

# Contraction and Reaction in Generalized Schrödinger Bridges

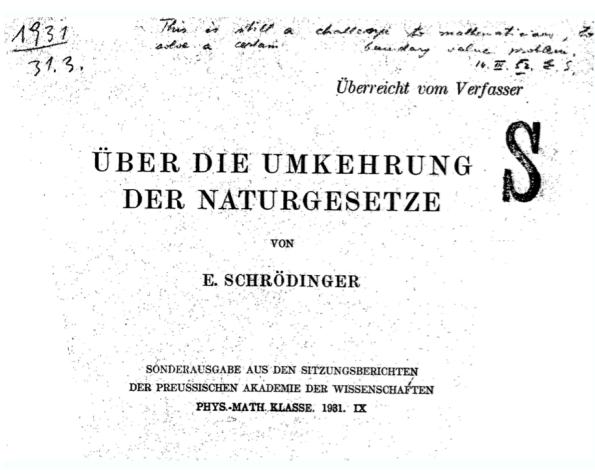
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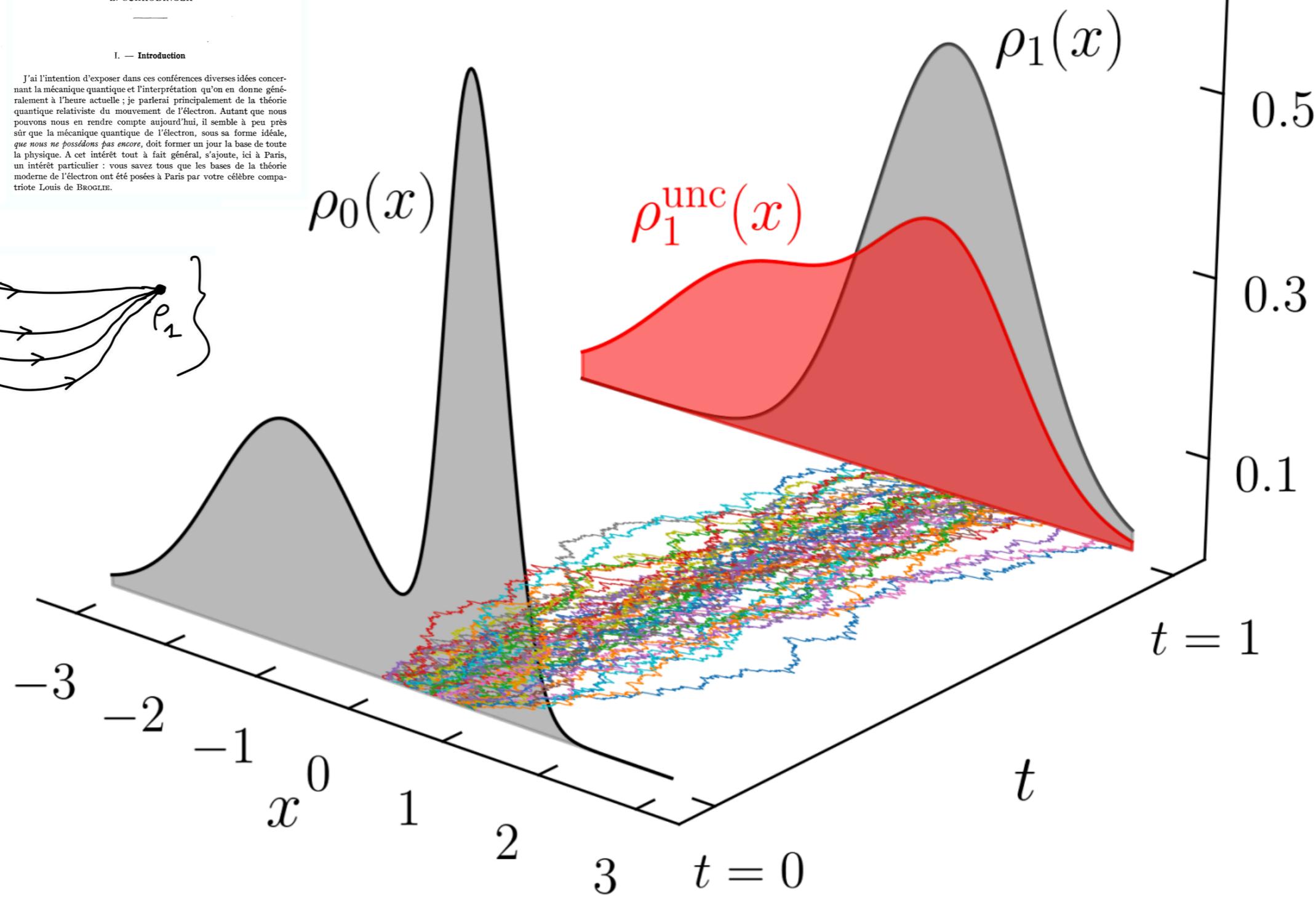
Advancement to Ph.D. candidacy

January 30, 2024

# What is a Schrödinger Bridge Problem (SBP)



$$\mathcal{P}_{01} := \left\{ \rho_0 \rightarrow \rho_1 \right\}$$



Most likely evolution between 2 distributional snapshots

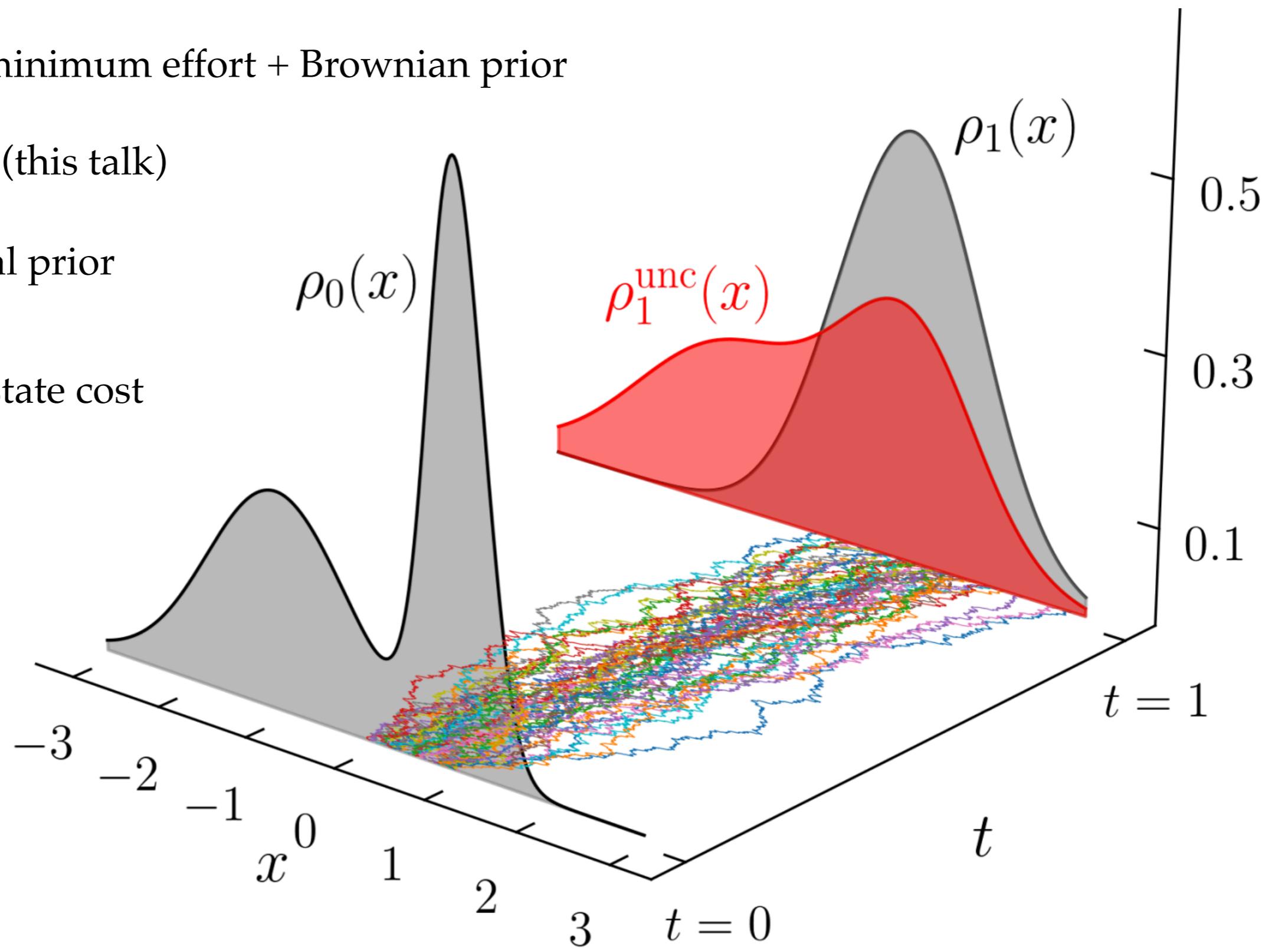
# This talk: Generalized SBP

Classical SBP = minimum effort + Brownian prior

Generalized SBP (this talk)

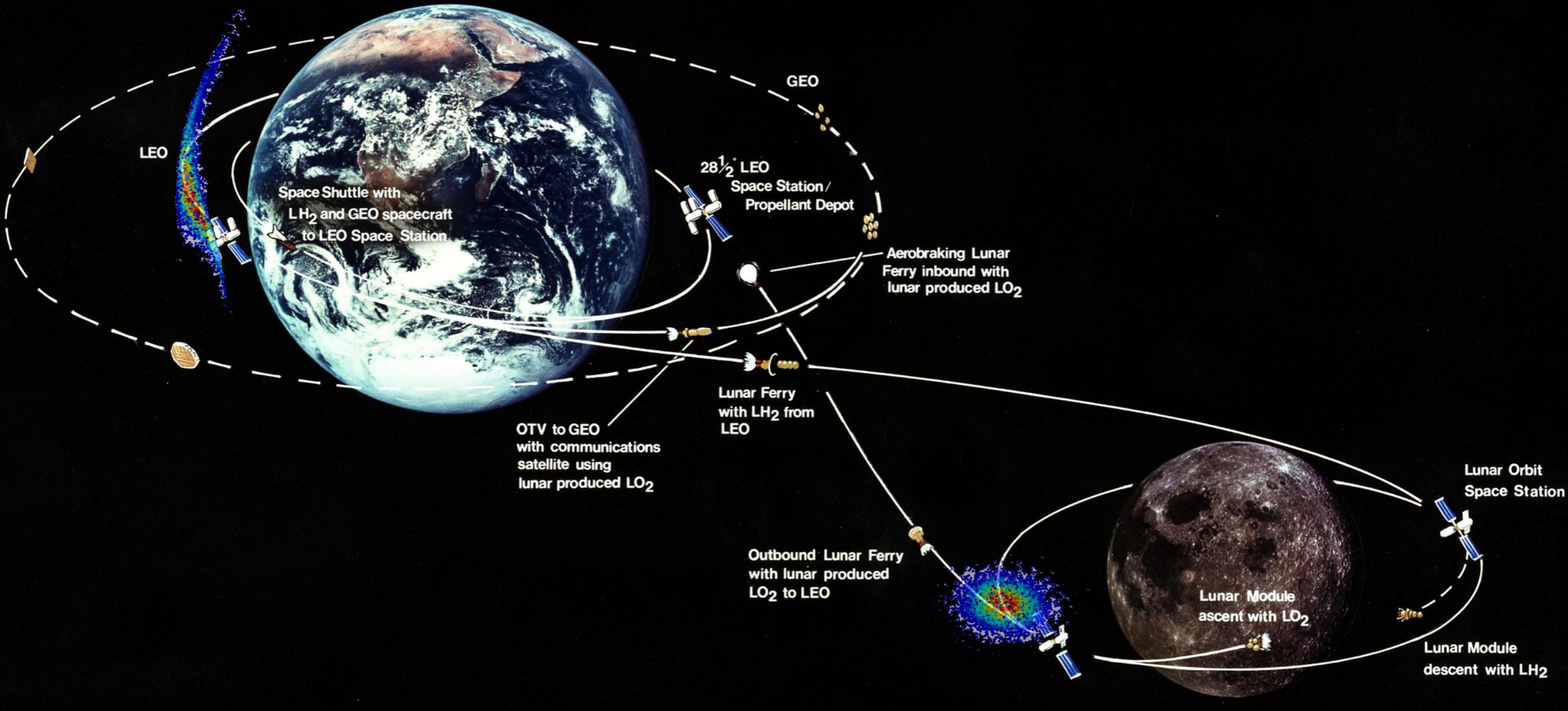
More general prior

Additional state cost



Most likely evolution between 2 distributional snapshots

# Motivating Application: Generalized SBP



Stochastic guidance and control of a spacecraft

# Background

# Optimal Mass Transport (OMT)

Static (Monge) formulation [1781]

$$\begin{aligned} & \arg \inf_{\substack{\text{measurable } \tau: \mathbb{R}^n \mapsto \mathbb{R}^n}} \mathbb{E}_{\rho_0} \frac{1}{2} |\mathbf{x}_0 - \tau(\mathbf{x}_0)|^2 \\ & \text{subject to} \quad \mathbf{x}_0 \sim \rho_0, \quad \tau(\mathbf{x}_0) \sim \rho_1 \end{aligned}$$

