

# Generalized Schrödinger bridges in stochastic thermodynamics

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based on

*Journal of Statistical Physics* **191**, p. 117, (2024). arXiv: 2403.00679

in collaboration with

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# Standing on the shoulders of giants

144 Sitzung der physikalisch-mathematischen Klasse vom 12. März 1931

## Über die Umkehrung der Naturgesetze.

VON E. SCHRÖDINGER.

**Einleitung.** Wenn für ein diffundierendes oder in Brownscher Bewegung begriffenes Teilchen die Aufenthaltswahrscheinlichkeit im Abszissenbereich  $(x; x + dx)$  zur Zeit  $t_0$

$$w(x, t_0) dx$$

gegeben ist,

$$w(x, t_0) = w_0(x),$$

so ist sie für  $t > t_0$  diejenige Lösung  $w(x, t)$  der Diffusionsgleichung

$$D \frac{\partial^2 w}{\partial x^2} = \frac{\partial w}{\partial t}, \quad (1)$$

welche für  $t = t_0$  der vorgegebenen Funktion  $w_0(x)$  gleich wird. Über

“if I have seen further [than others], it is by standing on the shoulders of giants.”

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1675 Letter  
from Sir Isaac Newton  
to Robert Hooke

English translation Chetrite, Muratore-Ginanneschi, and Schwieger, *The European Physical*

*Journal H* **46**, pp. 1–29, (2021). arXiv: 2105.12617

# Schrödinger's particle migration model

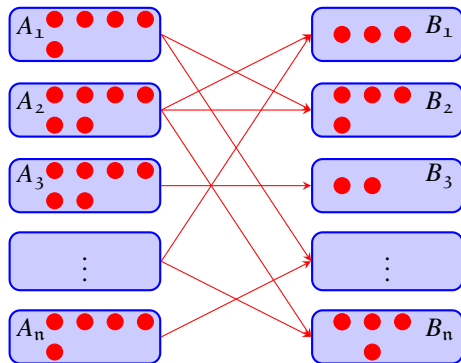
- Two sets of  $n$  boxes

$$\{A_i\}_{i=1}^n \quad \& \quad \{B_i\}_{i=1}^n$$

- $N$  particles initially randomly located in  $\{A_i\}_{i=1}^n$

- Each *migration* is an independent event

$$g(j|i) = \Pr(\text{be in } B_j \mid \text{been in } A_i)$$



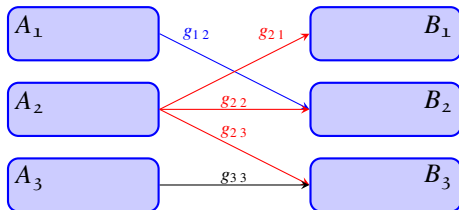
# Schrödinger's bridge problem

**H.1** : Assign initial marginal

$$\tilde{\mathcal{C}}_A = \mathbf{a}$$

**H.2** : Assign final marginal

$$\tilde{\mathcal{C}}_B = \mathbf{b}$$



**Q** : Determine  $\mathbf{K} = (k(i|j))$  “close to”  $\mathbf{G} = (g(i|j))$  realizing the migration

**Schrödinger's solution: minimize**

$$D_{KL}(\mathbf{K}||\mathbf{G}) = \sum_{i,j=1}^n k(j|i) w_o(i) \ln \frac{k(j|i)}{g(j|i)}$$

*“The so-called irreversible laws of nature, if one interprets them statistically, do actually not privilege any time direction.”*

## Modern formulations

# Cost of the transition depends on the dynamics

## Divergence from a reference process

$\mathcal{P}, \mathcal{Q} =$  path measures

$$K(\mathcal{P} \parallel \mathcal{Q}) = E_{\mathcal{P}} \ln \frac{d\mathcal{P}}{d\mathcal{Q}}$$

Föllmer, "Time reversal on Wiener space" *Stochastic Processes, Mathematics and Physics* vol. **1158**, pp. 119–129, (1986).

Dai Pra, *Applied Mathematics and Optimization* **23**, pp. 313–329, (1991).

Léonard, *Discrete and Continuous Dynamical Systems - Series A* **34**, pp. 1533–1574, (2014). arXiv: 1308.0215

Peyré and Cuturi, *Foundations and Trends in Machine Learning* **11**, pp. 355–607, (2019). arXiv: 1803.00567

Chen, Georgiou, and Pavon, *SIAM Review* **63**, pp. 249–313, (2021). ETC.

