \int U(x)p(x)\mathrm{d}x - k_B T\mathcal{S}(p)$$

Second law:

$$\Delta\mathcal{S}_{\text{tot}} = \Delta\mathcal{S}_{\text{sys}} + \Delta\mathcal{S}_{\text{env}} \geq 0 \quad \Longleftrightarrow \quad \mathcal{W} - \Delta\mathcal{F} = \mathcal{W}_{\text{diss}} \geq 0$$

Question: how to prove and refine 2nd law for overdamped Langevin eq.?

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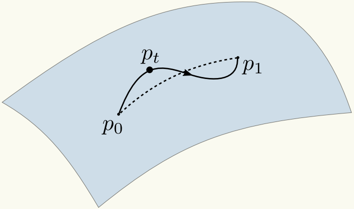

- Wasserstein Riemannian metric:

$$\|\frac{\partial p}{\partial t}\|_{\mathrm{W}}^2 := \int \|\nabla \phi\|^2 p \, \mathrm{d}x, \quad \text{where} \quad \frac{\partial p}{\partial t} + \nabla \cdot (p \nabla \phi) = 0$$

- Length of a curve:

$$\mathsf{length}_{\mathrm{W}}(p_{[0,1]}) := \int_0^1 \|\frac{\partial p}{\partial t}\|_{\mathrm{W}} \mathrm{d}t$$

- 2-Wasserstein distance:

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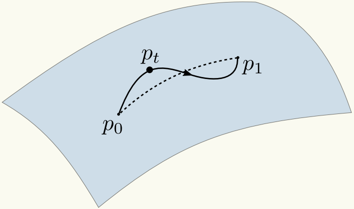

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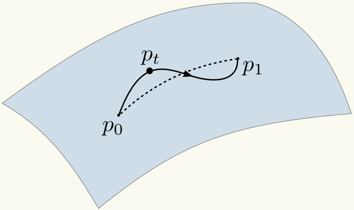

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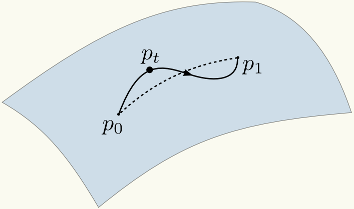

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- Fokker-planck eq. is the Wasserstein gradient flow of the free energy

$$\frac{\partial p}{\partial t} = -\frac{1}{\gamma}\nabla_W \mathcal{F}(p,U)$$

- If U is constant, the time-derivative of free energy along Fokker-Planck flow is

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathcal{F}(p,U) = -\gamma\|\frac{\partial p}{\partial t}\|^2_{\mathrm{W}}$$

- When U is time-varying,

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2nd law and Wasserstein geometry

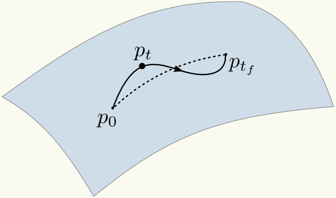
2nd law for finite-time transitions

We have the identity

$$\mathcal{W} - \Delta\mathcal{F} = \gamma \int_0^{t_f} \|\frac{\partial p}{\partial t}\|_{\mathrm{W}}^2 \mathrm{d}t$$

and the bounds

$$\mathcal{W} - \Delta\mathcal{F} \geq \frac{\gamma}{t_f} \mathsf{length}_{\mathrm{W}}(p_{[0,t_f]})^2 \geq \frac{\gamma}{t_f} \mathrm{W}_2(p_0, p_{t_f})^2$$



- This is refinement of the second law for finite-time non-equilibrium transitions
- The bound is achieved when moving with constant velocity along the geodesic
- RHS converges to zero as transition time $t_f \to \infty$ (quasi-static limit)

E. Aurell, C. Mejía-Monasterio, and P. Muratore-Ginanneschi, Optimal protocols and optimal transport in stochastic thermodynamics, Phys. Rev. Lett, 2011
Y. Chen, T. Georgiou, and A. Tannenbaum, "Stochastic control and non-equilibrium thermodynamics: fundamental limits," IEEE TAC, 2019.
R. Fu, A. Taghvaei, Y. Chen, and T. T. Georgiou, "Maximal power output of a stochastic thermodynamic engine", Automatica, 2021.