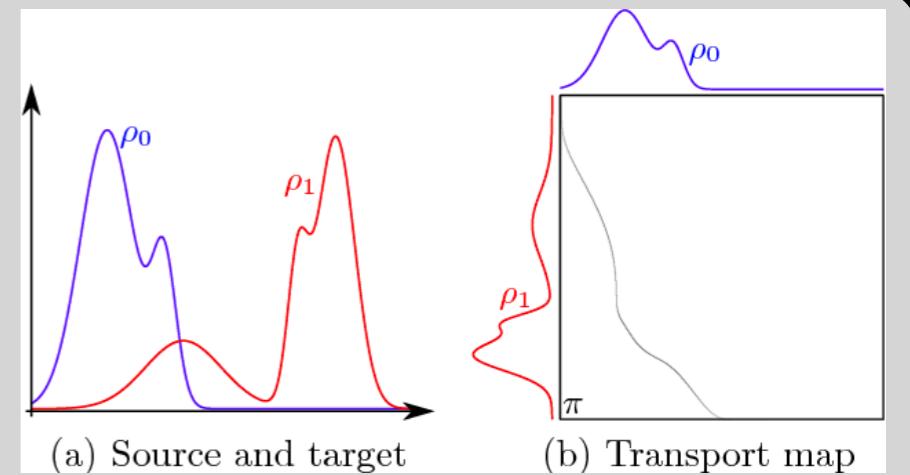


Image credit: Justin Solomon

# Optimal Mass Transport (OMT)

Static (Monge) formulation [1781]

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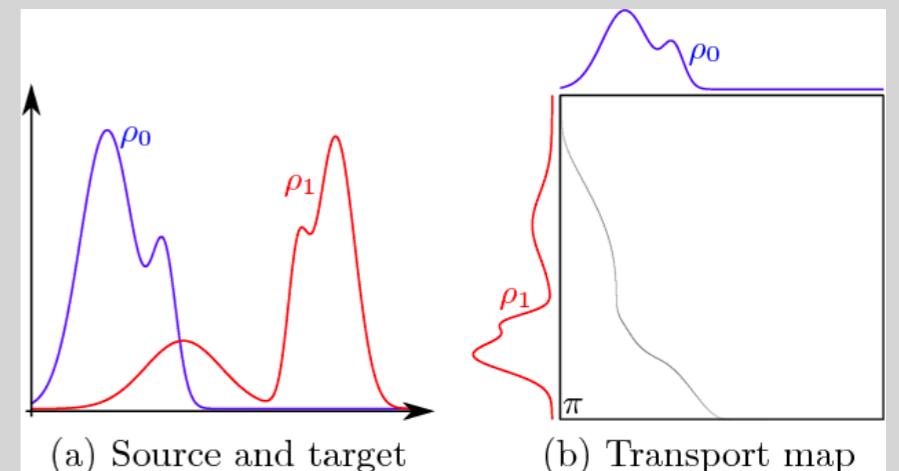


Image credit: Justin Solomon

Static (Kantorovich-Rubinstein) reformulation [1941]

$$\begin{aligned} \arg \inf_{\pi \in \Pi(\rho_0, \rho_1)} & \mathbb{E}_{\pi} \frac{1}{2} |\mathbf{x}_0 - \mathbf{x}_1|^2 \\ \text{subject to} & \quad \mathbf{x}_0 \sim \rho_0, \quad \mathbf{x}_1 \sim \rho_1 \end{aligned}$$

Infinite dimensional linear program

# Optimal Mass Transport (OMT)

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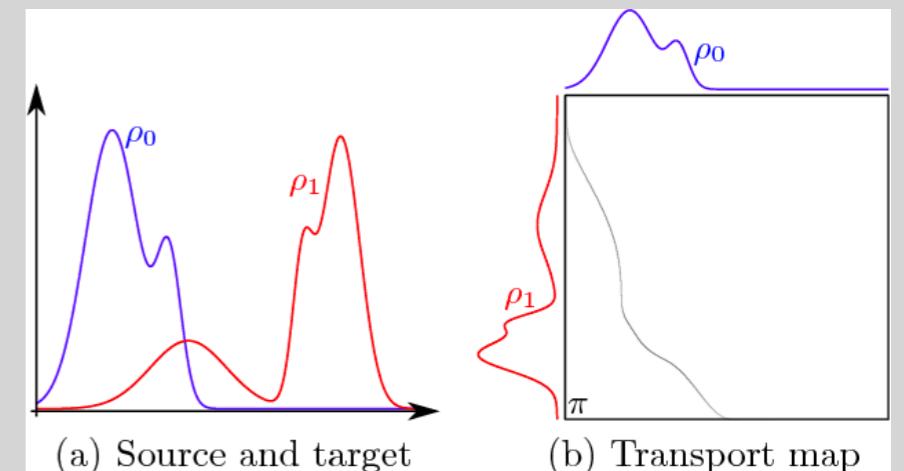


Image credit: Justin Solomon

Static (Kantorovich-Rubinstein) reformulation [1941]

$$\begin{aligned} & \arg \inf_{\pi \in \Pi(\rho_0, \rho_1)} \mathbb{E}_{\pi} \frac{1}{2} |\mathbf{x}_0 - \mathbf{x}_1|^2 \\ \text{subject to } & \quad \mathbf{x}_0 \sim \rho_0, \quad \mathbf{x}_1 \sim \rho_1 \end{aligned}$$

Infinite dimensional linear program

Dynamic (Benamou-Brenier) formulation [1999]

$$\arg \inf_{(\rho, \mathbf{v}) \in \mathcal{P}_{01} \times \mathcal{V}} \int_{t_0}^{t_1} \int_{\mathbb{R}^n} \frac{1}{2} |\mathbf{v}|^2 \rho(\mathbf{x}, t) d\mathbf{x} dt$$

$$\frac{\partial \rho}{\partial t} + \nabla_{\mathbf{x}} \cdot (\rho \mathbf{v}) = 0,$$

$$\rho(\mathbf{x}, t = t_0) = \rho_0, \quad \rho(\mathbf{x}, t = t_1) = \rho_1$$

Stochastic optimal control problem

# Classical SBP as Stochastic Optimal Control

$$\operatorname{arginf}_{(\rho, \mathbf{v}) \in \mathcal{P}_{01} \times \mathcal{V}} \int_{t_0}^{t_1} \int_{\mathbb{R}^n} \frac{1}{2} |\mathbf{v}|^2 \rho(\mathbf{x}, t) d\mathbf{x} dt$$

$$\frac{\partial \rho}{\partial t} + \nabla_{\mathbf{x}} \cdot (\rho \mathbf{v}) = \varepsilon \Delta_{\mathbf{x}} \rho, \quad \varepsilon > 0,$$

$$\rho(\mathbf{x}, t = t_0) = \rho_0, \quad \rho(\mathbf{x}, t = t_1) = \rho_1,$$

Fokker-Planck-Kolmogorov PDE

Controlled sample path dynamics

$$d\mathbf{x} = \mathbf{v}(\mathbf{x}, t) dt + \sqrt{2\varepsilon} d\mathbf{w}(t)$$

# Classical OMT vs. Classical SBP

## Classical OMT

$$\arg \inf_{(\rho, \mathbf{v}) \in \mathcal{P}_{01} \times \mathcal{V}} \int_{t_0}^{t_1} \int_{\mathbb{R}^n} \frac{1}{2} |\mathbf{v}|^2 \rho(\mathbf{x}, t) d\mathbf{x} dt$$
$$\frac{\partial \rho}{\partial t} + \nabla_{\mathbf{x}} \cdot (\rho \mathbf{v}) = 0, \quad \text{Liouville PDE}$$
$$\rho(\mathbf{x}, t = t_0) = \rho_0, \quad \rho(\mathbf{x}, t = t_1) = \rho_1$$

## Classical SBP

$$\operatorname{arginf}_{(\rho, \mathbf{v}) \in \mathcal{P}_{01} \times \mathcal{V}} \int_{t_0}^{t_1} \int_{\mathbb{R}^n} \frac{1}{2} |\mathbf{v}|^2 \rho(\mathbf{x}, t) d\mathbf{x} dt$$
$$\frac{\partial \rho}{\partial t} + \nabla_{\mathbf{x}} \cdot (\rho \mathbf{v}) = \varepsilon \Delta_{\mathbf{x}} \rho, \quad \varepsilon > 0, \quad \text{Fokker-Planck-Kolmogorov PDE}$$
$$\rho(\mathbf{x}, t = t_0) = \rho_0, \quad \rho(\mathbf{x}, t = t_1) = \rho_1,$$

# Generalized SBP

$$\arg \inf_{(\rho, \mathbf{v}) \in \mathcal{P}_{01} \times \mathcal{V}} \int_{t_0}^{t_1} \int_{\mathbb{R}^n} \left( \frac{1}{2} |\mathbf{v}|^2 + q(\mathbf{x}) \right) \rho(\mathbf{x}, t) d\mathbf{x} dt$$

$$\frac{\partial \rho}{\partial t} + \nabla_{\mathbf{x}} \cdot (\rho \mathbf{f}(\mathbf{x}, t, \mathbf{v})) = \varepsilon \langle \text{Hess}, \mathbf{g} \mathbf{g}^\top \rho \rangle$$
$$\sum_{i,j} \frac{\partial^2}{\partial x_i \partial x_j} \left( (\mathbf{g} \mathbf{g}^\top)_{ij} \rho \right)$$

$$\rho(\mathbf{x}, t = t_0) = \rho_0, \quad \rho(\mathbf{x}, t = t_1) = \rho_1$$



Controlled sample path dynamics

$$d\mathbf{x} = \mathbf{f}(\mathbf{x}, t, \mathbf{v}) dt + \sqrt{2\varepsilon} \mathbf{g}(\mathbf{x}, t, \mathbf{v}) dw(t)$$

# Linear SBP: Contraction Coefficient

# Related works

Y. Chen, T. Georgiou, and M. Pavon, “Entropic and displacement interpolation: a computational approach using the Hilbert metric,” *SIAM Journal on Applied Mathematics*, vol. 76, no. 6, pp. 2375–2396, 2016

