On extremals of the entropy production by “Langevin–Kramers” dynamics

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Outline

1. Physical motivation and previous results
   - Stochastic Thermodynamics of Langevin–Smoluchowski models
   - Relation with optimal mass transport

2. Entropy production by Langevin–Kramers
   - Stochastic Thermodynamics of Langevin–Kramers models
   - An explicitly solvable case

3. The “over-damped” Langevin–Smoluchowski limit
   - Multiscale perturbation theory

4. Conclusions

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Small systems and Optimization

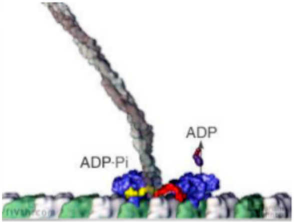
- At mesoscopic scales, the size of the fluctuations are of the same order of the magnitude of the observables.
- Nonequilibrium fluctuation relations imply that dynamical fluctuations contrary to the thermodynamic forces are likely to occur in small systems.

Molecular motors

Convert chemical energy into mechanical motion. Cyclic isothermal operation at fairly high efficiency.

Nano engines

Cyclic or steady operation in the presence of gradients or not. What is the cycle that maximizes the output power?



A kinesin motor walking along a microtubule
Bustamante, et al. Physics Today, 2005, 58, 43-48

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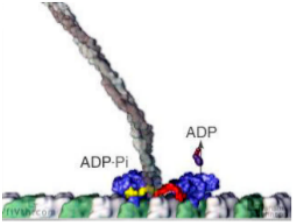

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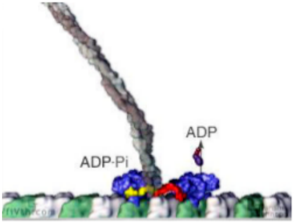

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From fluctuation relations to optimal control: ground-breaking and stepping stones

Fluctuation relations, time reversal and stochastic thermodynamics

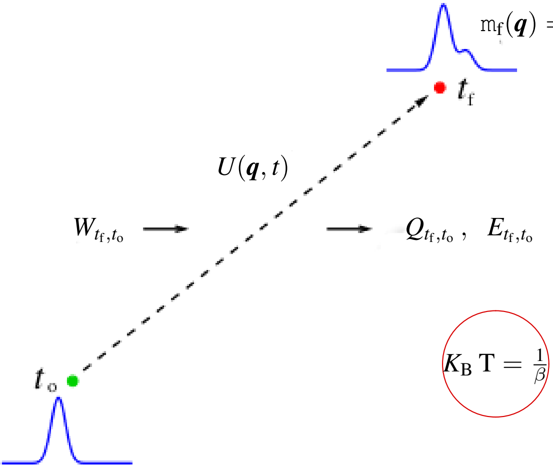
- Gallavotti & Cohen, Phys. Rev. Lett., 74, 2694-2697 (1995).
- Jarzynski, Phys. Rev. Lett., 78, 2690-2693 (1997).
- Kurchan, J. Phys. A, 31, 3719 (1998).
- Lebowitz & Spohn, Stat. Phys., 95, 333-365 (1999).
- Maes et al., J. Math. Phys., 41, 1528-1554 (2000).
- Chétrite & Gawdzki, Comm. Math. Phys., 282, 469-51 (2008).

Optimal control of finite-time thermodynamics

- Schmiedl & Seifert, Phys. Rev. Lett., 98, 108301 (2007).

Transition between two assigned states in a finite time horizon $[t_{\mathrm{o}}\,,\,t_{\mathrm{f}}]$

$$\mathrm{m}_{\mathrm{f}}(\boldsymbol{q}) = \left(\frac{\beta}{2\,\pi}\right)^{d/2} e^{-\beta\,S_{\mathrm{f}}(\boldsymbol{q})}$$



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Schrödinger, “Über die Umkehrung der Naturgesetze”
Sitz.-Ber. d Preuss. Akad. d. Wiss., Phys.-math. Klasse, 1931

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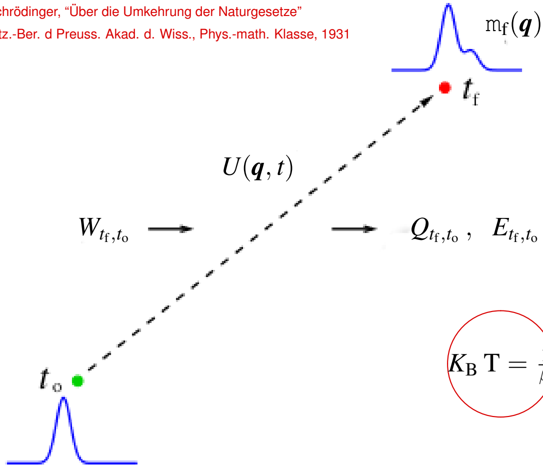

$$K_B\,\mathrm{T} = \frac{1}{\beta}$$

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Stochastic Thermodynamics Sekimoto, Prog. Theor. Phys. Suppl. 130, 17 (1998)

$$d\boldsymbol{\xi}_t = -\partial_{\boldsymbol{\xi}_t} U(\boldsymbol{\xi}_t, t)\,\frac{dt}{\tau} + \sqrt{\frac{2}{\beta\,\tau}}\,d\boldsymbol{\omega}_t$$

