

# Optimal control of non-equilibrium processes in stochastic thermodynamics.

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<https://wiki.helsinki.fi/display/mathphys/paolo>

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# Outline of the talk

## Background: from time reversal of Markov Processes to Stochastic Thermodynamics

- Schrödinger & Nelson. Scope: interpretation of Q.M.
- Kolmogorov: from time reversal to detailed balance.
- A **recent different** application: non-equilibrium thermodynamics of small systems.
- The “Cost” of deterministic time reversal

## Control of thermodynamic processes

- Over-damped dynamics: Work, Heat, Entropy production.
- “Coercivity” and control.
- A simple “universal” result.

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# Schrödinger's diffusion problem

E. Schrödinger. "Über die Umkehrung der Naturgesetze". In: *Sitzungsberichte der preussischen Akademie der Wissenschaften, physikalische mathematische Klasse* 8.9 (1931), pp. 144–153. DOI: 10.1002/ange.19310443014

- Given two probability densities

$$m_o(d^d x) = m(d^d x, t_o) \quad \& \quad m_f(d^d x) = m(d^d x, t_f)$$

at the end-points of a time interval  $[t_o, t_f]$ ,

- find the interpolating diffusion

$$m(d^d x, t) \quad \forall t \in [t_o, t_f]$$

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# Reciprocal diffusion processes

Let  $\{\xi_t; t \in [t_0, t_f]\}$  be an e.g.  $\mathbb{R}^d$ -valued diffusion process

$$p(d^d x, t | \mathbf{x}_1, t_1) = P(\xi_t \in [\mathbf{x}, \mathbf{x} + d\mathbf{x}] | \xi_{t_1} = \mathbf{x}_1)$$

Schrödinger's (math-refinements:<sup>1</sup> see also e.g.<sup>2</sup>) finding:

$$q(d^d x_n, t_n, \dots, d^d x_1, t_1 | m_o, m_f) = \psi[m_o, m_f](d^d x_o) \bar{\psi}[m_o, m_f](d^d x_f) \prod_{i=1}^{n-1} p(d^d x_{i+1}, t | \mathbf{x}_i, t_i)$$

The auxiliary scalar fields

$$\psi[m_o, m_f](d^d x_o) \quad \& \quad \bar{\psi}[m_o, m_f](d^d x_f)$$

are Lagrange multipliers imposing the boundary conditions.

<sup>1</sup> Bernstein. 1932; Jamison. 1974.

<sup>2</sup> Dai Pra. 1991; Krener. 1997.

# Kolmogorov analysis of time-reversal

A. N. Kolmogorov. "Zur Umkehrbarkeit der statistischen Naturgesetze". In: *Mathematische Annalen* 113 (1 1937), pp. 766–772. doi:

10.1007/BF01571664

- Fix two densities  $m_o, m_f$  at the end-points of  $[t_i, t_f]$ .
- The **time reversed Markov** evolution must satisfy<sup>3</sup> for any  $t_o \leq t_1 \leq t_2 \leq t_f$ :

$$m(\mathbf{x}_2, t_2) \tilde{p}(\mathbf{x}_1, t_1 | \mathbf{x}_2, t_2) = p(\mathbf{x}_2, t_2 | \mathbf{x}_1, t_1) m(\mathbf{x}_1, t_1)$$

- **Add** the hypotheses
  - the diffusion is time-stationary:  $p(\mathbf{x}_2, t_2 | \mathbf{x}_1, t_1) = p(\mathbf{x}_2, t_2 - t_1 | \mathbf{x}_1, 0)$
  - $m(\mathbf{x}, t) = m_*(\mathbf{x}) > 0$  is stationary.

Question: under which conditions

$$\tilde{p}(\mathbf{x}_1, 0 | \mathbf{x}_2, t_2 - t_1) = p(\mathbf{x}_1, t_2 - t_1 | \mathbf{x}_2, 0)$$

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# Kolmogorov's covariant characterization of a diffusion

## Multiplicative noise warning:

Even for an  $\mathbb{R}^d$ -valued process  $\xi$  the scale of the noise imposes a “Riemannian” metric  $g : d\mathbf{x} \otimes d\mathbf{x}$  on the space.

$$\lim_{dt \downarrow 0} \mathbb{E} \left\{ \frac{\xi_{t+dt} - \xi_t}{dt} \middle| \xi_t = \mathbf{x} \right\} = \left( \mathbf{f} - \frac{1}{2} \Gamma : g^{-1} \right) (\mathbf{x})$$

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Christoffel symbols of  $g$

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here: strictly positive definite

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# Edward Nelson's time reversal for smooth diffusions