M. Kuang and E. G. Tabak, “Preconditioning of optimal transport,” *SIAM Journal on Scientific Computing*, vol. 39, no. 4, pp. A1793–A1810, 2017

# Linear SBP

$$\arg \inf_{(\rho, \mathbf{v}) \in \mathcal{P}_{01} \times \mathcal{V}} \int_{t_0}^{t_1} \int_{\mathbb{R}^n} \frac{1}{2} |\mathbf{v}|^2 \rho(\mathbf{x}, t) d\mathbf{x} dt$$

$$\frac{\partial \rho}{\partial t} + \nabla_{\mathbf{x}} \cdot (\rho(\mathbf{A}(t)\mathbf{x} + \mathbf{B}(t)\mathbf{v})) = \varepsilon \langle \text{Hess}, \mathbf{B}(t)\mathbf{B}(t)^\top \rho \rangle$$

resp. compact supports  $\mathcal{X}_0, \mathcal{X}_1$

$$\rho(\mathbf{x}, t = t_0) = \rho_0, \quad \rho(\mathbf{x}, t = t_1) = \rho_1$$

## Controlled sample path dynamics

$$d\mathbf{x}(t) = (\mathbf{A}(t)\mathbf{x}(t) + \mathbf{B}(t)\mathbf{v}(\mathbf{x}, t))dt + \sqrt{2\varepsilon} \mathbf{B}(t)d\mathbf{w}(t)$$

State transition matrix  $\Phi_{t\tau} := \Phi(t, \tau) \quad \forall t_0 \leq \tau \leq t \leq t_1$

Assume controllability:  $\mathbf{M}_{10} := \int_{t_0}^{t_1} \Phi_{t_1\tau} \mathbf{B}(\tau) \mathbf{B}^\top(\tau) \Phi_{t_1\tau}^\top d\tau \succ 0$

Classical SBP is special case:  $\mathbf{A}(t) \equiv \mathbf{0}, \mathbf{B}(t) \equiv \mathbf{I}$

# Structure of the Solution for Linear SBP

Optimally controlled joint state PDF:  $\rho_\varepsilon^{\text{opt}}(\cdot, t) = \widehat{\varphi}_\varepsilon(\cdot, t)\varphi_\varepsilon(\cdot, t)$

Optimal control:  $\mathbf{v}_\varepsilon^{\text{opt}}(\cdot, t) = 2\varepsilon \nabla_{\mathbf{x}} \log \varphi_\varepsilon(\cdot, t)$

  
**Schrödinger factors**

Define:  $\widehat{\varphi}_{\varepsilon,0}(\cdot) := \widehat{\varphi}_\varepsilon(\cdot, t = t_0)$ ,  $\varphi_{\varepsilon,1}(\cdot) := \varphi_\varepsilon(\cdot, t = t_1)$

## Schrödinger system

$$\rho_0(\mathbf{x}) = \widehat{\varphi}_{\varepsilon,0}(\mathbf{x}) \int_{\mathbb{R}^n} k(t_0, \mathbf{x}, t_1, \mathbf{y}) \varphi_{\varepsilon,1}(\mathbf{y}) d\mathbf{y}$$

**Markov kernel**

$$\rho_1(\mathbf{x}) = \varphi_{\varepsilon,1}(\mathbf{x}) \int_{\mathbb{R}^n} k(t_0, \mathbf{y}, t_1, \mathbf{x}) \widehat{\varphi}_{\varepsilon,0}(\mathbf{y}) d\mathbf{y}$$

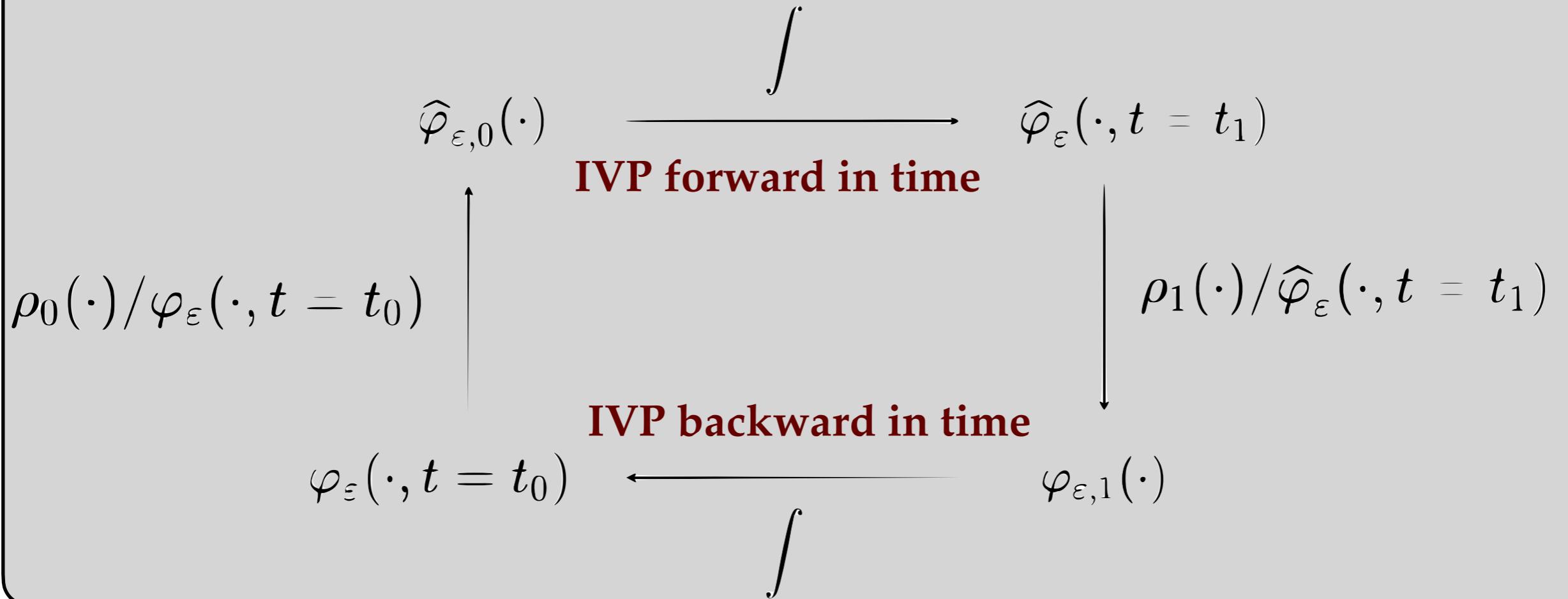
**Coupled nonlinear  
integral equations**

Here

$$k(t_0, \mathbf{x}_0, t_1, \mathbf{x}_1) := \frac{\exp\left(-\frac{(\Phi_{t_1 t_0} \mathbf{x}_0 - \mathbf{x}_1)^\top \mathbf{M}_{10}^{-1} (\Phi_{t_1 t_0} \mathbf{x}_0 - \mathbf{x}_1)}{4\varepsilon}\right)}{\sqrt{(4\pi\varepsilon)^n \det(\mathbf{M}_{10})}}$$

# Contractive Fixed Point Algorithm

Fixed point recursion over pair  $(\varphi_{\varepsilon,1}, \widehat{\varphi}_{\varepsilon,0})$



Guaranteed linear convergence with contraction rate  $\kappa \in (0, 1)$

But exact rate depends on problem data  $(\mathcal{X}_0, \mathcal{X}_1, \varepsilon, \mathbf{A}(t), \mathbf{B}(t))$

Worst case contraction coefficient  $\gamma := \sup_{\text{Linear SBPs with fixed } (\mathcal{X}_0, \mathcal{X}_1, \varepsilon, \mathbf{A}(t), \mathbf{B}(t))} \kappa$

# $\gamma$ in Classical SBP

Let

$$\alpha_B = \frac{\exp(-\tilde{\alpha}_B/(4\varepsilon))}{\sqrt{(4\pi\varepsilon)^n}}, \quad \beta_B = \frac{\exp(-\tilde{\beta}_B/(4\varepsilon))}{\sqrt{(4\pi\varepsilon)^n}}.$$

where

$$\tilde{\beta}_B := \min_{\mathbf{x}_0 \in \mathcal{X}_0, \mathbf{x}_1 \in \mathcal{X}_1} |\mathbf{x}_0 - \mathbf{x}_1|^2 \quad \text{and} \quad \tilde{\alpha}_B := \max_{\mathbf{x}_0 \in \mathcal{X}_0, \mathbf{x}_1 \in \mathcal{X}_1} |\mathbf{x}_0 - \mathbf{x}_1|^2$$

$$\gamma_B := \tanh^2 \left( \frac{1}{2} \log \left( \frac{\beta_B}{\alpha_B} \right) \right) \in (0, 1)$$

Chen, Georgiou, Pavon, SIAM J. Applied Math, 2016

# $\gamma$ in Linear SBP

Thm. (informal)

Let

$$\tilde{\alpha}_L := \max_{\mathbf{x}_0 \in \mathcal{X}_0, \mathbf{x}_1 \in \mathcal{X}_1} (\Phi_{t_1 t_0} \mathbf{x}_0 - \mathbf{x}_1)^\top M_{10}^{-1} (\Phi_{t_1 t_0} \mathbf{x}_0 - \mathbf{x}_1)$$

↑  
**State transition matrix**

↑  
**Controllability Gramian**

$$\tilde{\beta}_L := \min_{\mathbf{x}_0 \in \mathcal{X}_0, \mathbf{x}_1 \in \mathcal{X}_1} (\Phi_{t_1 t_0} \mathbf{x}_0 - \mathbf{x}_1)^\top M_{10}^{-1} (\Phi_{t_1 t_0} \mathbf{x}_0 - \mathbf{x}_1)$$

Then

$$\gamma_L = \tanh^2 \left( \frac{\tilde{\alpha}_L - \tilde{\beta}_L}{8\varepsilon} \right)$$

# $\gamma$ in Linear SBP

Thm. (informal)

Let

$$\tilde{\alpha}_L := \max_{\mathbf{x}_0 \in \mathcal{X}_0, \mathbf{x}_1 \in \mathcal{X}_1} (\Phi_{t_1 t_0} \mathbf{x}_0 - \mathbf{x}_1)^\top M_{10}^{-1} (\Phi_{t_1 t_0} \mathbf{x}_0 - \mathbf{x}_1)$$

$$\tilde{\beta}_L := \min_{\mathbf{x}_0 \in \mathcal{X}_0, \mathbf{x}_1 \in \mathcal{X}_1} (\Phi_{t_1 t_0} \mathbf{x}_0 - \mathbf{x}_1)^\top M_{10}^{-1} (\Phi_{t_1 t_0} \mathbf{x}_0 - \mathbf{x}_1)$$

Then

$$\gamma_L = \tanh^2 \left( \frac{\tilde{\alpha}_L - \tilde{\beta}_L}{8\varepsilon} \right)$$

Note:

$$\begin{aligned} \mathbf{A}(t) &\equiv \mathbf{0} \\ \mathbf{B}(t) &\equiv \mathbf{I} \end{aligned}$$

$$\begin{aligned} \Phi_{t_1 t_0} &= \mathbf{I} \\ M_{10} &= \frac{1}{t_1 - t_0} \mathbf{I} \end{aligned}$$

$$\begin{aligned} \tilde{\alpha}_B &:= \max_{\mathbf{x}_0 \in \mathcal{X}_0, \mathbf{x}_1 \in \mathcal{X}_1} \frac{1}{t_1 - t_0} |\mathbf{x}_0 - \mathbf{x}_1|^2 \\ \tilde{\beta}_B &:= \min_{\mathbf{x}_0 \in \mathcal{X}_0, \mathbf{x}_1 \in \mathcal{X}_1} \frac{1}{t_1 - t_0} |\mathbf{x}_0 - \mathbf{x}_1|^2 \end{aligned}$$