Fluctuating heat release during the horizon $[t_o\,,\,t_f]$

$$Q_{t_f,t_o} = -\int_{t_o}^{t_f} d\xi_t \overset{\circ}{\cdot} \partial_{\xi_t} U(\xi_t, t)$$

Fluctuating work during the horizon $[t_o\,,\,t_f]$

$$W_{t_f,t_o} = \int_{t_o}^{t_f} dt\,\partial_t U(\xi_t, t)$$

First law of thermodynamics in $[t_o\,,\,t_f]$

$$W_{t_f,t_o} - Q_{t_f,t_o} = U\left(\xi_{t_f}, t_f\right) - U\left(\xi_{t_o}, t_o\right)$$

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Wiener increment

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Second law

Entropy production and current velocity

$$\mathrm{E}Q_{t_\mathrm{f},t_\mathrm{o}} + \frac{1}{\beta}\mathrm{E}\ln\frac{\mathrm{m}_\mathrm{o}(\boldsymbol{\xi}_{t_\mathrm{o}})}{\mathrm{m}_\mathrm{f}(\boldsymbol{\xi}_{t_\mathrm{f}})} = \mathrm{E}\int_{t_\mathrm{o}}^{t_\mathrm{f}}\frac{\mathrm{d}t}{\tau}\;\parallel \boldsymbol{v} \parallel^2(\boldsymbol{\xi}_t,t)\;\geq\;0$$

$$\boldsymbol{v}(\boldsymbol{q},t) = -\partial_{\boldsymbol{q}}\left\{U(\boldsymbol{q},t) + \frac{1}{\beta}\ln\frac{(2\,\pi)^{d/2}\,\mathrm{m}(\boldsymbol{q},t)}{\beta^{d/2}}\right\} \equiv -\partial_{\boldsymbol{q}}(U-S)(\boldsymbol{q},t)$$

Properties of the current velocity, E. Nelson, “Dynamical Theories of Brownian Motion” 1967

$$\frac{\boldsymbol{v}(\boldsymbol{q},t)}{\tau} := \lim_{\mathrm{d}t\downarrow 0}\mathrm{E}_{\boldsymbol{\xi}_t=\boldsymbol{q}}\frac{\boldsymbol{\xi}_{t+\mathrm{d}t}-\boldsymbol{\xi}_{t-\mathrm{d}t}}{2\,\mathrm{d}t}$$

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Minimal entropy production in a finite time transition

$$\mathcal{E} = \beta \int_{t_o}^{t_f} \frac{dt}{\tau} \int_{\mathbb{R}^{2d}} d^{2d}x \, m(\boldsymbol{x}, t) \parallel \boldsymbol{v} \parallel^2 (\boldsymbol{x}, t)$$

- $\boldsymbol{v}$ is the control protocol.
- $\mathcal{E}$ is coercive in $\boldsymbol{v}$: current velocity kinetic energy.
- Admissible protocols: we restrict to differentiable (viscosity sense) $\boldsymbol{v}$
- Optimal control is local and deterministic: Hamilton–Jacobi equations.

Monge–Ampère–Kantorovich equations

$$\partial_t (U - S) - \frac{\parallel \partial_{\boldsymbol{q}} (U - S) \parallel^2}{2\,\tau} = 0$$

$$\partial_t m - \frac{1}{\tau} \partial_{\boldsymbol{q}} \cdot [m \, \partial_{\boldsymbol{q}} (U - S)] = 0$$

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Previuosly encountered in optimal mass transport:

Frisch et al, Nature 417, 260 (2002)

Brenier et al, MNRAS 346, 501 (2003)

Villani, “Optimal transport: old and new”, (2009)

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- Cassical physical systems obey Newton's law.
- Langevin–Kramers dynamics: thermal stirring coupled to momentum dynamics.
- How does the symplectic structure affect the selection of the optimal control?

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Langevin–Kramers “metriplectic” stochastic dynamics

$$H : \mathbb{R}^{2d} \times \mathbb{R}_+ \mapsto \mathbb{R}$$

$$\mathrm{d}\chi_t = (\mathsf{J} - \mathsf{G}) \cdot \partial_{\chi_t} H \frac{\mathrm{d}t}{\tau} + \sqrt{\frac{2}{\beta\,\tau}}\,\mathsf{G}^{1/2} \cdot \mathrm{d}\boldsymbol{\omega}_t$$

$$\mathsf{J} = \begin{bmatrix} 0 & 1_d \\ -1_d & 0 \end{bmatrix} \qquad \mathsf{G} = \begin{bmatrix} 0 & 0 \\ 0 & 1_d \end{bmatrix}$$