## Mean entropy production (stochastic thermodynamics)

$\mathcal{P}_{\mathcal{R}} =$  time reversal + path reversal of  $\mathcal{P}$

$$\mathcal{E} = K(\mathcal{P} \parallel \mathcal{P}_{\mathcal{R}}) = E_{\mathcal{P}} \ln \frac{d\mathcal{P}}{d\mathcal{P}_{\mathcal{R}}}$$

Maes, Redig, and Mofaert, *Journal of Mathematical Physics* **41**, pp. 1528–1554, (2000).

Chétrite and Gawędzki, *Communications in Mathematical Physics* **282**, pp. 469–518, (2008). arXiv: 0707.2725

Peliti and Pigolotti, *Stochastic Thermodynamics*, Princeton University Press, (2020). ETC.

# Mechanical Langevin-Kramers (underdamped) dynamics

Zwanzig, *Journal of Statistical Physics* **9**, pp. 215–220, (1973).

Cépas and Kurchan, *European Physical Journal B: Condensed Matter and Complex Systems* **2**, pp. 221–223, (1998). arXiv: cond-mat/9706296

## Kinematics compatible with thermalization

$$d\mathbf{q}_t = \frac{\mathbf{p}_t}{m} dt - \frac{g\tau}{m} (\partial U_t)(-\mathbf{q}_t) dt + \sqrt{\frac{2g\tau}{m\beta}} d\mathbf{w}_t$$

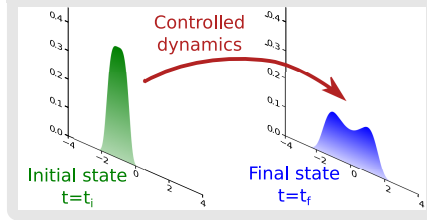
$$d\mathbf{p}_t = - \left( \frac{\mathbf{p}_t}{\tau} + (\partial U_t)(\mathbf{q}_t) \right) dt + \sqrt{\frac{2m}{\tau\beta}} d\boldsymbol{\omega}_t$$

## Physical motivation: open system in a bipartite environment

Cuccoli et al., *Physical Review E* **64**, p. 066124, (2001). (bipartite environment: Josephson junctions)

# Generalized Schrödinger bridges

Find a **mechanical potential** steering the transition at **minimum cost** in a given time horizon



- **Cost: divergence from a free diffusion**

$$K(\mathcal{P} \parallel \mathcal{Q}) = C \mathbb{E}_{\mathcal{P}} \int_{t_i}^{t_f} dt \|(\partial U_t)(\mathbf{q}_t)\|^2$$

$$C = \frac{\beta \tau (1 + g)}{4 m}$$

- **Cost: entropy production – convexity problem!!**

$$\mathcal{E} = \mathbb{E}_{\mathcal{P}} \ln \frac{p_{t_f}(\mathbf{q}_{t_f}, \mathbf{p}_{t_f})}{f_{t_f}(\mathbf{q}_{t_f}, \mathbf{p}_{t_f})} + \mathbb{E}_{\mathcal{P}} \int_{t_i}^{t_f} dt \left( \frac{\beta \|\mathbf{p}_t\|^2}{m \tau} - \frac{d}{\tau} \right)$$

$$+ \frac{\beta g \tau}{m} \mathbb{E}_{\mathcal{P}} \int_{t_i}^{t_f} dt \left( \|(\partial U)(\mathbf{q}_t)\|^2 - \frac{(\partial^2 U)(\mathbf{q}_t)}{\beta} \right)$$



# Universal bound on the mean entropy production

## Lower bound by Wasserstein 2-distance between the end PDFs

$$\mathcal{E}(\text{underdamped}) \geq \frac{m\beta}{(1+g)\tau} \frac{\mathbb{E}_{\mathcal{P}} \left\| \mathbf{q}_{t_\ell} - \mathbf{q}_{t_\iota} \right\|^2}{t_\ell - t_\iota} = \mathcal{E}(\text{overdamped})$$

Aurell, Mejía-Monasterio, and Muratore-Ginanneschi, *Physical Review Letters* **106**, p. 250601, (2011). arXiv: 1012.2037

Aurell et al., *Journal of Statistical Physics* **147**, pp. 487–505, (2012). arXiv: 1201.3207

Chen, Georgiou, and Pavon, *Journal of Optimization Theory and Applications* **169**, pp. 671–691, (2016). arXiv: 1412.4430

} overdamped maps into optimal mass transport

Proofs:

Muratore-Ginanneschi, *Journal of Statistical Mechanics: Theory and Experiment* **2014**, P05013, (2014). arXiv: 1401.3394

Dechant and Sasa, *Physical Review E* **97**, p. 062101, (2018). arXiv: 1803.09447

Gawedzki, “Improved 2nd Law of Stochastic Thermodynamics for underdamped Langevin process”, (2021)

Muratore-Ginanneschi and Peliti, *Journal of Statistical Mechanics: Theory and Experiment* **Aug 2023**, p. 083202, (2023). arXiv: 2302.08290

## For a bipartite classical system exceeds that of a part

$$S(\text{Pr}(\xi, \eta)) = S(\text{Pr}(\xi)) + S(\text{Pr}(\eta|\xi)) \geq S(\text{Pr}(\xi))$$

## First order conditions for optimality (stationary conditions)

Muratore-Ginanneschi, *Journal of Statistical Mechanics: Theory and Experiment* **2014**, P05013, (2014). arXiv: 1401.3394  
Muratore-Ginanneschi and Schwieger, *Physical Review E* **90**, 060102(R), (2014). arXiv: 1408.5298

# Mapping to a variational problem (model problem)

## “Adjoint equation method”

$$\mathcal{A}[\mathcal{P}, V, U] = \mathbb{E}_{\mathcal{P}} \left( V_{t_L}(\mathbf{q}_{t_L}, \mathbf{p}_{t_L}) - V_{t_f}(\mathbf{q}_{t_f}, \mathbf{p}_{t_f}) \right) + \mathbb{E}_{\mathcal{P}} \int_{t_L}^{t_f} dt \left( \frac{\beta \tau}{4m} \|(\partial U_t)(\mathbf{q}_t)\|^2 + (D V_t)(\mathbf{q}_t, \mathbf{p}_t) \right)$$

Mean forward derivative

Serrin, “Mathematical Principles of Classical Fluid Mechanics”, Springer Science + Business Media, (1959).

Seliger and Whitham, *Proceedings of the Royal Society A: Mathematical, Physical and Engineering Sciences* **305**, pp. 1–25, (1968).

Bismut, *SIAM Review* **20**, pp. 62–78, (1978).

equivalently (modulo technicalities)

## Fokker-Planck control: $\mathbf{x} = [\mathbf{q}, \mathbf{p}]$

$$\mathcal{A}[f, U, V] = \int_{t_L}^{t_f} dt \int_{\mathbb{R}^{2d}} d^{2d} \mathbf{x} \left( \frac{\beta \tau}{4m} \|(\partial U_t)(\mathbf{q})\|^2 - V_t(\mathbf{x}) \left( \partial_t - \mathfrak{L}_x^\dagger \right) f_t(\mathbf{x}) \right)$$

Fokker-Planck

Lagrange multiplier

Breitenbach and Borzi, *Computational Optimization and Applications* **76**, 499–533, (2020).

Daudin, *Journal de Mathématiques Pures et Appliquées* **175**, 37–75, (2023). arXiv: 2109.14978

# Mechanical potentials only depend upon “position”

**Fokker–Planck evolution of the density:**

$$(\partial_t - \mathfrak{L}_x^\dagger) f_t(\mathbf{x}) = 0$$

**Value function equation:**

$$(\partial_t + \mathfrak{L}_x) V_t(\mathbf{x}) + \frac{\beta \tau}{4m} \|(\partial U_t)(\mathbf{q})\|^2 = 0$$

**Condition specifying the optimal control potential ( $g = 0$ ):**

$$\left( (\partial \ln \tilde{f}_t)(\mathbf{q}) + \partial_{\mathbf{q}} \right) \cdot \left( \int_{\mathbb{R}^d} d^d \mathbf{p} \frac{f_t(\mathbf{q}, \mathbf{p})}{\tilde{f}_t(\mathbf{q})} \partial_{\mathbf{p}} V_t(\mathbf{q}, \mathbf{p}) - \frac{\beta \tau}{2m} (\partial U_t)(\mathbf{q}) \right) = 0$$

$$\tilde{f}_t(\mathbf{q}) = \int_{\mathbb{R}^d} d^d \mathbf{p} f_t(\mathbf{q}, \mathbf{p}) \quad (\text{position marginal pdf})$$