# Control-theoretic Interpretation for $\gamma_L$

$$\tilde{\alpha}_L := \max_{\mathbf{x}_0 \in \mathcal{X}_0, \mathbf{x}_1 \in \mathcal{X}_1} (\Phi_{t_1 t_0} \mathbf{x}_0 - \mathbf{x}_1)^\top \mathbf{M}_{10}^{-1} (\Phi_{t_1 t_0} \mathbf{x}_0 - \mathbf{x}_1)$$

$$\tilde{\beta}_L := \min_{\mathbf{x}_0 \in \mathcal{X}_0, \mathbf{x}_1 \in \mathcal{X}_1} (\Phi_{t_1 t_0} \mathbf{x}_0 - \mathbf{x}_1)^\top \mathbf{M}_{10}^{-1} (\Phi_{t_1 t_0} \mathbf{x}_0 - \mathbf{x}_1)$$


$$\underset{\mathbf{v}}{\text{minimum}} \int_{t_0}^{t_1} \frac{1}{2} |\mathbf{v}|^2 dt$$

$$\begin{aligned} \text{subject to } \quad & \dot{\mathbf{x}} = \mathbf{A}(t) \mathbf{x} + \mathbf{B}(t) \mathbf{v} \\ & \mathbf{x}(t = t_0) = \mathbf{x}_0, \mathbf{x}(t = t_1) = \mathbf{x}_1 \end{aligned}$$

Minimum cost for deterministic OCP

# Control-theoretic Interpretation for $\gamma_L$

$$\gamma_L = \tanh^2 \left( \frac{\tilde{\alpha}_L - \tilde{\beta}_L}{8\varepsilon} \right)$$

Range of optimal state transfer cost

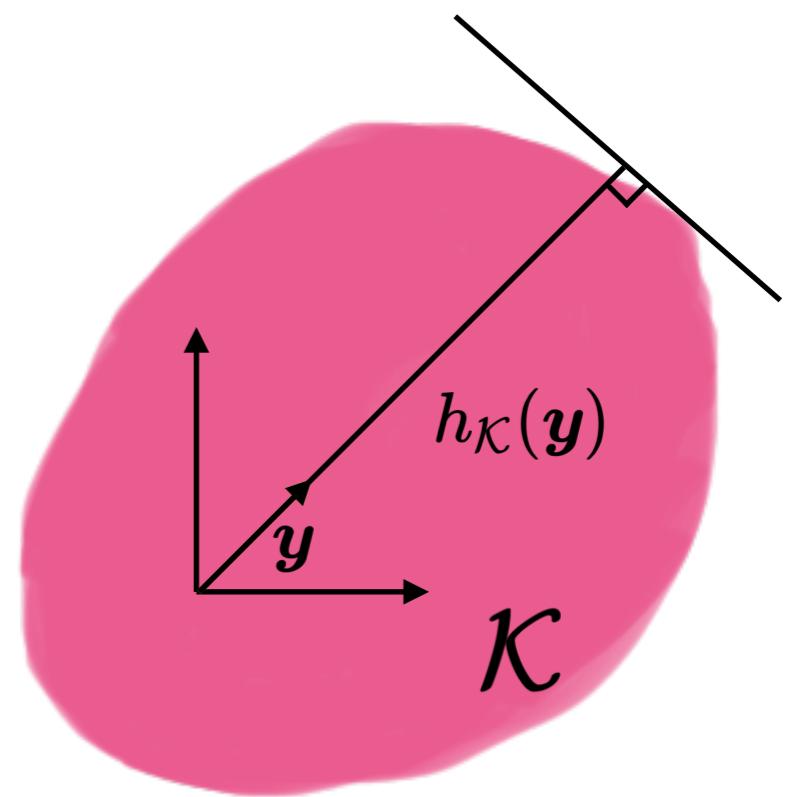
Process noise

Conforms with intuition:

$$\tilde{\alpha}_L - \tilde{\beta}_L \uparrow \quad \Rightarrow \quad \gamma_L \uparrow$$

$$\varepsilon \uparrow \quad \Rightarrow \quad \gamma_L \downarrow$$

# Support Functions



The support function  $h_{\mathcal{K}}(\cdot)$  for closed convex set  $\mathcal{K}$  is

$$h_{\mathcal{K}}(\mathbf{y}) := \sup_{\mathbf{x} \in \mathcal{K}} \langle \mathbf{y}, \mathbf{x} \rangle, \quad \mathbf{y} \in \mathbb{R}^n$$

e.g., distance from the origin to a supporting hyperplane of  $\mathcal{K}$  with normal in direction of  $\mathbf{y}$

# $\gamma$ in Linear SBP

$$\gamma_L = \tanh^2 \left( \frac{\tilde{\alpha}_L - \tilde{\beta}_L}{8\varepsilon} \right)$$

Thm. (informal)

With support functions of  $\mathcal{X}_0$  and  $\mathcal{X}_1$ , and Euclidean unit sphere  $\mathcal{S}^{n-1}$

$$\begin{aligned}\tilde{\alpha}_L &= \left\{ \max_{\mathbf{y} \in \mathcal{S}^{n-1}} (h_{\mathcal{X}_0}(\Phi_{t_1 t_0}^\top \mathbf{M}_{10}^{-1/2} \mathbf{y}) + h_{\mathcal{X}_1}(-\mathbf{M}_{10}^{-1/2} \mathbf{y})) \right\}^2 \\ \tilde{\beta}_L &= \left\{ \min_{\mathbf{y} \in \mathcal{S}^{n-1}} (h_{\mathcal{X}_0}(\Phi_{t_1 t_0}^\top \mathbf{M}_{10}^{-1/2} \mathbf{y}) + h_{\mathcal{X}_1}(-\mathbf{M}_{10}^{-1/2} \mathbf{y})) \right\}^2\end{aligned}$$

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Note:

$$\Phi_{t_1 t_0} = \mathbf{I}$$

$$\mathbf{M}_{10} = \frac{1}{t_1 - t_0} \mathbf{I}$$



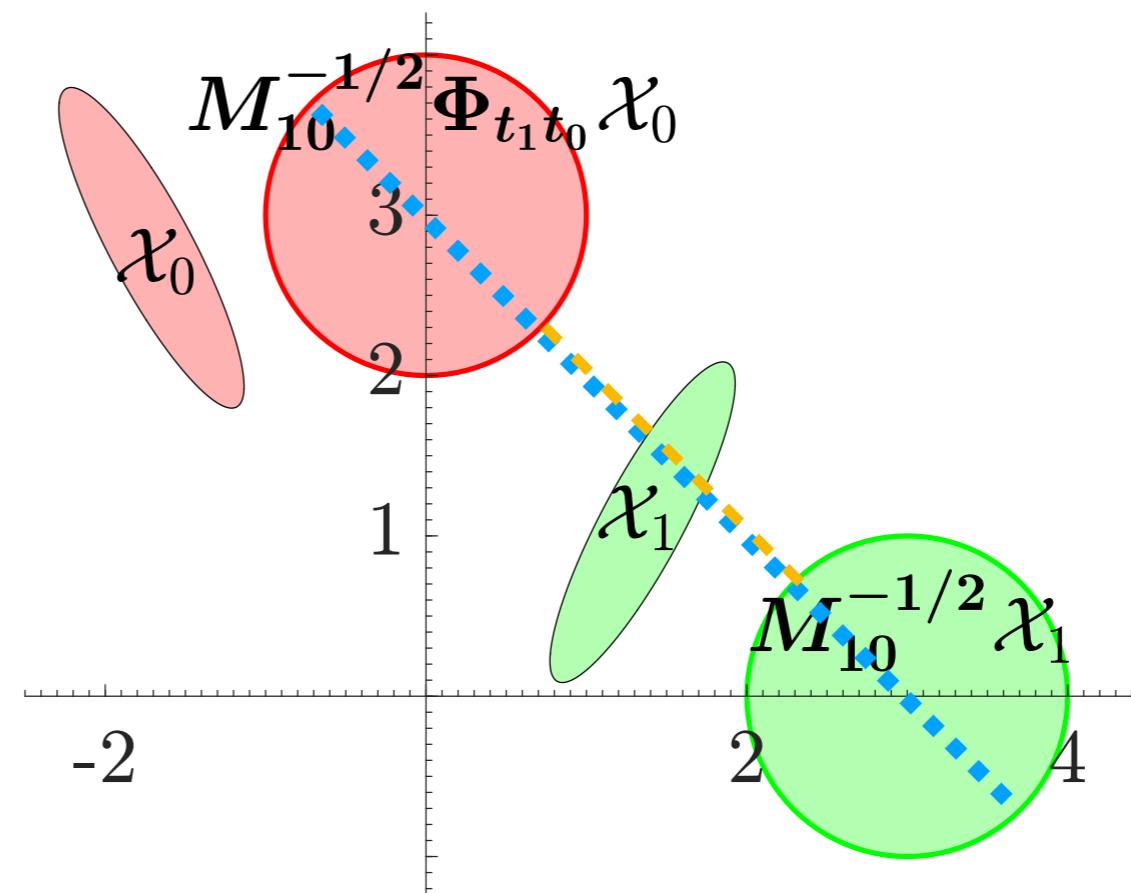
$$\begin{aligned}\tilde{\alpha}_B &= \frac{1}{t_1 - t_0} \left\{ \max_{\mathbf{y} \in \mathcal{S}^{n-1}} (h_{\mathcal{X}_0}(\mathbf{y}) + h_{\mathcal{X}_1}(-\mathbf{y})) \right\}^2 \\ \tilde{\beta}_B &= \frac{1}{t_1 - t_0} \left\{ \min_{\mathbf{y} \in \mathcal{S}^{n-1}} (h_{\mathcal{X}_0}(\mathbf{y}) + h_{\mathcal{X}_1}(-\mathbf{y})) \right\}^2\end{aligned}$$

# Geometric Interpretation for $\gamma_L$

$$\gamma_L = \tanh^2 \left( \frac{\tilde{\alpha}_L - \tilde{\beta}_L}{8\varepsilon} \right)$$

**Geometric interpretation:**

$\tilde{\alpha}_L$  and  $\tilde{\beta}_L$  can be considered the maximum and minimal separation of  $M_{10}^{-1/2} \Phi_{t_1 t_0} \mathcal{X}_0$  and  $M_{10}^{-1/2} \mathcal{X}_1$