Scalar generator of the process $\chi_t \mapsto \boldsymbol{x} = [\boldsymbol{q}\,,\boldsymbol{p}]^{\dagger} \in \mathbb{R}^{2d}$ with $\boldsymbol{q}\,,\boldsymbol{p} \in \mathbb{R}^{d}$

$$(\mathfrak{L}f)(\boldsymbol{x},t) = \Big\{ \underbrace{(\partial_{\boldsymbol{x}} H) \cdot \mathsf{J}^{\dagger} \cdot \partial_{\boldsymbol{x}}}_{\text{Symplectic structure}} \quad \underbrace{-(\partial_{\boldsymbol{x}} H) \cdot \mathsf{G} \cdot \partial_{\boldsymbol{x}} + \frac{1}{\beta}\,\mathsf{G} : \partial_{\boldsymbol{x}} \otimes \partial_{\boldsymbol{x}}}_{\text{Dissipative "metric" structure}} \Big\} f(\boldsymbol{x},t)$$

Symplectic structure: $\sum_{i=1}^{d}[(\partial_{p_i}H)\partial_{q_i} - (\partial_{q_i}H)\partial_{p_i}]$

Dissipative "metric" structure: $\sum_{i=1}^{d}[-(\partial_{p_i}H)\partial_{p_i} + \frac{1}{\beta}\partial_{p_i}^2]$

Thermodynamics

Natural involution associated to time reversal

$[\boldsymbol{q},\boldsymbol{p}] \mapsto [\boldsymbol{q},-\boldsymbol{p}]$

First law

$$W_{t_f,t_o} = \int_{t_o}^{t_f} \mathrm{d}t\, \partial_t H(\boldsymbol{\xi}_t, t)$$

$$Q_{t_f,t_o} = -\int_{t_o}^{t_f} \mathrm{d}\chi_t \overset{\diamond}{\cdot} \partial_{\chi_t} H(\boldsymbol{\xi}_t, t)$$

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Entropy production as utility functional

Relation with non-equilibrium Helmholtz energy

$$A(\boldsymbol{x},t) = (H - S)(\boldsymbol{x},t) = H(\boldsymbol{x},t) + \frac{1}{\beta} \ln \frac{(2\,\pi)^d\, \mathrm{m}(\boldsymbol{x},t)}{\beta^d}$$

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Symplectic structure ⇒ incompressible component

Non explicitly coercive: no penalty on large $\partial_q A$

$$\mathsf{G} \cdot \partial_{\boldsymbol{x}} A \equiv \begin{bmatrix} 0 \\ \partial_p A \end{bmatrix}$$

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Symplectic structure $\Rightarrow$ incompressible component

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Difficulties

- Absence of explicit coercivity on all degrees of freedom
  1. We require smooth evolution between the initial $\mathrm{m_o}$ and final $\mathrm{m_f}$ density
  2. We restrict admissible Hamiltonian to $C^{(2,1)}(\mathbb{R}^{2d}, \mathbb{R}_+) \cap \mathbb{L}^2(\mathbb{R}^{2d}, \mathrm{m}\, \mathrm{d}^{2d}x)$
- Entropy production depends only on the compressible component of the current velocity
  - $\Rightarrow$ control problem does not reduce to a deterministic one: H governs both the compressible and incompressible components.
  - Imposing kinetic+potential form of H leads to singular control.
- Presence of incompressible component in the control
  - $\Rightarrow$ Non-local constraint on the dynamics

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- Entropy production depends only on the compressible component of the current velocity
  - $\Rightarrow$ control problem does not reduce to a deterministic one: H governs both the compressible and incompressible components.
  - Imposing kinetic+potential form of H leads to singular control.
- Presence of incompressible component in the control
  - $\Rightarrow$ Non-local constraint on the dynamics

Difficulties

- Absence of explicit coercivity on all degrees of freedom
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Example: incompressible Euler equation

Bloch et al, IEEE Decision & Control Proceedings, (2000)

$$\mathcal{A} = \int_{t_o}^{t_f} \mathrm{d}t \int_{\mathbb{R}^d} \mathrm{d}^d x \, \{ \| \boldsymbol{v}(\boldsymbol{x},t) \|^2 + K(\boldsymbol{x},t) \partial_{\boldsymbol{x}} \boldsymbol{v}(\boldsymbol{x},t) \}$$
$$+ \int_{t_o}^{t_f} \mathrm{d}t \int_{\mathbb{R}^d} \mathrm{d}^d x \, \boldsymbol{\Phi}_t(\boldsymbol{x},t_o) \cdot \Big(\boldsymbol{v}(\boldsymbol{X}_t(\boldsymbol{x},t_o),t) - \dot{\boldsymbol{X}}_t(\boldsymbol{x},t_o) \Big)$$

Variations for $\boldsymbol{X}'_{t_o} = \boldsymbol{X}'_{t_f}$

K – variation	$\partial_{\boldsymbol{x}} \cdot \boldsymbol{v} = 0$
$\boldsymbol{\Phi}$ – variation	$\dot{\boldsymbol{X}}_t - \boldsymbol{v}(\boldsymbol{X}_t,t) = 0$
$\boldsymbol{X}_t$ – variation	$\dot{\boldsymbol{\Phi}}_t(\boldsymbol{x},t_o) + \boldsymbol{\Phi}_t(\boldsymbol{x},t_o) \cdot (\partial_{\boldsymbol{X}_t} \otimes \boldsymbol{v})(\boldsymbol{X}_t(\boldsymbol{x},t_o),t) = 0$
$\boldsymbol{v}$ – variation	$2\,\boldsymbol{v}(\boldsymbol{x},t) + \boldsymbol{\Phi}_t(\boldsymbol{X}_t^{-1}(\boldsymbol{x},t_o),t) - \partial_{\boldsymbol{x}} K(\boldsymbol{x},t) = 0$