E. Nelson. *Dynamical Theories of Brownian Motion*. second edition. Princeton University Press, 2001, p. 148

## Mean backward derivatives

$$\lim_{dt \downarrow 0} \mathbb{E} \left\{ \frac{\xi_t - \xi_{t-dt}}{dt} \middle| \xi_t = \mathbf{x} \right\} = \left( \tilde{\mathbf{f}} + \frac{1}{2} \Gamma : \mathbf{g}^{-1} \right) (\mathbf{x})$$

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- Assigning  $(m_o, m_f)$  at  $t_o \leq t_f$  specifies  $\tilde{\mathbf{f}}$  in terms of  $\mathbf{f}$ .
- Ito lemma in local coordinates becomes  $(d\xi_t = \xi_t - \xi_{t-dt})$

$$\begin{aligned} F(\xi_t, t) - F(\xi_{t-dt}, t-dt) &= d\xi_t \cdot \partial_{\xi_t} F(\xi_t, t) \\ &+ dt \partial_t F(\xi_t, t) - \frac{1}{2} d \prec \xi_t \otimes \xi_t \succ : \partial_{\xi_t} \otimes \partial_{\xi_t} F(\xi_t, t) \end{aligned}$$

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# Backward drift via Girsanov formula: covariant Wiener measure

Suppose as above that  $g$  be

- strictly positive definite;
- time independent.

The (Eells-Elworthy<sup>4</sup>) development map

$$d\omega_t = e_t \diamond d\beta_t$$

$$de_t = -\Gamma : e_t \otimes d\omega_t$$

gives a **covariant** description of a  $d$ -dimensional Riemann manifold-valued Wiener process.

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Stratonovich differential (pointing to  $d\beta_t$ ) → Standard "Euclidean" Brownian motion

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Christoffel symbols of  $g$  (pointing to  $-\Gamma$ )      Stratonovich differential (pointing to  $d\omega_t$ )

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Christoffel symbols of  $g$       Stratonovich differential

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The important aspect here is covariance, the manifold may well be  $\mathbb{R}^d$

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- The Wiener process  $\omega \equiv \{\omega_t; t \in [t_0, t_f]\}$  is invariant under time reversal.
- Semi-martingale  $\xi \equiv \{\xi_t; t \in [t_0, t_f]\}$  absolutely continuous w.r.t.  $\omega$  with non-vanishing covariant drift  $f$ . Girsanov formula permits to write for any n-tuple  $t_0 \leq t_1 \leq \dots \leq t_n \leq t_f$

$$E F(\xi_{t_1}, \dots, \xi_{t_n}) = E \frac{dP_\xi}{dP_\omega} F(\omega_{t_1}, \dots, \omega_{t_n})$$

- Let  $(m_0 = \sqrt{\det g_n}, m_f := \sqrt{\det g_n})$  at  $t_0 \leq t_f$  be assigned (as before)

scalar density: w.r.t. the invariant volume

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- Let  $(n_o = \sqrt{\det \mathbf{g}_n}, n_f := \sqrt{\det \tilde{\mathbf{g}}_n})$  at  $t_0 \leq t_f$  be assigned (as before)

$$\begin{aligned} \frac{dP_\xi}{dP_\omega} &= n_o(\omega_{t_0}) e^{\int_{t_0}^{t_f} \left[ (\mathbf{g} \cdot \mathbf{f})(\omega_t, t) \cdot (e \cdot d\beta_t) - \frac{\|\mathbf{f}(\omega_t, t)\|_{\mathbf{g}}^2}{2} dt \right]} \\ &= n_f(\omega_{t_f}) e^{\int_{t_0}^{t_f} \left[ (\mathbf{g} \cdot \tilde{\mathbf{f}})(\omega_t, t) \cdot (e \cdot d\beta_t) - \frac{\|\tilde{\mathbf{f}}(\omega_t, t)\|_{\tilde{\mathbf{g}}}^2}{2} dt \right]} \\ &\Rightarrow (\mathbf{f} - \tilde{\mathbf{f}})(\mathbf{x}, t) = \mathbf{g}^{-1}(\mathbf{x}) \cdot \partial_{\mathbf{x}} \ln n(\mathbf{x}, t) \end{aligned}$$

Annotations:

- scalar density: w.r.t. the invariant volume (pointing to  $n_o$  and  $n_f$ )
- Ito integral w.r.t. Euclidean Wiener process (pointing to the  $d\beta_t$  term in the first integral)
- post-point differential: martingale with respect to the "future" filtration (pointing to the  $e \cdot d\beta_t$  term in the second integral)
- scalar density (pointing to  $n(\mathbf{x}, t)$ )