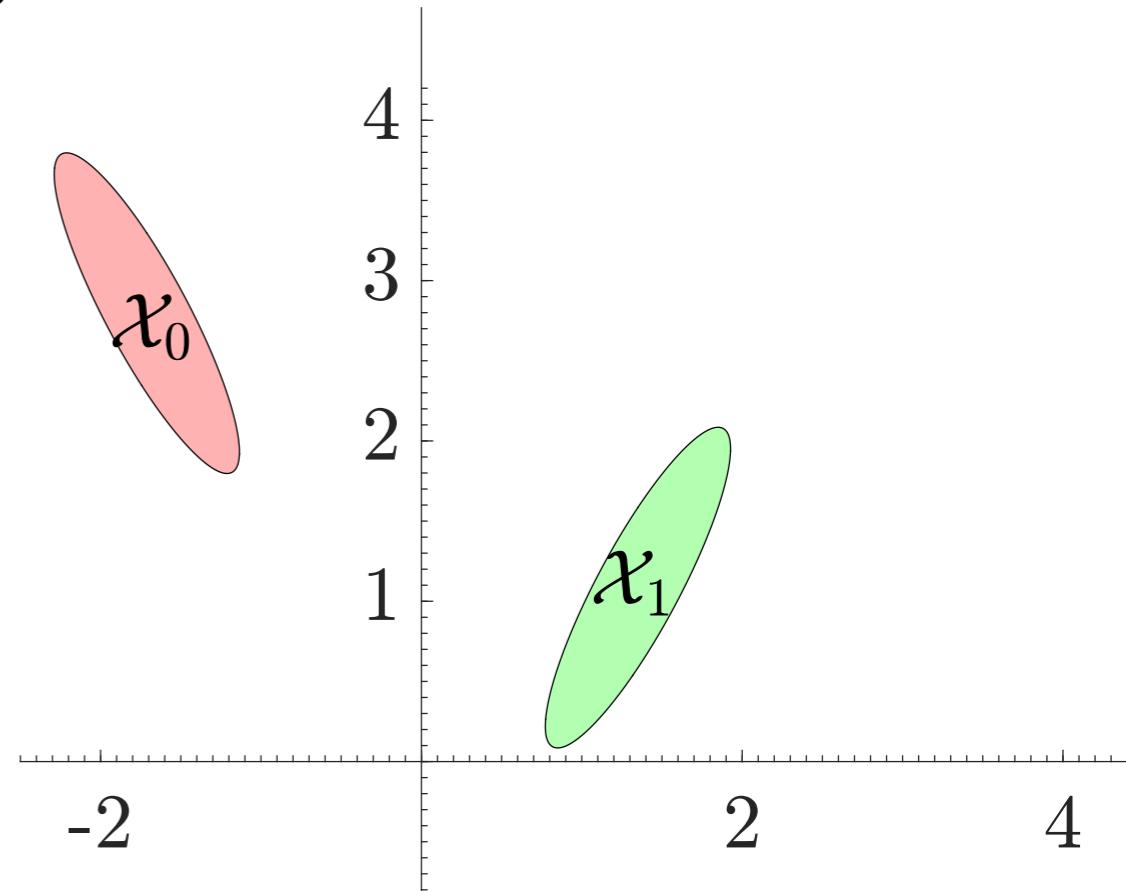
# Applications to Preconditioning:

Preconditioning to improve optimal transport algorithms  
~ Kuang and Tabak, *SIAM J. Scientific Computing*, 2017

Example: Linear SBP:  $\varepsilon = 0.5$

$$d\mathbf{x}(t) = \begin{bmatrix} 0 & 1 \\ 0 & 0 \end{bmatrix} \mathbf{x}(t) dt + \sqrt{2\varepsilon} \begin{bmatrix} 0 \\ 1 \end{bmatrix} d\mathbf{w}(t)$$

$$\Phi_{t_1 t_0} = \begin{bmatrix} 1 & 1 \\ 0 & 1 \end{bmatrix}, \quad M_{10}^{-1} = \begin{bmatrix} 12 & -6 \\ -6 & 4 \end{bmatrix}.$$



# Applications to Preconditioning:

Preconditioning to improve optimal transport algorithms  
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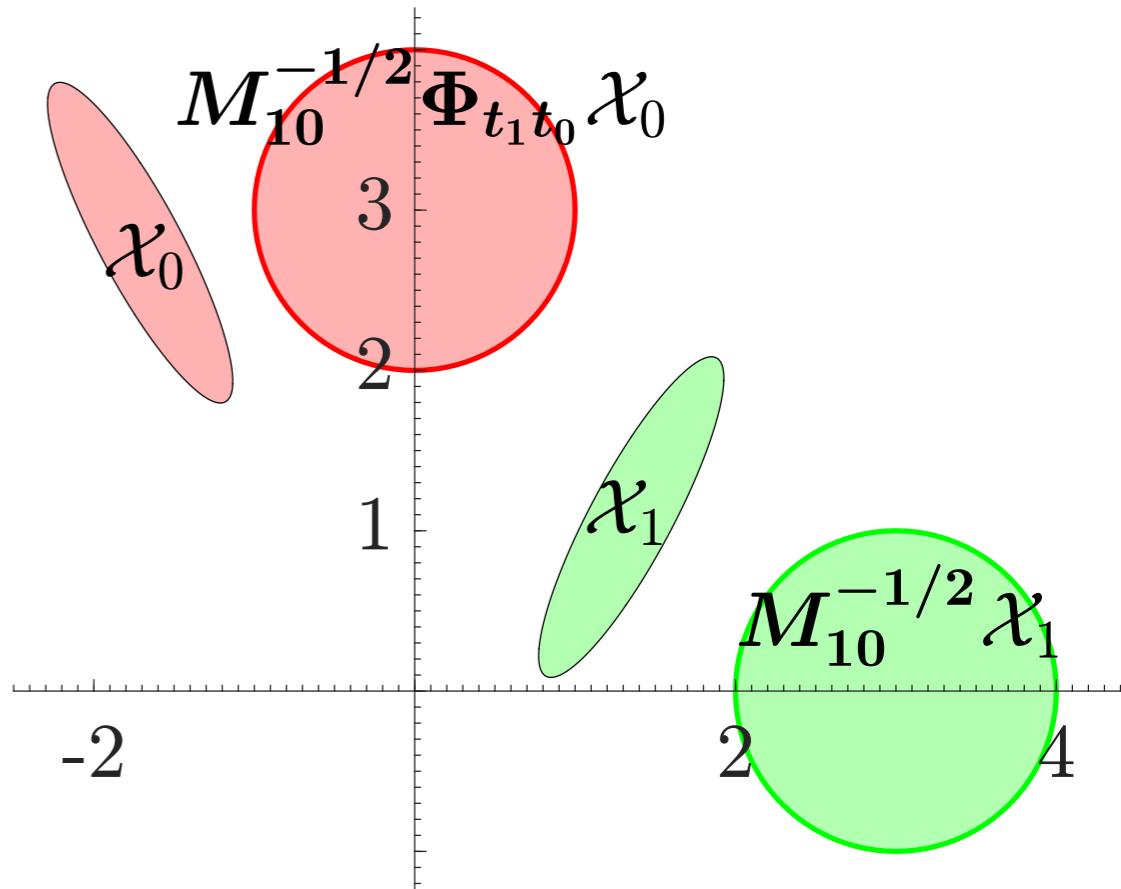
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$$\Phi_{t_1 t_0} = \begin{bmatrix} 1 & 1 \\ 0 & 1 \end{bmatrix}, \quad M_{10}^{-1} = \begin{bmatrix} 12 & -6 \\ -6 & 4 \end{bmatrix}.$$

No Preconditioning:

$$\begin{aligned} \tilde{\alpha}_L &= 2 + 2\sqrt{3} & \longrightarrow & \gamma_L = \tanh^2(1) \approx 0.580 \\ \tilde{\beta}_L &= -2 + 2\sqrt{3} \end{aligned}$$



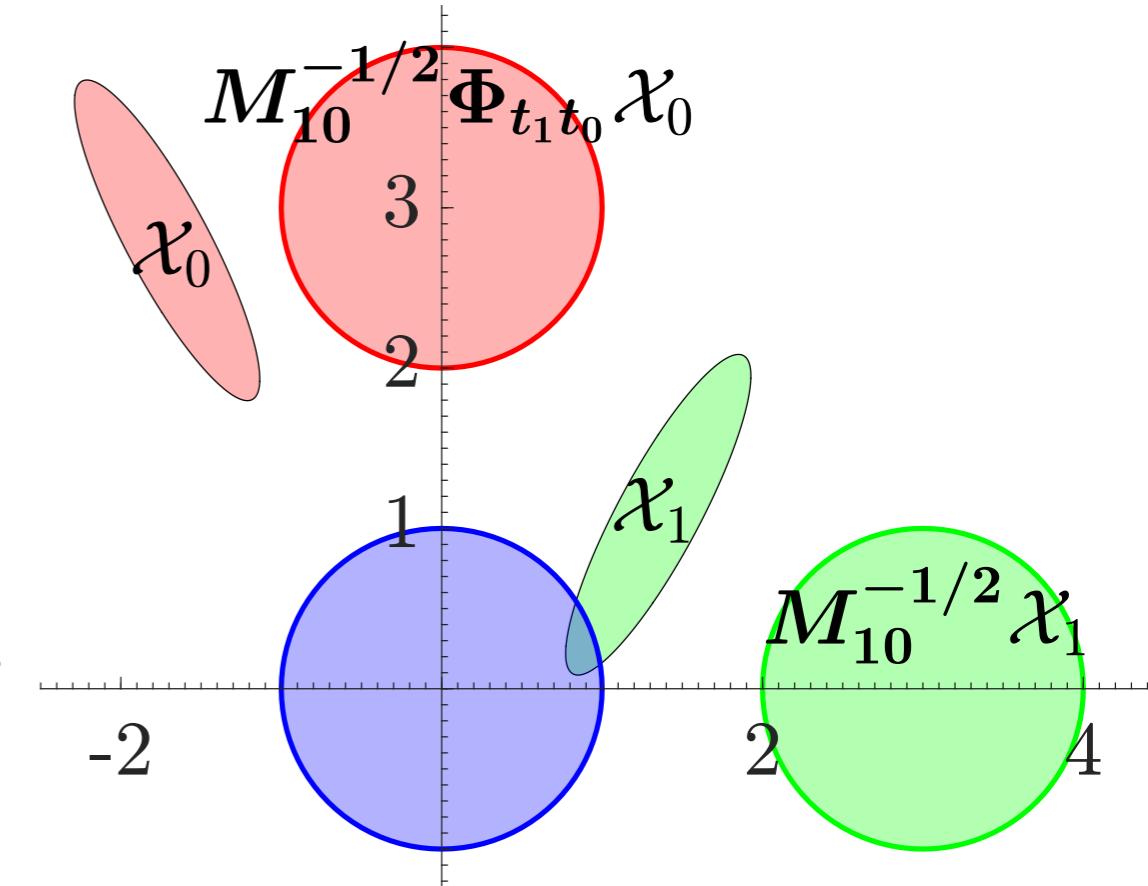
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$$\Phi_{t_1 t_0} = \begin{bmatrix} 1 & 1 \\ 0 & 1 \end{bmatrix}, \quad M_{10}^{-1} = \begin{bmatrix} 12 & -6 \\ -6 & 4 \end{bmatrix}.$$



With Preconditioning:

$$\tilde{\alpha}_L^{\text{precond}} = 2, \quad \tilde{\beta}_L^{\text{precond}} = 0 \quad \longrightarrow \quad \gamma_L^{\text{precond}} = \tanh^2(0.5) = 0.214$$

# **SBP with State Cost**

# Related works

Dawson, D., Gorostiza, L., and Wakolbinger, A., “Schrödinger processes and large deviations,” *Journal of mathematical physics*, Vol. 31, No. 10, 1990, pp. 2385–2388.  
<https://doi.org/10.1063/1.528840>

Aebi, R., and Nagasawa, M., “Large deviations and the propagation of chaos for Schrödinger processes,” *Probability Theory and Related Fields*, Vol. 94, No. 1, 1992, pp. 53–68. <https://doi.org/10.1007/BF01222509>

# SBP with State Cost

$$\arg \inf_{(\rho, \mathbf{v}) \in \mathcal{P}_{01} \times \mathcal{V}} \int_{t_0}^{t_1} \int_{\mathbb{R}^n} \left( \frac{1}{2} |\mathbf{v}|^2 + q(\mathbf{x}) \right) \rho(\mathbf{x}, t) d\mathbf{x} dt$$

$$\frac{\partial \rho}{\partial t} + \nabla_{\mathbf{x}} \cdot (\rho \mathbf{v}) = \varepsilon \Delta_{\mathbf{x}} \rho$$

$$\mathbf{x}(t = t_0) \sim \rho_0 \text{ (given)}, \quad \mathbf{x}(t = t_1) \sim \rho_1 \text{ (given)}$$