Eulerian Lagrange multiplier: $\boldsymbol{w}(\boldsymbol{x},t) = \boldsymbol{\Phi}_t(\boldsymbol{X}_t^{-1}(\boldsymbol{x},t_o),t)$

$$\partial_t \boldsymbol{w} + \boldsymbol{v} \cdot \partial_{\boldsymbol{x}} \boldsymbol{w} + (\partial_{\boldsymbol{x}} \otimes \boldsymbol{v}) \cdot \boldsymbol{w} = 0$$
$$\Rightarrow \partial_t \boldsymbol{v} + \boldsymbol{v} \cdot \partial_{\boldsymbol{x}} = -\partial_{\boldsymbol{x}} \wp(K)$$

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Pontryagin-Bismut variational approach

$$
\begin{aligned}
&\mathcal{A}(\mathtt{m}, V, \boldsymbol{j}, H, \boldsymbol{X}, \boldsymbol{\Phi}) \\
&= \int_{t_o}^{t_f} \frac{\mathrm{d}t}{\tau} \int_{\mathbb{R}^{2\,d}} \mathrm{d}^{2\,d}x \, \left\{ \mathtt{m} \, \| \, \partial_{\boldsymbol{x}}(H - S) \, \|_{\mathsf{G}}^{2} - V \left(\tau \, \partial_t - \mathfrak{L}^{\dagger} \right) \mathtt{m} \right\} \\
&+ \int_{\mathrm{R}^{2d}} \mathrm{d}^{2d} x_o \, \mathtt{m}_o(\boldsymbol{x}_o) \, \mathrm{E}^{(\omega)}_{\boldsymbol{X}_{t_o} = \boldsymbol{x}_o} \int_{t_o}^{t_f} \boldsymbol{\Phi}_t \cdot \left\{ \mathrm{d}\boldsymbol{X}_t - \frac{\mathrm{d}t}{\tau} \, (\mathsf{J} - \mathsf{G}) \cdot \partial_{\boldsymbol{X}_t} H \right\} \\
&+ \boldsymbol{\jmath} \cdot \int_{\mathrm{R}^{2d}} \mathrm{d}^{2d} x \, \left\{ \mathtt{m}_f(\boldsymbol{x}) \, \boldsymbol{x} - \mathtt{m}_o(\boldsymbol{x}) \, \mathrm{E}^{(\omega)}_{\boldsymbol{X}_{t_o} = \boldsymbol{x}} \boldsymbol{X}_{t_f} \right\}
\end{aligned}
$$

with the auxiliary constraint

$$
\mathrm{d}\boldsymbol{\Phi}_t = \boldsymbol{u} \, \mathrm{d}t + \sqrt{\frac{2}{\beta \, \tau}} \mathsf{Y} \cdot \mathrm{d}\boldsymbol{\omega}_t
$$

and

$$
\boldsymbol{X}'_{t_o} = \boldsymbol{X}'_{t_f} \overset{\text{in some sense}}{=} 0
$$

Numquam ponenda est pluralitas sine necessitate

William of Ockham, Quaestiones et decisiones in quattuor libros Sententiarum Petri Lombardi

Reduction Ansatz

$$\mathbf{\Phi}_t = 0$$

Equivalent Pontryagin functional

$$\mathcal{A}(\mathrm{m}, V, \jmath, H) = \int_{\mathbb{R}^{2d}} \mathrm{d}^{2d}x\, \mathrm{m_f}(\boldsymbol{x})\, V(\boldsymbol{x}, t)$$

$$+ \int_{t_o}^{t_f} \frac{\mathrm{d}t}{\tau} \int_{\mathbb{R}^{2\,d}} \mathrm{d}^{2\,d}x\, \mathrm{m}(\boldsymbol{x}, t)\, \left\{ \| \mathsf{G} \cdot \partial_{\boldsymbol{x}}(H - S) \|^2 + (\tau\, \partial_t + \mathfrak{L})\, V \right\} (\boldsymbol{x}, t)$$

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Guerra & Morato, Phys. Rev. D, 27, 1774-1786, (1983)

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Extremal equations

$$\mathfrak{D}^{(S)} = -\beta\,(\partial_x S)\cdot \mathsf{G}\cdot\partial_x + \mathsf{G} : \partial_x \otimes \partial_x$$

$$(S\,,V)_{\mathrm{P}} + \frac{1}{\beta}\mathfrak{D}^{(S)}(V - 2A) = 0$$ "non- local constraint"

$$\tau\,\partial_t V + (A\,,V)_{\mathrm{P}} - \partial_x A\cdot\mathsf{G}\cdot\partial_x V + \parallel \mathsf{G}\cdot\partial_x A \parallel^2 = 0$$

$$\tau\,\partial_t S + (A\,,S)_{\mathrm{P}} + \frac{1}{\beta}\mathfrak{D}^{(S)}A = 0$$