**Boundary conditions: kinematically compatible with equilibria**

$$f_{t_\iota}(\mathbf{x}) = \frac{e^{-\beta \left( \frac{\|\mathbf{p}\|^2}{2m} + U_\iota(\mathbf{q}) \right)}}{Z_\iota} \quad \& \quad f_{t_\ell}(\mathbf{x}) = \frac{e^{-\beta \left( \frac{\|\mathbf{p}\|^2}{2m} + U_\ell(\mathbf{q}) \right)}}{Z_\ell}$$

# Takeaways

- Similar equations (more cumbersome!) hold for the entropy production.
- For the entropy production  $g$ -regularization guarantees convexity in the control.
- Convexity in the control  $\implies$  **existence** of stationary eqs.
- **Q**: uniqueness of solutions? (boundary not Cauchy problem!)
- Equations are **non-local**: average over momenta.
- Gaussian case: optimal potential equation reduces to a **Lyapunov equation**.
- Equations have the correct overdamped ( $\varepsilon \searrow 0$ ) limit:

$$\lim_{g \searrow 0} \lim_{\varepsilon \searrow 0} \underline{\text{underdamped stationary eqs}} = \underline{\text{overdamped stationary eqs}}$$

Muratore-Ginanneschi and Schwieger, *Physical Review E* **90**, 060102(R), (2014). arXiv: 1408.5298

# Analytical treatment: finite-time Poincaré-Lindstedt expansion around over-damped limit

Sanders, Baldovin, and Muratore-Ginanneschi, *Journal of Statistical Physics* **191**, p. 117, (2024). arXiv: 2403.00679  
Sanders, Baldovin, and Muratore-Ginanneschi, *Eprint* , , (2024). arXiv: 2407.15678

# Non dimensional variables identify a small parameter

$$t = \tau t \quad \& \quad p = \sqrt{\frac{m}{\beta}} p \quad \& \quad q = L q \quad \& \quad U_t = \frac{1}{\beta} U_t$$
$$\varepsilon = \sqrt{\frac{\tau^2}{m \beta L^2}}$$

## Optimal control equations in the 1d case

$$\partial_t f_t - \partial_p (p + \partial_p) f_t = \varepsilon \left( (\partial_q U) \partial_p - p \partial_q \right) f_t$$

$$\partial_t V_t - (p \partial_p - \partial_p^2) V_t = \varepsilon \left( (\partial_q U) \partial_p - p \partial_q \right) V_t - \frac{\varepsilon^2}{4} \|(\partial U_t)(q)\|$$

$$\int_{\mathbb{R}} dp \frac{f_t(p, q)}{\tilde{f}_t(q)} \partial_q V_t(p, q) = \frac{\varepsilon}{2} (\partial U_t)(q)$$

# Hierarchy in configuration space

Expansion in Hermite polynomials  $\{H_n\}_{n=0}^{\infty}$  unfolds the optimal control equations in an infinite hierarchy

$$\partial_t f_t^{(n)} = \mathcal{F}_n(f_t^{(n-1)}, f_t^{(n)}, f_t^{(n+1)}, \partial_q U_t)$$

$$\partial_t v_t^{(n)} = \mathcal{V}_n(v_t^{(n-1)}, v_t^{(n)}, v_t^{(n+1)}, \partial_q U_t)$$

$$\frac{\varepsilon}{2}(\partial U_t)(q) - \sum_{n=0}^{\infty} (n+1)! \frac{f_t^{(n)}(q) v_t^{(n+1)}(q)}{f_t^{(0)}(q)} = 0$$

$$f_t(p, q) = \frac{e^{-\frac{p^2}{2}}}{\sqrt{2\pi}} \sum_{n=0}^{\infty} f_t^{(n)}(q) H_n(p)$$

$$f_{t_\iota}^{(n)}(q) = \delta_{n,0} \frac{e^{-U_\iota(q)}}{Z_\iota}$$

$$f_{t_\ell}^{(n)}(q) = \delta_{n,0} \frac{e^{-U_\ell(q)}}{Z_\ell}$$

$$V_t(p, q) = \sum_{n=0}^{\infty} v_t^{(n)}(q) H_n(p)$$

no b.c.