## Controlled sample path dynamics

$$d\mathbf{x} = \mathbf{v}(\mathbf{x}, t) dt + \sqrt{2\varepsilon} d\mathbf{w}(t)$$

# Solution for the SBP with State Cost

Thm. (informal)

SBP with state cost admits a unique solution

Proof idea:

Reformulate as Kullback-Leibler minimization over path space:

$$\arg \inf_{\mathbb{P} \in \Pi_{01}} D_{\text{KL}} \left( \mathbb{P} \parallel \frac{\exp \left( -\frac{1}{2\varepsilon} \int_{t_0}^{t_1} q(\mathbf{x}) dt \right) \mathbb{W}}{Z} \right)$$

large deviation principle

# Conditions for Optimality

Necessary conditions of optimality for the SBP with state cost

The pair  $(\rho_\varepsilon^{\text{opt}}, \mathbf{v}_\varepsilon^{\text{opt}})$  solves the coupled nonlinear PDEs

$$\frac{\partial \psi_\varepsilon}{\partial t} + \frac{1}{2} |\nabla_{\mathbf{x}} \psi_\varepsilon|^2 + \varepsilon \Delta_{\mathbf{x}} \psi_\varepsilon = q(\mathbf{x})$$

$$\frac{\partial \rho_\varepsilon^{\text{opt}}}{\partial t} + \nabla_{\mathbf{x}} \cdot (\rho_\varepsilon^{\text{opt}} \nabla_{\mathbf{x}} \psi_\varepsilon) = \varepsilon \Delta_{\mathbf{x}} \rho_\varepsilon^{\text{opt}}$$

with boundary conditions

$$\rho_\varepsilon^{\text{opt}}(\mathbf{x}, t = t_0) = \rho_0(\mathbf{x})$$

$$\rho_\varepsilon^{\text{opt}}(\mathbf{x}, t = t_1) = \rho_1(\mathbf{x})$$

# Structure of the solution for SBP with State Cost

Boundary-coupled system of linear PDEs for the Schrödinger factors

**Reaction-diffusion PDEs**

$$\frac{\partial \hat{\varphi}_\varepsilon}{\partial t} = \left( \varepsilon \Delta_{\mathbf{x}} - \frac{1}{2\varepsilon} q(\mathbf{x}) \right) \hat{\varphi}_\varepsilon \xleftarrow{\textcolor{red}{\mathcal{L}_{\text{forward}} \hat{\varphi}}} \hat{\varphi}$$

$$\frac{\partial \varphi_\varepsilon}{\partial t} = \left( -\varepsilon \Delta_{\mathbf{x}} + \frac{1}{2\varepsilon} q(\mathbf{x}) \right) \varphi_\varepsilon \xleftarrow{\textcolor{red}{\mathcal{L}_{\text{backward}} \varphi}} \varphi$$

$$\hat{\varphi}_\varepsilon(\cdot, t = t_0) \varphi_\varepsilon(\cdot, t = t_0) = \rho_0$$

$$\hat{\varphi}_\varepsilon(\cdot, t = t_1) \varphi_\varepsilon(\cdot, t = t_1) = \rho_1.$$

Optimally controlled joint state PDF

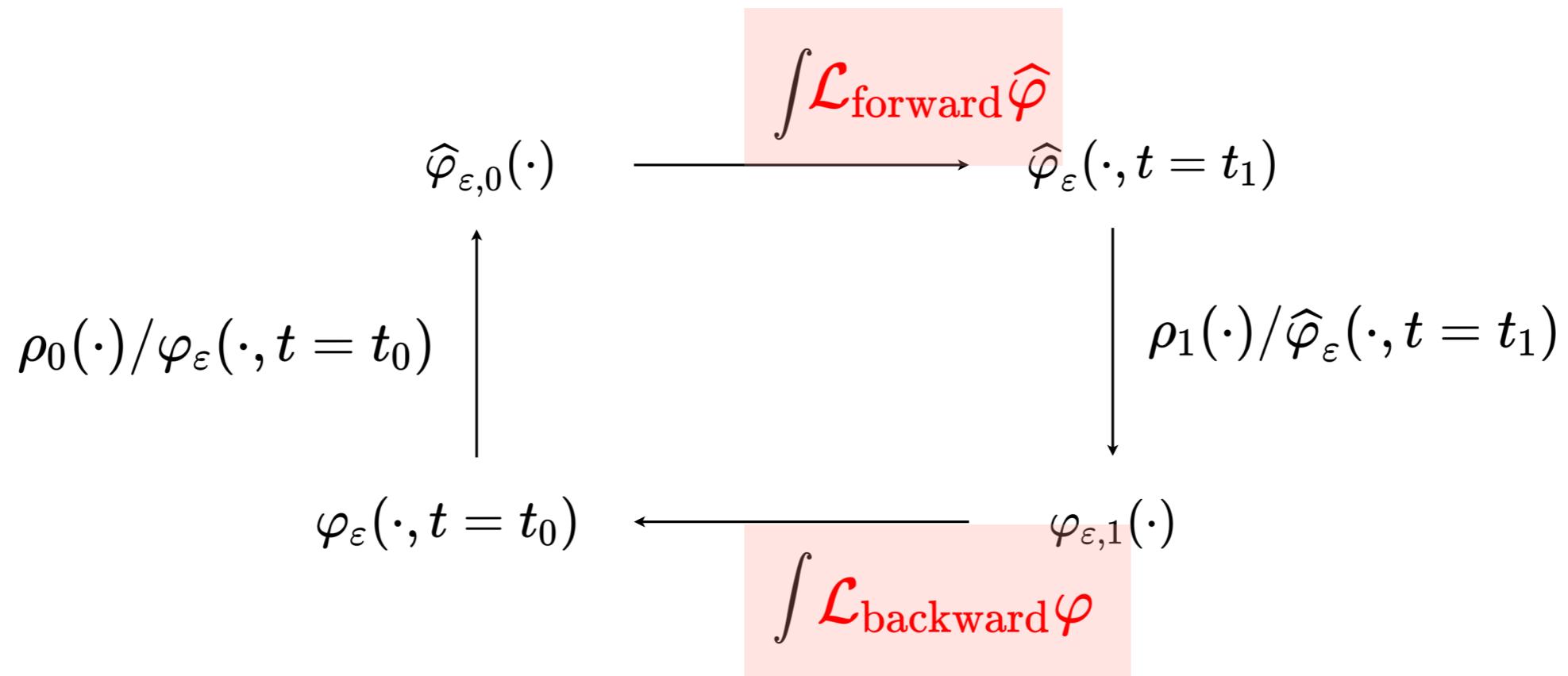
$$\rho_\varepsilon^{\text{opt}}(\cdot, t) = \hat{\varphi}_\varepsilon(\cdot, t) \varphi_\varepsilon(\cdot, t)$$

Optimal control

$$\mathbf{v}_\varepsilon^{\text{opt}}(\cdot, t) = 2\varepsilon \nabla_{\mathbf{x}} \log \varphi_\varepsilon(\cdot, t)$$

# Algorithm

Fixed point recursion over pair  $(\varphi_{\varepsilon,1}, \widehat{\varphi}_{\varepsilon,0})$



Schrödinger system:

$$\rho_0(\mathbf{x}) = \widehat{\varphi}_{\varepsilon,0}(\mathbf{x}) \int_{\mathbb{R}^n} k(t_0, \mathbf{x}, t_1, \mathbf{y}) \varphi_{\varepsilon,1}(\mathbf{y}) d\mathbf{y}$$

$$\rho_1(\mathbf{x}) = \varphi_{\varepsilon,1}(\mathbf{x}) \int_{\mathbb{R}^n} k(t_0, \mathbf{y}, t_1, \mathbf{x}) \widehat{\varphi}_{\varepsilon,0}(\mathbf{y}) d\mathbf{y}$$

# Fredholm Integral Equation of 2nd Kind

Thm. (informal)

Solution of linear reaction-diffusion PDE IVP with state-dependent reaction rate:

$$\frac{\partial u}{\partial t} = a\Delta_x u + q(\mathbf{x})u, \quad \mathbf{x} \in \mathbb{R}^n, \quad u(\mathbf{x}, t = t_0) = u_0(\mathbf{x}) \text{ given}$$

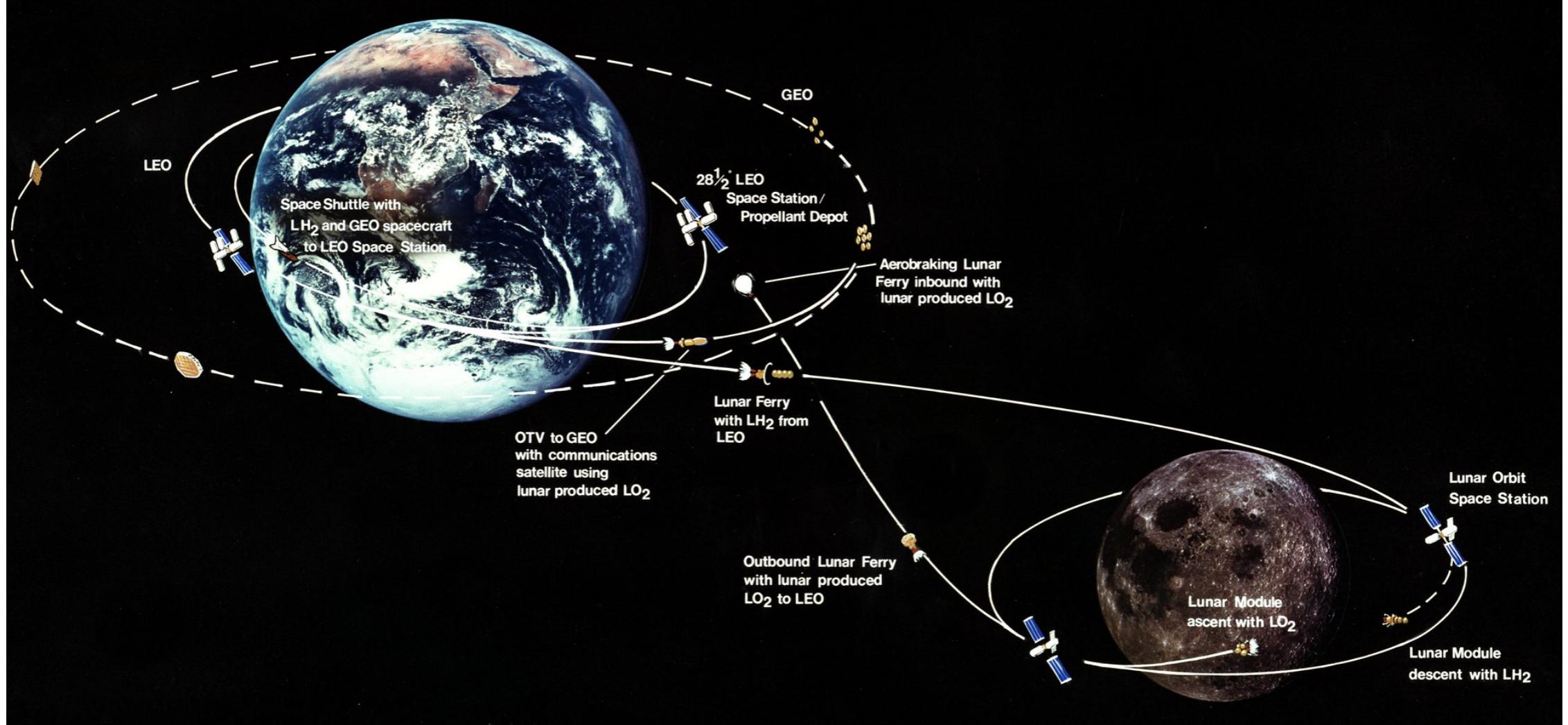
admits space-time Fredholm integral representation

$$u(\mathbf{x}, t) = \underbrace{\frac{1}{\sqrt{(4\pi at)^n}} \int_{\mathbb{R}^n} \exp\left(-\frac{|\mathbf{x} - \mathbf{y}|^2}{4at}\right) u_0(\mathbf{y}) d\mathbf{y}}_{\text{term 1}} \\ + \underbrace{\int_{t_0}^t \frac{1}{\sqrt{(4\pi a(t - \tau))^n}} \int_{\mathbb{R}^n} \exp\left(-\frac{|\mathbf{x} - \mathbf{y}|^2}{4a(t - \tau)}\right) q(\mathbf{y}) u(\mathbf{y}, \tau) d\mathbf{y} d\tau}_{\text{term 2}}$$