Non coercivity: extremal independent of $\partial_q A$

$$\sum_{i=1}^{d}\left\{(\partial_{p_i}S)\partial_{q_i}V - (\partial_{q_i}S)\partial_{p_i}V - \left[(\partial_{p_i}S)\partial_{p_i} - \frac{1}{\beta}\partial_{p_i}\right](V - 2A)\right\} = 0$$

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Extremal equations

$\mathfrak{D}^{(S)} = -\beta\,(\partial_{\boldsymbol{x}} S)\cdot \mathsf{G}\cdot\partial_{\boldsymbol{x}} + \mathsf{G} : \partial_{\boldsymbol{x}}\otimes\partial_{\boldsymbol{x}}$ Langevin–Smoluchowski case

$$V - 2A = 0$$

"local constraint"

$$\tau\,\partial_t V - \partial_{\boldsymbol{x}} A\cdot\mathsf{G}\cdot\partial_{\boldsymbol{x}} V + \parallel \mathsf{G}\cdot\partial_{\boldsymbol{x}} A \parallel^2 = 0$$

$$\tau\,\partial_t S + \frac{1}{\beta}\mathfrak{D}^{(S)} A = 0$$

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An explicitly solvable case

Boundary conditions

$$\mathrm{m_i}(\boldsymbol{x}) = \frac{\beta}{2\,\pi} e^{-\beta\, S_{\mathrm{i}}(\boldsymbol{x})} \qquad \mathrm{i} = \mathrm{o}, \mathrm{f}$$

with

$$S_{\mathrm{i}}(p,q) = \frac{(p-\mu_{p;\mathrm{i}})^2}{2\,\sigma_{p;\mathrm{i}}^2\,\cos^2\theta_{\mathrm{i}}} + \frac{(q-\mu_{q;\mathrm{i}})^2}{2\,\sigma_{q;\mathrm{i}}^2\,\cos^2\theta_{\mathrm{i}}} - \tanh\theta_{\mathrm{i}}\,\frac{(p-\mu_{p;\mathrm{i}})(q-\mu_{q;\mathrm{i}})}{\sigma_{p;\mathrm{i}}\,\sigma_{q;\mathrm{i}}\,\cos\theta_{\mathrm{i}}} - \frac{1}{\beta}\ln\left(\frac{1}{2\,\pi\,\sigma_{p;\mathrm{i}}\,\sigma_{q;\mathrm{i}}\,\cos\theta_{\mathrm{i}}}\right)$$

Decorrelated zero mean statistics of the initial state

$$\mu_{p;\mathrm{o}} = \mu_{p;\mathrm{o}} = \theta_{\mathrm{o}} = 0$$

Solution by quadratic Ansätze

The extremal equations foliate into a solvable hierarchy of DE's

$$y_t := \frac{\partial_p^2 A}{\partial_p^2 S} \quad \text{resolve the hierarchy for 2nd order monomials}$$

$$\ddddot{y}_t\,\dot{y}_t^2 - 2\,\dot{y}_t\,\ddot{y}_t\,\dddot{y}_t + \ddot{y}_t^3 = 0$$

$$\Rightarrow y_t = \tau\,\Omega\,\{c_0 + c_1\,\Omega\,t + c_1\,[\sin(\Omega\,t + \varphi) - \sin\varphi]\}$$

Family of extremals parametrized by $\partial_p\partial_q S$ and $\mu_{p;t}$

$$\partial_p^2 S = \frac{16\,\cos^2\frac{\varphi}{2}\,\cos^2\frac{\Omega\,t+\varphi}{2}}{\left\{4\,\sigma_{p;\mathrm{o}}\cos^2\frac{\varphi}{2} + \sigma_{q;\mathrm{o}}\left[\Omega\,t + \sin(\Omega\,t+\varphi) - \sin\varphi\right]\right\}^2} \geq 0$$

$$\partial_q^2 S = \frac{\cos^2\frac{\varphi}{2}}{\sigma_{q;\mathrm{o}}^2\,\cos^2\frac{\Omega\,t+\varphi}{2}} + \frac{(\partial_p\partial_q S)^2}{\partial_p^2 S} \geq 0$$

$$\mu_{q;t} = \frac{\mu_{\mathrm{f}}t}{t_{\mathrm{f}}}$$

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$$\partial_q^2 S = \frac{\cos^2\frac{\varphi}{2}}{\sigma_{q;\mathrm{o}}^2\,\cos^2\frac{\Omega\,t+\varphi}{2}} + \frac{(\partial_p\partial_q S)^2}{\partial_p^2 S} \geq 0$$

$$\mu_{q;t} = \frac{\mu_{\mathrm{f}} t}{t_{\mathrm{f}}}$$

Exact value of the entropy production

$$\frac{\mathcal{E}_{t_{\mathrm{f}},t_{\mathrm{o}}}}{\beta} = \frac{\mu_{q;\mathrm{f}}^2\,\tau}{t_{\mathrm{f}}} + \frac{\sigma_{q;\mathrm{o}}^2\,\Omega^2\,\tau\,t_{\mathrm{f}}}{4\,\beta\,\cos^2\frac{\varphi}{2}}$$