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- Background on stochastic thermodynamics
- 2nd law of thermodynamics and Wasserstein geometry
- Energy harvesting from anisotropic fluctuations

Thermodynamic model
Brownian gyrator

Model:

$$\gamma \mathrm{d}X_t = -\nabla_x U(t, X_t, Y_t)\mathrm{d}t + \sqrt{2k_B T_x}\mathrm{d}B_t^x$$
$$\gamma \mathrm{d}Y_t = -\nabla_y U(t, X_t, Y_t)\mathrm{d}t + \sqrt{2k_B T_y}\mathrm{d}B_t^y$$

- 2-dimensional system with potential $U(t, x, y)$
- anisotropic fluctuations $\Delta T := T_x - T_y > 0$

Steady-state:

R. Filliger and P. Reimann, "Brownian Gyrator: A Minimal Heat Engine on the Nanoscale" Phys. Rev. Lett, 2007

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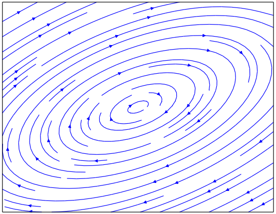

Steady-state:

- system reaches a non-equilibrium steady-state (NESS)

$$\nabla \cdot (pv) = 0, \quad \text{but} \quad v \neq 0 \quad \text{circulation}$$

- circulation mediates transfer of energy from one degree of freedom to the other

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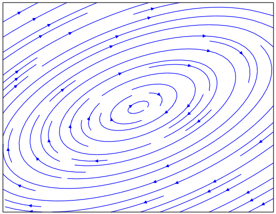

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Problem formulation

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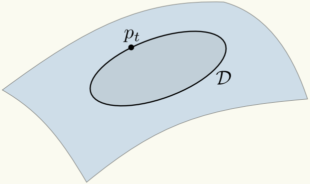


Objective: Design the potential to extract maximum work over cyclic transitions

$$\mathcal{W}_{\mathsf{out}} = -\int_0^{t_f} \int \frac{\partial U}{\partial t} p \, \mathrm{d}x \, \mathrm{d}t$$

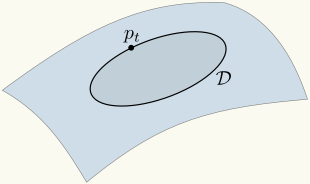
Geometric formulation

Extracted work over the cycle is equal to

$$\mathcal{W}_{\mathsf{out}} = \underbrace{\int_0^{t_f} \int \langle k_B T \nabla \log p, \nabla \phi \rangle \, p \mathrm{d}x \, \mathrm{d}t}_{\text{heat uptake}} - \underbrace{\gamma \int_0^{t_f} \| \frac{\partial p}{\partial t} \|_W^2 \, \mathrm{d}t}_{\text{dissipation}}$$

Problem formulation

$$\frac{\partial p}{\partial t} = \gamma^{-1}\nabla \cdot (p\nabla U + k_B T \nabla p)$$
$$= \nabla \cdot (p\nabla \phi)$$



Objective: Design the potential to extract maximum work over cyclic transitions

$$\mathcal{W}_{\text{out}} = -\int_0^{t_f} \int \frac{\partial U}{\partial t} p \, \mathrm{d}x \, \mathrm{d}t$$

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Restriction to Gaussian distributions

- Consider restriction to 2-dim Gaussian dist. $N(0,\Sigma)$ with $\det(\Sigma)=1$
- Parametrize the covariance matrix with $(r,\theta)\in[0,\infty)\times[0,2\pi)$:

$$\Sigma(r,\theta)=R(-\frac{\theta}{2})\begin{bmatrix}e^r & 0\\ 0 & e^{-r}\end{bmatrix}R(\frac{\theta}{2})$$

- Define (weighted) area and perimeter of a closed curve $\mathcal{D}$ as

$$\mathcal{A}_f(\mathcal{D})=\int_{\mathcal{D}}f(r,\theta)\sqrt{\det(g)}\mathrm{d}\theta\mathrm{d}r,\quad \ell(\mathcal{D})=\oint_{\partial\mathcal{D}}\|\mathrm{d}s\|_g$$

where

density $f(r,\theta)=\dfrac{\sin(\theta)\tanh(r)}{\cosh(r)}$, and metric $g(r,\theta)=\begin{bmatrix}\cosh(r) & 0\\ 0 & \sinh(r)\tanh(r)\end{bmatrix}$

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- Maximizing work output is equivalent to

$$\max_{\mathcal{D}} \ \{\mathcal{A}_f(\mathcal{D}) - \mu \ell(\mathcal{D})^2\}$$