# Poincaré-Lindstedt method Wycoff and Báalazs, Physica A 146, pp 175-200, (1987)

Slow times, e.g.  $\varepsilon^2 t$ , treated as independent variables

$$f_t^{(n)}(q) = e^{-n t} f_{\varepsilon^2 t, \dots}^{(n:0)}(q) + \sum_{k=1}^{\infty} \varepsilon^k f_{t, \varepsilon^2 t, \dots}^{(n:k)}(q)$$

$$v_t^{(n)}(q) = e^{-n(t_f - t)} v_{\varepsilon^2 t, \dots}^{(n:k)}(q) + \sum_{k=1}^{\infty} \varepsilon^k v_{t, \varepsilon^2 t, \dots}^{(n:k)}(q)$$

$$U_t(q) = U_{\varepsilon^2 t}^{(k)}(q) + \sum_{k=1}^{\infty} \varepsilon^k U_{t, \varepsilon^2 t, \dots}^{(k)}(q)$$

Cancellation of saecular terms (no need for slow variable  $\varepsilon t$ )

$$f_{t_l, \varepsilon^2 t, \dots}^{(n:i)}(q) = f_{t_f, \varepsilon^2 t, \dots}^{(n:i)}(q) = 0 \quad \forall n > 0 \quad (\text{boundary conditions})$$

$$v_{t_l, \varepsilon^2 t, \dots}^{(n:i)}(q) = v_{t_f, \varepsilon^2 t, \dots}^{(n:i)}(q) \quad \forall n \quad (\text{cost only when the potential varies})$$

$$\mathcal{A}_* = \sum_{i=0}^{\infty} \varepsilon^i \int_{\mathbb{R}^{2d}} dq \left( v_{\varepsilon^2 t_l, \dots}^{(0:i)}(q) f_l^{(0:0)}(q) - v_{\varepsilon^2 t_f, \dots}^{(0:i)}(q) f_f^{(0:0)}(q) \right)$$

# Perturbative intertwining of hierarchy elements

## Leading order

$$\begin{aligned}f_t^{(0)}(q) &= f_{\varepsilon^2 t}^{(0:0)}(q) + \varepsilon^2 f_{t, \varepsilon^2 t}^{(0:2)}(q) + \mathcal{O}(\varepsilon^3) & v_t^{(0)}(q) &= v_{\varepsilon^2 t}^{(0:0)}(q) + \mathcal{O}(\varepsilon^2) \\f_t^{(1)}(q) &= \varepsilon f_{t, \varepsilon^2 t}^{(1:1)}(q) + \mathcal{O}(\varepsilon^2) & v_t^{(1)}(q) &= \varepsilon v_{t, \varepsilon^2 t}^{(1:1)}(q) + \mathcal{O}(\varepsilon^2) \\f_t^{(2)}(q) &= \varepsilon^2 f_{t, \varepsilon^2 t}^{(2:2)}(q) + \mathcal{O}(\varepsilon^3) & v_t^{(2)}(q) &= v_{\varepsilon^2 t}^{(2:0)}(q) e^{-2(t_f - t)} + \mathcal{O}(\varepsilon) \\f_t^{(n)}(q) &= o(\varepsilon^2) \quad \forall n \geq 3 & v_t^{(n)}(q) &= v_{\varepsilon^2 t}^{(n:0)}(q) e^{-n(t_f - t)} + \mathcal{O}(\varepsilon)\end{aligned}$$

## Meaning of color code

Solutions of “cell” problem w.r.t. slow time  $\varepsilon^2 t$  and  $q$  at order  $\mathcal{O}(\varepsilon^2)$ .

Solutions of differential problem only w.r.t. fast time  $t$  at order  $\mathcal{O}(\varepsilon)$  where

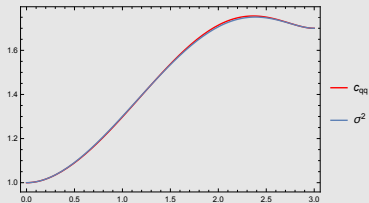
$f_{\varepsilon^2 t}^{(0:0)}(q)$ ,  $v_{\varepsilon^2 t}^{(0:0)}(q)$  and  $v_{\varepsilon^2 t}^{(2:0)}(q)$  only appear as parameters.

Fixed by imposing that  $f_{\varepsilon^2 t}^{(2:2)}$  satisfies the boundary conditions.

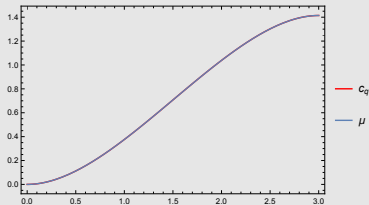
Enslaved or higher order quantities.