Constraints imposed by the boundary conditions

$$\sigma_{p;\mathrm{f}}^2 = \frac{\left\{4\,\sigma_{p;\mathrm{o}}\cos^2\frac{\varphi}{2} + \sigma_{q;\mathrm{o}}\left[\Omega\,t_{\mathrm{f}} + \sin(\Omega\,t_{\mathrm{f}}+\varphi) - \sin\varphi\right]\right\}^2}{16\,\cos^2\theta_{\mathrm{f}}\,\cos^2\frac{\varphi}{2}\,\cos^2\frac{\Omega\,t_{\mathrm{f}}+\varphi}{2}}$$

$$\frac{\sigma_{q;\mathrm{f}}^2}{\sigma_{q;\mathrm{o}}^2} = \frac{\cos^2\frac{\Omega\,t_{\mathrm{f}}+\varphi}{2}}{\cos^2\frac{\varphi}{2}}$$

Exact value of the entropy production

Independent of $\partial_q \partial_p S$ & $\mu_{p,t}$: self-consistency of the extremal.

$$\frac{\mathcal{E}_{t_\mathrm{f},t_\mathrm{o}}}{\beta} = \frac{\mu_{q;\mathrm{f}}^2\,\tau}{t_\mathrm{f}} + \frac{\sigma_{q;\mathrm{o}}^2\,\Omega^2\,\tau\,t_\mathrm{f}}{4\,\beta\,\cos^2\frac{\varphi}{2}}$$

Constraints imposed by the boundary conditions

$$\sigma_{p;\mathrm{f}}^2 = \frac{\left\{4\,\sigma_{p;\mathrm{o}}\cos^2\frac{\varphi}{2} + \sigma_{q;\mathrm{o}}\left[\Omega\,t_\mathrm{f} + \sin(\Omega\,t_\mathrm{f}+\varphi) - \sin\varphi\right]\right\}^2}{16\,\cos^2\theta_\mathrm{f}\,\cos^2\frac{\varphi}{2}\,\cos^2\frac{\Omega\,t_\mathrm{f}+\varphi}{2}}$$

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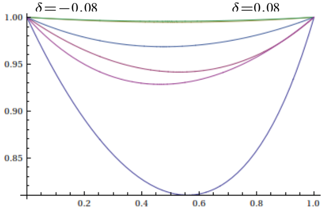
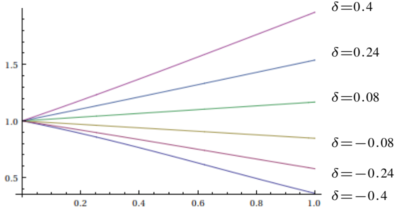
A special case: $\sigma_{p;\mathrm{o}} = \sigma_{p;\mathrm{f}}$ & $\lambda = \sigma_{p;\mathrm{o}}/\sigma_{q;\mathrm{o}}$

$$\frac{\mathcal{E}_{t_\mathrm{f},0}}{\beta} = \frac{\mu_{q;\mathrm{f}}^2\,\tau}{t_\mathrm{f}} + \frac{\tau\,(1+\lambda^2)\,(\sigma_{q;\mathrm{f}} - \sigma_{q;\mathrm{f}})^2}{\beta\, t_\mathrm{f}} - \frac{\tau\,\lambda^2\,(\sigma_{q;\mathrm{f}} - \sigma_{q;\mathrm{o}})^3}{\beta\,\sigma_{q;\mathrm{o}}\, t_\mathrm{f}} + O(\sigma_{q;\mathrm{f}} - \sigma_{q;\mathrm{o}})^4$$



(a) Momentum variance $\sigma^2_{p;t}$



(b) Position variance $\sigma^2_{q;t}$ for $\partial_q\partial_p S = 0$

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Wide scale separation: $\lambda = \sigma_{p;o}/\sigma_{q;o} \ll 1$

$$\frac{\mathcal{E}_{t_f,0}}{\beta} = \frac{\mu_{q;f}^2\,\tau}{t_f} + \frac{(\sigma_{q;f} - \sigma_{q;o})^2}{\beta\, t_f} + o\,(\lambda)$$

with

$$(\partial_q A)(0,q,t)\big|_{\mu_{p;t}=0} = -\frac{\mu_{q;f} + \frac{q\,(\sigma_{q;f}-\sigma_{q;o})}{\sigma_{q;o}}}{1 + \frac{t\,(\sigma_{q;f}-\sigma_{q;o})}{t_f\,\sigma_{q;o}}}\,\frac{\tau}{t_f} + o\,(\lambda)$$

$$(\partial_p A)(0,q,t)\big|_{\mu_{p;t}=0} = -\,(\partial_p A)(0,q,t)\big|_{\mu_{p;t}=0} + o\,(\lambda)$$

$$(\partial_q S)(0,q,t) = \frac{\left(q - \frac{\mu_{q;f}\,t}{t_f}\right)}{\sigma_{q;o}^2\left[1 + \frac{t\,(\sigma_{q;f}-\sigma_{q;o})}{t_f\,\sigma_{q;o}}\right]^2} + o(\lambda)$$

for $\beta \parallel \boldsymbol{p} \parallel \ll \lambda \ll 1$ we recover the entropy production of the optimally controlled Langevin–Smoluchowski model