# A change of perspective: non-equilibrium thermodynamics of small systems

- molecular fluctuations play a fundamental role for transport processes (phase transitions, nucleation, chemical reactions, DNA mutations).
- dynamical fluctuations contrary to the thermodynamic forces are likely to occur in small systems.
- nano-scales: size of the fluctuations are of the same order of the magnitude of the observables

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# The statistical “cost” of deterministic reversal

## Girsanov martingale and time reversal

$$\int_{t_0}^{t_f} (\mathbf{g} \cdot \mathbf{f}) \cdot (\mathbf{e} \cdot d\beta_t) \quad \Rightarrow \quad \int_{t_0}^{t_f} (\mathbf{g} \cdot \tilde{\mathbf{f}}) \cdot (\mathbf{e} \cdot d\beta_t)$$

What if we replace  $\tilde{\mathbf{f}}$  with  $-\mathbf{f}$  ?

$$\int_{t_0}^{t_f} (\mathbf{g} \cdot \mathbf{f}) \cdot (\mathbf{e} \cdot d\beta_t) =$$

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Log-Cost of the deterministic reversal for  $\xi$

$$\mathcal{J}[\xi] = 2 \int_{t_0}^{t_f} d\xi \cdot \mathbf{g} \cdot \mathbf{f}$$

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# Thermodynamics of over-damped dynamics

Suppose

$$\mathbf{f}(\mathbf{x}, t) = -(\mathbf{g}^{-1} \cdot \partial_{\mathbf{x}} U)(\mathbf{x}, t)$$

then

$$\begin{aligned} \mathcal{J}[\xi] &= -2 \int_{t_0}^{t_f} d\xi \diamond (\partial_{\xi_t} U)(\xi_t, t) \\ &= -2[U(\xi_{t_f}, t_f) - U(\xi_{t_0}, t_0)] + 2 \int_{t_0}^{t_f} dt (\partial_t U)(\xi_t, t) \end{aligned}$$

## Sekimoto's interpretation

$$\mathcal{W} := \int_{t_0}^{t_f} dt (\partial_t U)(\xi_t, t) \quad \text{work}$$

$$\mathcal{Q} := - \int_{t_0}^{t_f} d\xi \diamond (\partial_{\xi_t} U)(\xi_t, t) \quad \text{heat}$$

# “Natural” parametrization of the Heat

## Heat and development map

$$\begin{aligned}
 \mathcal{Q} &= - \int_{t_0}^{t_f} d\xi \diamond (\partial_{\xi_t} U)(\xi_t, t) \\
 &= \int_{t_0}^{t_f} \left\{ -(\mathbf{e} \cdot d\beta)_t \cdot (\partial_{\xi_t} U)(\xi_t, t) + \left( \|\mathbf{g} \cdot \partial_{\xi_t} U\|_{\mathbf{g}}^2 - \frac{1}{2} \Delta_{\xi_t} U \right) dt \right\}
 \end{aligned}$$

hence

$$\mathbb{E} \mathcal{Q} = \int_{t_0}^{t_f} \left\{ \|\mathbf{g}^{-1} \cdot \partial_{\xi_t} U\|_{\mathbf{g}}^2 + \frac{1}{2} (\partial_{\xi_t} \ln n) \cdot \mathbf{g}^{-1} \cdot (\partial_{\xi_t} U) \right\} dt$$

covariant density

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$d\mathbf{e} = -\Gamma : \mathbf{e} \otimes d\xi$

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vanishes on average

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# “Natural” parametrization of the Heat

## Nelson's current and osmotic velocity

$$\mathbf{v} = \frac{\mathbf{f} + \tilde{\mathbf{f}}}{2} \quad \& \quad \mathbf{u} = \frac{\mathbf{f} - \tilde{\mathbf{f}}}{2} = \frac{1}{2} \mathbf{g}^{-1} \partial_{\mathbf{x}} \ln n$$

$$\partial_t n + \nabla_{\mathbf{x}} \cdot (\mathbf{v} n) = 0$$

- current  $\mathbf{v}$  and osmotic velocities  $\mathbf{u}$  transform as vector fields
- $\mathbf{v}$  behaves as the velocity field of a deterministic ensemble.