# Case Study

# Probabilistic Lambert's Problem

# Lambert's Problem

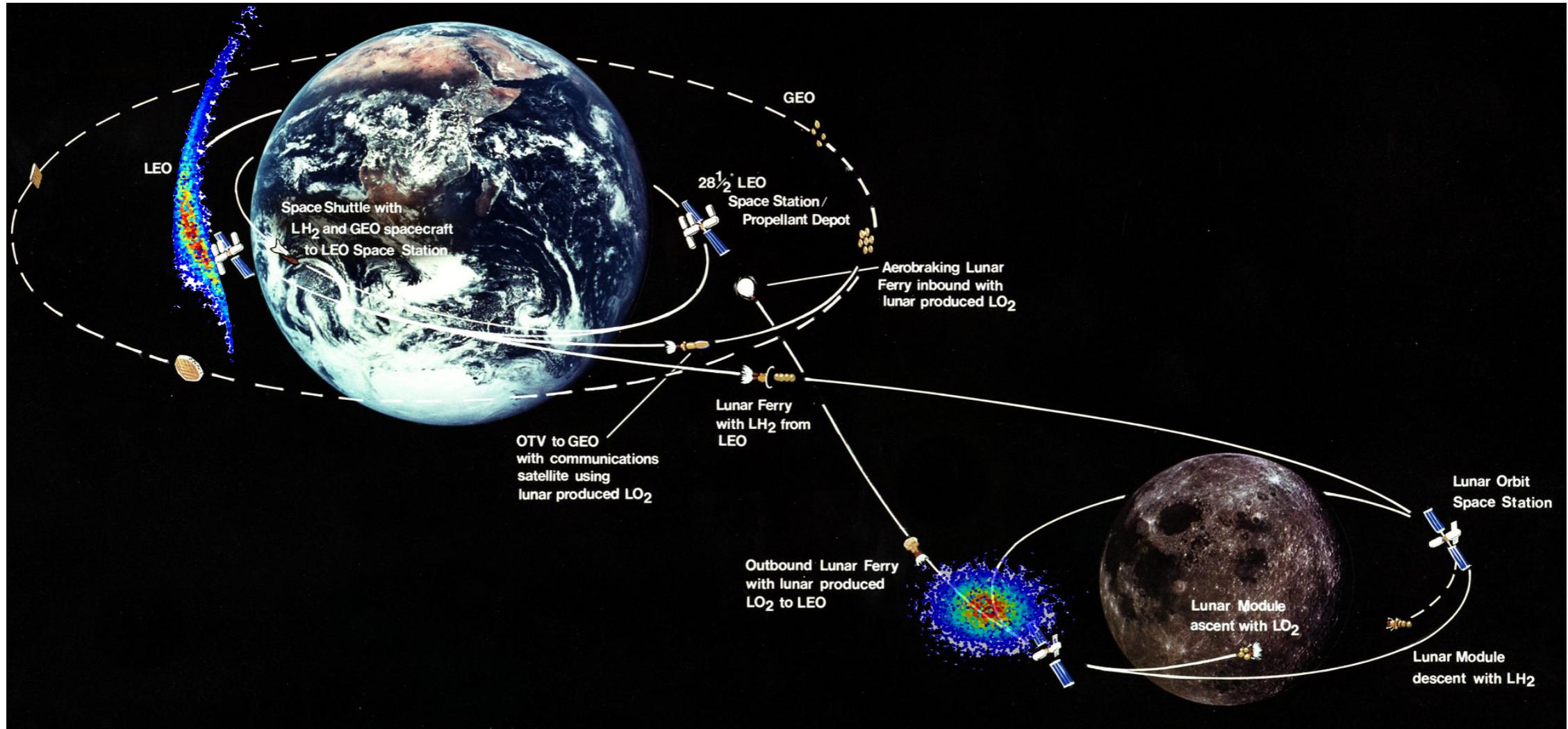


3D position coordinate  $\mathbf{x} := \begin{pmatrix} x \\ y \\ z \end{pmatrix} \in \mathbb{R}^3$

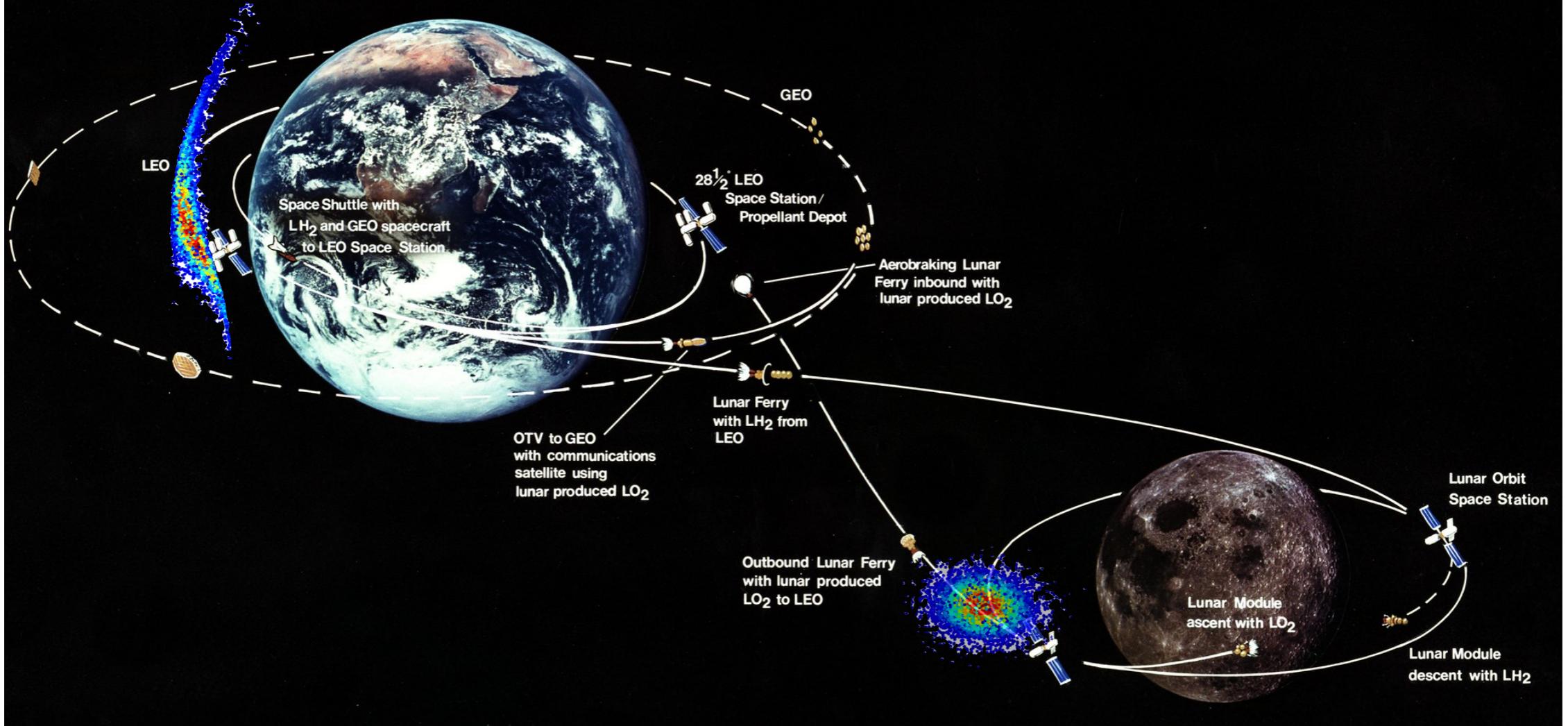
Find velocity control policy  $\dot{\mathbf{x}} := \mathbf{v}(\mathbf{r}, t)$  such that

$$\ddot{\mathbf{x}} = -\nabla_{\mathbf{x}} V(\mathbf{x}), \quad \mathbf{x}(t = t_0) = \mathbf{x}_0 \text{ (given)}, \quad \mathbf{x}(t = t_1) = \mathbf{x}_1 \text{ (given)}$$

# Probabilistic Lambert's Problem



# Probabilistic Lambert's Problem



3D position coordinate  $\mathbf{x} := \begin{pmatrix} x \\ y \\ z \end{pmatrix} \in \mathbb{R}^3$

Find velocity control policy  $\dot{\mathbf{x}} := \mathbf{v}(\mathbf{r}, t)$  such that

$$\ddot{\mathbf{x}} = -\nabla_{\mathbf{x}} V(\mathbf{x}), \quad \mathbf{x}(t = t_0) \sim \rho_0 \text{ (given)}, \quad \mathbf{x}(t = t_1) \sim \rho_1 \text{ (given)}$$

# Connection with OMT

Lambert Problem  $\Leftrightarrow$  Deterministic OCP

Reformulate Lambert's problem as deterministic OCP

[Bando and Yamakawa, JGCD, 2010]

$$\ddot{\mathbf{x}} = -\nabla_{\mathbf{x}} V(\mathbf{x}), \quad \mathbf{x}(t = t_0) = \mathbf{x}_0 \text{ (given)}, \quad \mathbf{x}(t = t_1) = \mathbf{x}_1 \text{ (given)}$$



$$\arg \inf_{\mathbf{v}} \int_{t_0}^{t_1} \left( \frac{1}{2} |\mathbf{v}|^2 - V(\mathbf{x}) \right) dt$$

$$\dot{\mathbf{x}} = \mathbf{v}$$

Potential as state cost

$$\mathbf{x}(t = t_0) = \mathbf{x}_0 \text{ (given)}, \quad \mathbf{x}(t = t_1) = \mathbf{x}_1 \text{ (given)}$$

# Lambertian OMT (L-OMT)

Probabilistic Lambert's Problem  $\Leftrightarrow$  Generalized OMT

$$\ddot{\mathbf{x}} = -\nabla_{\mathbf{x}} V(\mathbf{x}), \quad \mathbf{x}(t = t_0) \sim \rho_0 \text{ (given)}, \quad \mathbf{x}(t = t_1) \sim \rho_1 \text{ (given)}$$

$\Updownarrow$

$$\arg \inf_{(\rho, \mathbf{v}) \in \mathcal{P}_{01} \times \mathcal{V}} \int_{t_0}^{t_1} \int_{\mathbb{R}^n} \left( \frac{1}{2} |\mathbf{v}|^2 - V(\mathbf{x}) \right) \rho(\mathbf{x}, t) d\mathbf{x} dt$$

$V = 0$  is OMT

$$\dot{\mathbf{x}} = \mathbf{v}$$

$$\mathbf{x}(t = t_0) = \mathbf{x}_0 \text{ (given)}, \quad \mathbf{x}(t = t_1) = \mathbf{x}_1 \text{ (given)}$$