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A multiscale reminder

Pavliotis & Stuart, “Multiscale methods: averaging and homogenization” (2008)

$$\partial_t u = \left\{ \mathfrak{O}_0 + \frac{1}{\varepsilon}\mathfrak{O}_1 + \frac{1}{\varepsilon^2}\mathfrak{O}_2 \right\} u$$

- $\mathfrak{O}_i \in \mathbb{R}^{d\times d}$, $i = 1, 2, 3$
- $\mathrm{Ker}\mathfrak{O}_0 = \mathrm{Ker}\mathfrak{O}_0^\dagger = 1$
- $r_0 \in \mathrm{Ker}\,\mathfrak{O}_0 \quad \& \quad l_0 \in \mathrm{Ker}\,\mathfrak{O}_0^\dagger$

$u = u_0 + \varepsilon\, u_1 + \varepsilon^2\, u_2 + \dots$

Assume centering condition: $(l_0\,, \mathfrak{O}_1 r_0) = 0$

$$\mathcal{O}(1/\varepsilon^2) \quad \mathfrak{O}_0\, u_0 = 0 \quad \Rightarrow \quad u_0 = \alpha(t)\, r_0$$

$$\mathcal{O}(1/\varepsilon) \quad \mathfrak{O}_0\, u_1 = -\mathfrak{O}_1\, u_0 \quad \Rightarrow \quad u_1 = \alpha(t)\, g \;\text{ s.t. }\; \mathfrak{O}_0\, g = \mathfrak{O}_1\, r_0$$

$$\mathcal{O}(1) \quad \mathfrak{O}_0 u_2 = -\partial_t u_0 - \mathfrak{O}_1 u_1 - \mathfrak{O}_2 u_0 \quad \Rightarrow \quad \partial_t \alpha = \frac{(l_0\,, \mathfrak{O}_2\, r_0 - \mathfrak{O}_1\, g)}{(l_0\,, r_0)}\alpha$$

by Fredholm’s alternative

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$\mathcal{O}(1/\varepsilon)$	$\mathfrak{O}_0\, u_1 = -\mathfrak{O}_1\, u_0$	$\Rightarrow$	$u_1 = \alpha(t)\, g$ s.t. $\mathfrak{O}_0\, g = \mathfrak{O}_1\, r_0$
$\mathcal{O}(1)$	$\mathfrak{O}_0 u_2 = -\partial_t u_0 - \mathfrak{O}_1 u_1 - \mathfrak{O}_2 u_0$	$\Rightarrow$	$\partial_t \alpha = \frac{(l_0\,, \mathfrak{O}_2\, r_0 - \mathfrak{O}_1\, g)}{(l_0\,, r_0)}\alpha$

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$\mathcal{O}(1/\varepsilon^2)$	$\mathfrak{O}_0\, u_0 = 0$	$\Rightarrow$	$u_0 = \alpha(t)\, r_0$
$\mathcal{O}(1/\varepsilon)$	$\mathfrak{O}_0\, u_1 = -\mathfrak{O}_1\, u_0$	$\Rightarrow$	$u_1 = \alpha(t)\, g$ s.t. $\mathfrak{O}_0\, g = \mathfrak{O}_1\, r_0$
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by Fredholm's alternative

Extremal eqs under wide scale separation

Boundary conditions: $\lambda \ll 1$

$$\mathrm{m_o}(\boldsymbol{p},\boldsymbol{q}) = \left(\frac{\beta}{2\,\pi\,\lambda}\right)^{d} e^{-\beta\,\frac{\|\boldsymbol{p}^2\|}{2\,\lambda^2}-\beta\,U_{\mathrm{o}}(\boldsymbol{q})} \qquad \mathrm{m_f}(\boldsymbol{p},\boldsymbol{q}) = \left(\frac{\beta}{2\,\pi\,\lambda}\right)^{d} e^{-\beta\,\frac{\|\boldsymbol{p}\|^2}{2\,\lambda^2}-\beta\,U_{\mathrm{f}}(\boldsymbol{q})}$$