## The “natural” representation of the Heat

$$\mathbb{E} Q = \mathbb{E} \ln n(\mathbf{x}_t, t) \Big|_{t_0}^{t_f} + \mathbb{E} \int_{t_0}^{t_f} dt \|\mathbf{v}\|_{\mathbf{g}}^2$$



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# Bounds and coercivity ( $\beta = 1$ )

## Bound for the Heat

$$EQ \geq E \ln n(\mathbf{x}_t, t) \Big|_{t_0}^{t_f} = -\text{variation of Shannon-Gibbs Entropy}$$

## Bound for the work

$$EW = E \left\{ U(\mathbf{x}_t, t) \Big|_{t_0}^{t_f} + Q \right\} \geq$$

$$E \left\{ U(\mathbf{x}_t, t) + \frac{1}{2} \ln n(\mathbf{x}_t, t) \right\} \Big|_{t_0}^{t_f} = \text{variation of equilibrium free energy}$$

## Current velocity: deviation from equilibrium

$$\mathbf{v} = -\mathbf{g}^{-1} \cdot \partial_{\mathbf{x}} \left( U + \frac{1}{2} \ln n \right) \quad \text{vanishes at equilibrium !!!}$$

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The Heat release between assigned end state is a convex functional of the current velocity.

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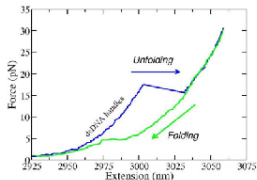
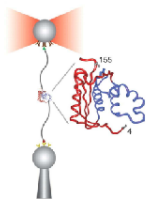
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# Physical motivations for control

## Nano motors

- mainly in steady operation
- what external control should be apply that maximizes the output power?
- operation under minimal dissipation
- efficiency at maximum power



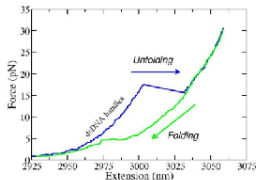
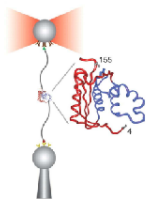
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- what external control should be apply that maximizes the output power?
- operation under minimal dissipation
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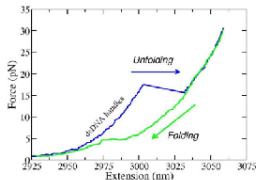
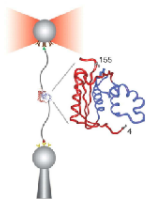


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# Physical motivations for control

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# Relation to hydrodynamical optimal transport I

- Heat minimization between fixed end-states  $(n_o, n_f)$  reduces to the **deterministic** control of

$$E\mathcal{S} = E \int_{t_o}^{t_f} dt \|\mathbf{v}\|_g^2$$

- The problem is well-posed in the space of smooth diffusions.
- The bound lower becomes tight if jump processes are admissible minimizers:
  - no penalty on acceleration.
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## Minimization in the space of smooth diffusions

- Suppose now  $g = I$
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- Suppose now  $g = I$
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$$\partial_t \varphi + \frac{1}{2} \|\partial_{\mathbf{x}}\varphi\|^2 = 0$$

$$\partial_t m + \partial_{\mathbf{x}} \cdot (m \partial_{\mathbf{x}}\varphi) = 0$$

$$m(\mathbf{x}, t_o) = m_o(\mathbf{x}) \quad \& \quad m(\mathbf{x}, t_f) = m_f(\mathbf{x})$$

# Relation to hydrodynamical optimal transport II

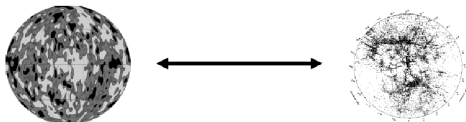
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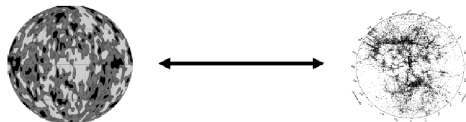


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# A “valley view” over optimal thermodynamic control

Ideas borrowed from instanton calculus in Quantum Field Theory.

$$\mathcal{A} := \int_{t_0}^{t_f} dt (\| \mathbf{v}_t \|^2 + \varepsilon \| \mathbf{a}_t \|^2) + \lambda \cdot \int_{t_0}^{t_f} dt \left[ \mathbf{v}_t - \frac{\phi(\mathbf{x}_o) - \mathbf{x}_o}{\Delta t} \right]$$

- $\dot{\mathbf{x}}_t = \mathbf{v}_t$
- $\lambda$  enforces  $\mathbf{x}_f = \phi(\mathbf{x}_o)$
- $\phi$  relates the initial and final states

$$m_f(\phi(\mathbf{x})) \left| \det \frac{\partial \phi(\mathbf{x})}{\partial \mathbf{x}} \right| = m_o(\mathbf{x})$$

- It is possible to impose boundary conditions on the state  $\mathbf{x}_{t_0} = \mathbf{x}_o$ ,  $\mathbf{x}_{t_f} = \mathbf{x}_f$  and on the initial and final velocities.

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# More about all the above

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