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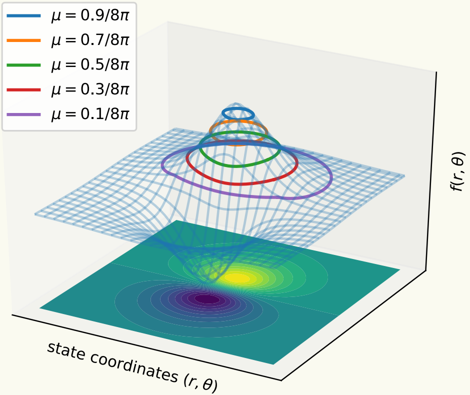

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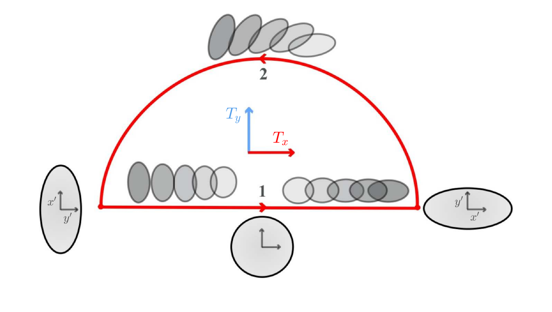
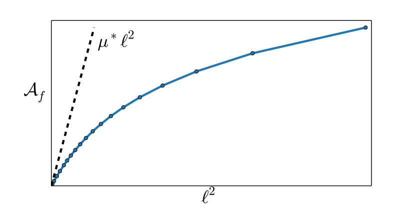


Maximum area as a function of length^2



- There exists a $\mu^* > 0$ such that

$$\mathcal{A}_f(\mathcal{D}) \leq \mu^* \ell(\mathcal{D})^2 \quad \forall \text{ closed curve } \mathcal{D}$$

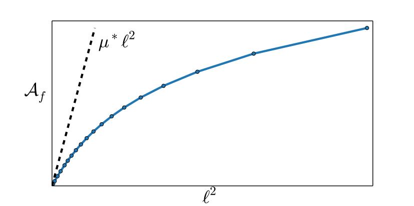
- Isoperimetric inequality implies a bound on the thermodynamic efficiency:

$$\eta := \frac{\mathcal{A}_f(\mathcal{D}) - \mu \ell(\mathcal{D})^2}{\mathcal{A}_f(\mathcal{D})} \leq 1 - \frac{1}{\mu^*}\frac{t_c}{t_f}$$

where $t_c = \dfrac{\gamma}{k_B \Delta T}$ is the characteristic time of the system.

Isoperimetric inequality
and its thermodynamic implications

Maximum area as a function of length^2



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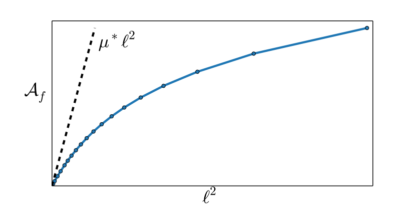

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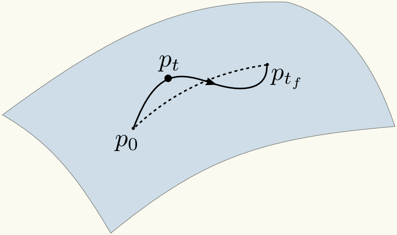
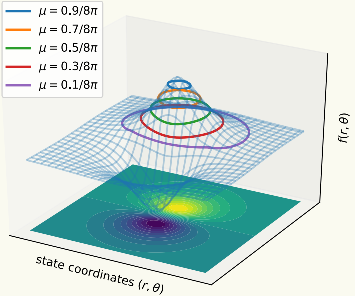
Summary and concluding remarks



$$\text{dissipation} = \int_0^{t_f} \|\frac{\partial p}{\partial t}\|_W^2 \mathrm{d}t$$



$$\mathcal{W}_{\text{out}} = k_B \Delta T(\mathcal{A}_f - \mu \ell^2)$$

Thank you for your attention!

O. Movilla Miangolarra, A. Taghvaei, Y. Chen, T. T. Georgiou "Energy harvesting from anisotropic fluctuations ", Phys. Rev. E., 2021
O. Movilla Miangolarra, A. Taghvaei, Y. Chen, T. T. Georgiou "Thermodynamic engine powered by anisotropic fluctuations ", Phys. Rev. E., Accepted
O. Movilla Miangolarra, A. Taghvaei, Y. Chen, T. T. Georgiou "Geometry of finite-time thermodynamic cycles with anisotropic thermal fluctuations", Control System Letters (L-CSS), Accepted