Multiscale asymptotic equations

$$A(\boldsymbol{x},t) = \sum_{i=0}^{2} \lambda^i A_{(i)}\left(\frac{\boldsymbol{p}}{\lambda},\boldsymbol{q},t\dots\right) + o(\lambda^2) := \tilde{A}\left(\tilde{\boldsymbol{p}},\boldsymbol{q},t\dots\right)$$

and similarly for V, S:

extremal condition eq. $\quad \frac{1}{\lambda}\widetilde{(\tilde{S},\tilde{V})}_{\mathrm{P}} + \frac{1}{\lambda^2\,\beta}\tilde{\mathfrak{D}}^{(\tilde{S})}(\tilde{V}-2\tilde{A}) = 0$

value function eq. $\quad \tau\,\partial_t\tilde{V} + \frac{1}{\lambda}\widetilde{(\tilde{A},\tilde{V})}_{\mathrm{P}} - \frac{1}{\lambda^2}\left(\partial_{\tilde{\boldsymbol{p}}}\tilde{A}\right)\cdot\partial_{\tilde{\boldsymbol{p}}}\left(\tilde{V}-\tilde{A}\right) = 0$

stochastic entropy eq. $\quad \tau\,\partial_t\tilde{S} + \frac{1}{\lambda}\widetilde{(\tilde{A},\tilde{S})}_{\mathrm{P}} + \frac{1}{\lambda^2\,\beta}\tilde{\mathfrak{D}}^{(\tilde{S})}\tilde{A} = 0$

Extremal eqs under wide scale separation

Boundary conditions: $\lambda \ll 1$

$$\mathrm{m}_{\mathrm{o}}(\boldsymbol{p},\boldsymbol{q}) = \left(\frac{\beta}{2\,\pi\,\lambda}\right)^{d} e^{-\beta\,\frac{\|\boldsymbol{p}^2\|}{2\,\lambda^2}-\beta\,U_{\mathrm{o}}(\boldsymbol{q})} \qquad \mathrm{m}_{\mathrm{f}}(\boldsymbol{p},\boldsymbol{q}) = \left(\frac{\beta}{2\,\pi\,\lambda}\right)^{d} e^{-\beta\,\frac{\|\boldsymbol{p}\|^2}{2\,\lambda^2}-\beta\,U_{\mathrm{f}}(\boldsymbol{q})}$$

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Centering condition

Ornstein-Uhlenbeck operator

$$\tilde{\mathfrak{D}}^{(S_0)} = -\tilde{\boldsymbol{p}} \cdot \partial_{\tilde{\boldsymbol{p}}} + \frac{1}{\beta}\partial^2_{\tilde{\boldsymbol{p}}} \qquad \begin{array}{ccc} 1 & \in & \mathrm{Ker}\mathfrak{D}^{(S_0)} \\ \exp\{-\frac{\beta\|\tilde{\boldsymbol{p}}\|^2}{2}\} & \in & \mathrm{Ker}\mathfrak{G}^{\dagger} \end{array}$$

$\mathcal{O}(1/\varepsilon^2)$

$$0 = \partial_{\tilde{\boldsymbol{p}}}\tilde{A}_{(0)} = \partial_{\tilde{\boldsymbol{p}}}\tilde{V}_{(0)} \quad \Rightarrow \quad \tilde{A}_{(0)}, \tilde{V}_{(0)} \in \mathrm{Ker}\mathfrak{D}$$

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$\mathcal{O}(1/\varepsilon)$: centering condition

$$\tilde{A}_{(1)} = -\tilde{\boldsymbol{p}} \cdot \partial_{\boldsymbol{q}}\tilde{A}_{(0)}$$

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Cell problem: Monge–Ampère–Kantorovich

$\mathcal{O}(1)$

value function eq.

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stochastic entropy eq.

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Averaging over Maxwell's distribution yields the cell problem

$$\tau \partial_t \tilde{S}_{(0)} - \partial_{\boldsymbol{q}} \tilde{A}_{(0)} \cdot \partial_{\boldsymbol{q}} \tilde{S}_{(0)} + \frac{1}{\beta} \partial_{\boldsymbol{q}}^2 \tilde{A}_{(0)} = 0$$

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$$\mathcal{E}_{t_f,0} = \beta \int_0^{t_f} \frac{dt}{\tau} \int_{\mathbb{R}^d} d^d q \, \beta^{d/2} e^{-\beta\, S_{(0,0)}} \parallel \partial_{\boldsymbol{q}} A_{(0)} \parallel^2 + O(\lambda)$$

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Summary

- Symplectic structure introduces non local constraint.
- Because of non-coercivity, parametric families of extremals.
- For large scale separations, both effects are weak $\Rightarrow$ recovery of the Langevin-Smoluchowski entropy production.

Open questions

- singular control ?

Heat release minimization by kinetic+potential Hamiltonian

$$\tau\,\partial_t V + \boldsymbol{p}\cdot\partial_{\boldsymbol{p}} V - (\boldsymbol{p} + \partial_{\boldsymbol{q}} U)\cdot\partial_{\boldsymbol{p}} V + \frac{1}{\beta}\partial_{\boldsymbol{p}}^2 V + \frac{\|\,\boldsymbol{p}\,\|^2}{2} = 0$$

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Some more about the foregoing

- Aurell, Mejia-Monasterio, M.-G., PRL 106, 250601 (2011)
- Aurell, Mejia-Monasterio, M.-G., PRE 85, 020103 (2012)
- Aurell, Gawedzki, Mejia-Monasterio, Mohayaee, M.-G., JSP 147, 487 (2012)
- M.-G., Mejia-Monasterio , Peliti, JSP 150, 181 (2013)
- M.G., J. Phys. A, 46, 275002 (2013)
- M.G., "On extremals of the entropy production by Langevin–Kramers dynamics", in preparation.

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