# Gaussian case (numerics vs semi-analytical)

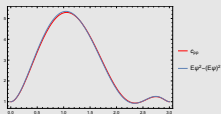
Cumulants exactly obey a finite set of ordinary differential equations



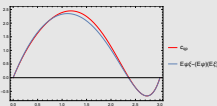
(a) position variance



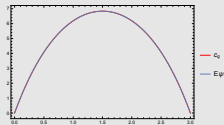
(b) position mean value



(c) momentum variance



(d) position momentum cross correlation



(e) momentum mean value

Figure: Horizon  $t_f = 3$ ,  $\varepsilon = 0.1$ , red curves: non-perturbative numerics

# Gaussian case

## Second order cumulants and their co-states (non-dimensional)

$$\begin{cases} \dot{x}_t^{(1)} = 2 \varepsilon x_t^{(2)} \\ \dot{x}_t^{(2)} = -x_t^{(2)} - \varepsilon (u_t^{(2)} x_t^{(1)} - x_t^{(3)}) \\ \dot{x}_t^{(3)} = 2 (1 - x_t^{(3)} - \varepsilon u_t^{(2)} x_t^{(2)}) \end{cases} \quad \begin{cases} \dot{y}_t^{(1)} = 2 \varepsilon y_t^{(2)} u_t^{(2)} \\ \dot{y}_t^{(2)} = -\varepsilon y_t^{(1)} + y_t^{(2)} + \varepsilon y_t^{(3)} u_t^{(2)} \\ \dot{y}_t^{(3)} = -2 \varepsilon y_t^{(2)} + 2 y_t^{(3)} \end{cases}$$

B.C.:  $\dot{x}_0^{(i)}$  &  $\dot{x}_{t_f}^{(i)}$   $i = 1, 2, 3$  assigned

## First order cumulants and their co-states (non-dimensional)

$$\begin{cases} \dot{x}_t^{(4)} = \varepsilon x_t^{(5)} \\ \dot{x}_t^{(5)} = -x_t^{(5)} + \varepsilon (u_t^{(1)} - u_t^{(2)} x_t^{(4)}) \end{cases} \quad \begin{cases} \dot{y}_t^{(4)} = y_t^{(2)} u_t^{(1)} + u_t^{(2)} y_t^{(5)} - \varepsilon u_t^{(2)} u_t^{(1)} \\ \dot{y}_t^{(5)} = y_t^{(5)} - \varepsilon y_t^{(4)} + \varepsilon y_t^{(3)} u_t^{(1)} \end{cases}$$

B.C.:  $\dot{x}_0^{(i)}$  &  $\dot{x}_{t_f}^{(i)}$   $i = 4, 5$  assigned

## Numerical analysis

Sanders, Baldovin, and Muratore-Ginanneschi, *Eprint* , , (2024). arXiv: 2407.15678

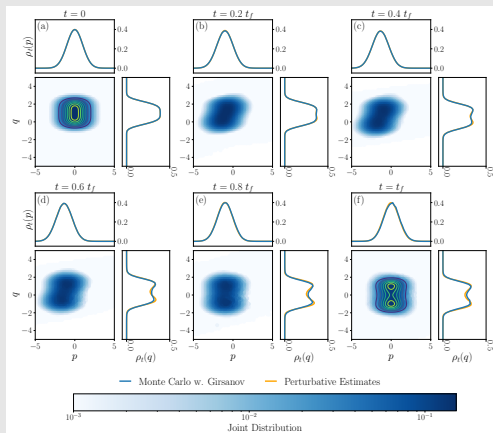
Sanders and Muratore-Ginanneschi, *Eprint* , , (2024). arXiv: 2411.08518

& in progress

# Self-consistence of perturbative drift

Sanders and Muratore-Ginanneschi, *Eprint*, (2024). arXiv: 2411.08518

## Landauer erasure at minimum divergence from free diffusion



Montecarlo method, we evolve  $M = 10\,000$  trajectories from a set of 2601 equally spaced points from the interval  $[-5, 5] \times [-5, 5]$ . We use a time step size  $h = 0.025$  and integrate over trajectories using an Euler-Maruyama discretization. We use  $t_L = 0$ ,  $t_f = 5$ ,  $\beta = 25$  and  $\tau = m = 1$ . The potential in the initial condition is given by with  $U_L(q) = \frac{1}{4}(q-1)^4$  and in the final condition with  $U_f(q) = \frac{1}{4}(q^2-1)^2$ .

## Exact numerical solution (in progress)

- Methods
  - Indirect methods: solution of the stationary equations (MonteCarlo +ML tools)
  - Direct methods: finding minimum of the cost functional (infinite optimization methods)
- Goal:
  - Underdamped half bridge.
  - Underdamped Landauer's erasure model in finite time.

THANKS, Julia & Marco





THANKS!