# Existence and Uniqueness of Solution for L-OMT

Thm. (informal)

L-OMT with negative potential admits a unique solution

Proof Idea:

Consider Lagrangian for L-OMT problem

Show that the Lagrangian is strictly convex and superlinear in  $\mathbf{v}$

Use Figalli's theory for Tonelli Lagrangians induced by action integrals

# Connection to SBP with state cost

$$\arg \inf_{(\rho, \mathbf{v}) \in \mathcal{P}_{01} \times \mathcal{V}} \int_{t_0}^{t_1} \int_{\mathbb{R}^n} \left( \frac{1}{2} |\mathbf{v}|^2 - V(\mathbf{x}) \right) \rho(\mathbf{x}, t) d\mathbf{x} dt$$

$$\frac{\partial \rho}{\partial t} + \nabla_{\mathbf{r}} \cdot (\rho \mathbf{v}) = 0,$$

$$\rho(t = t_0, \cdot) = \rho_0, \quad \rho(t = t_1, \cdot) = \rho_1$$

↳ Lambertian SBP (L-SBP)

$$\arg \inf_{(\rho, \mathbf{v}) \in \mathcal{P}_{01} \times \mathcal{V}} \int_{t_0}^{t_1} \int_{\mathbb{R}^n} \left( \frac{1}{2} |\mathbf{v}|^2 - V(\mathbf{x}) \right) \rho(\mathbf{x}, t) d\mathbf{x} dt$$

Regularization > 0

$$\frac{\partial \rho}{\partial t} + \nabla_{\mathbf{r}} \cdot (\rho \mathbf{v}) = \varepsilon \Delta_{\mathbf{r}} \rho,$$

$$\rho(t = t_0, \cdot) = \rho_0, \quad \rho(t = t_1, \cdot) = \rho_1$$

# L-SBP Solution

Thm. (informal) Existence and uniqueness of L-SBP is guaranteed

$$V(\mathbf{x}) = -\frac{\mu}{|\mathbf{x}|} \left( 1 + \frac{J_2 R_{\text{Earth}}^2}{2|\mathbf{x}|^2} \left( 1 - \frac{3z^2}{|\mathbf{x}|^2} \right) \right) \longrightarrow \begin{array}{l} \text{Bounded and} \\ \text{negative for} \\ |\mathbf{x}|^2 \geq R_{\text{Earth}}^2 \end{array}$$

Thm. (Necessary conditions of optimality for L-SBP)

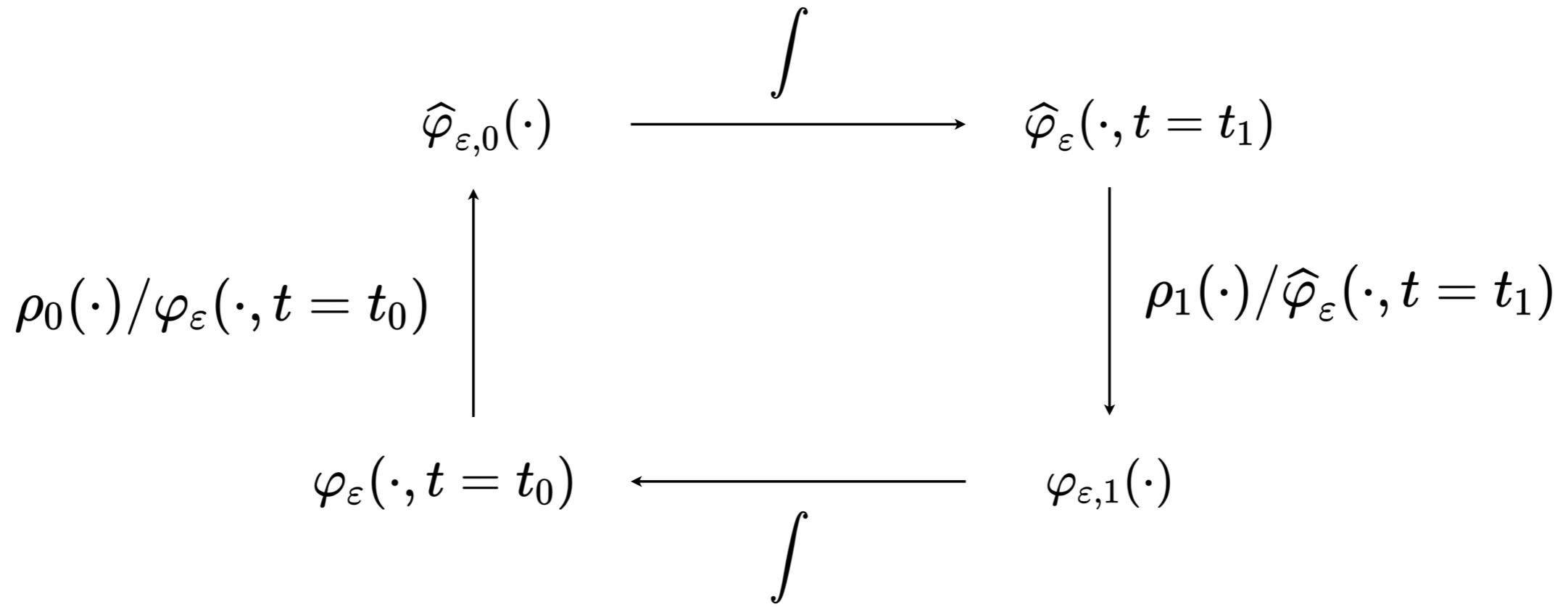
$$\frac{\partial \psi_\varepsilon}{\partial t} + \frac{1}{2} |\nabla_{\mathbf{x}} \psi_\varepsilon|^2 + \varepsilon \Delta_{\mathbf{x}} \psi_\varepsilon = -V(\mathbf{x})$$

$$\frac{\partial \rho_\varepsilon^{\text{opt}}}{\partial t} + \nabla_{\mathbf{x}} \cdot (\rho_\varepsilon^{\text{opt}} \nabla_{\mathbf{x}} \psi_\varepsilon) = \varepsilon \Delta_{\mathbf{x}} \rho_\varepsilon^{\text{opt}}$$

$$\rho_\varepsilon^{\text{opt}}(t = t_0, \cdot) = \rho_0, \quad \rho_\varepsilon^{\text{opt}}(t = t_1, \cdot) = \rho_1$$

# L-SBP Computation via Schrödinger Factors

Recursion over pair  $(\varphi_1, \hat{\varphi}_0)$



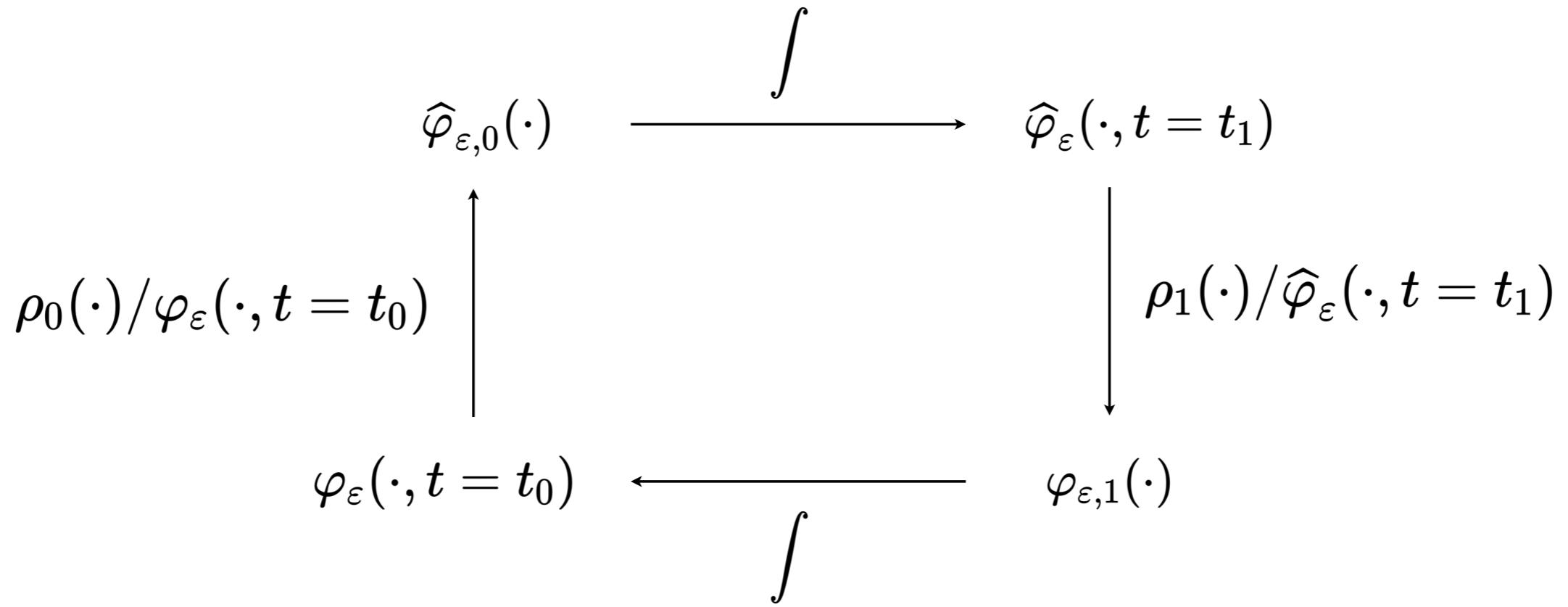
$$\frac{\partial \widehat{\varphi}_{\varepsilon}}{\partial t} = \left( \varepsilon \Delta_{\mathbf{x}} + \frac{1}{2\varepsilon} V(\mathbf{x}) \right) \widehat{\varphi}_{\varepsilon}$$

$$\frac{\partial \varphi_{\varepsilon}}{\partial t} = - \left( \varepsilon \Delta_{\mathbf{x}} + \frac{1}{2\varepsilon} V(\mathbf{x}) \right) \varphi_{\varepsilon}$$

$$\rho_{\varepsilon}^{\text{opt}}(t = t_0, \cdot) = \rho_0, \quad \rho_{\varepsilon}^{\text{opt}}(t = t_1, \cdot) = \rho_1$$

# L-SBP Computation via Schrödinger Factors

Recursion over pair  $(\varphi_1, \hat{\varphi}_0)$



**Thm. (Fredholm Integral Representation)**

$$\begin{aligned}
 \widehat{\varphi}_{\varepsilon}(\mathbf{x}, t) &= \frac{1}{\sqrt{(4\pi\varepsilon t)^3}} \int_{\mathbb{R}^3} \exp\left(-\frac{|\mathbf{x} - \tilde{\mathbf{x}}|^2}{4\varepsilon t}\right) \widehat{\varphi}_{\varepsilon,0}(\tilde{\mathbf{x}}) d\tilde{\mathbf{x}} \\
 &\quad - \int_{t_0}^t \frac{1}{2\varepsilon \sqrt{(4\pi\varepsilon(t-\tau))^3}} \int_{\mathbb{R}^3} \exp\left(-\frac{|\mathbf{x} - \tilde{\mathbf{x}}|^2}{4\varepsilon(t-\tau)}\right) V(\tilde{\mathbf{x}}) \widehat{\varphi}_{\varepsilon}(\tilde{\mathbf{x}}, \tau) d\tilde{\mathbf{x}} d\tau
 \end{aligned}$$

# Numerical Case Study

Prescribed time horizon  $[t_0, t_1] \equiv [0, 1]$  hours

Endpoint joint PDFs

$$\boldsymbol{x}_0 \sim \mathcal{N}(\mu_0, \Sigma_0)$$

$$\boldsymbol{x}_1 \sim \mathcal{N}(\mu_1, \Sigma_1)$$

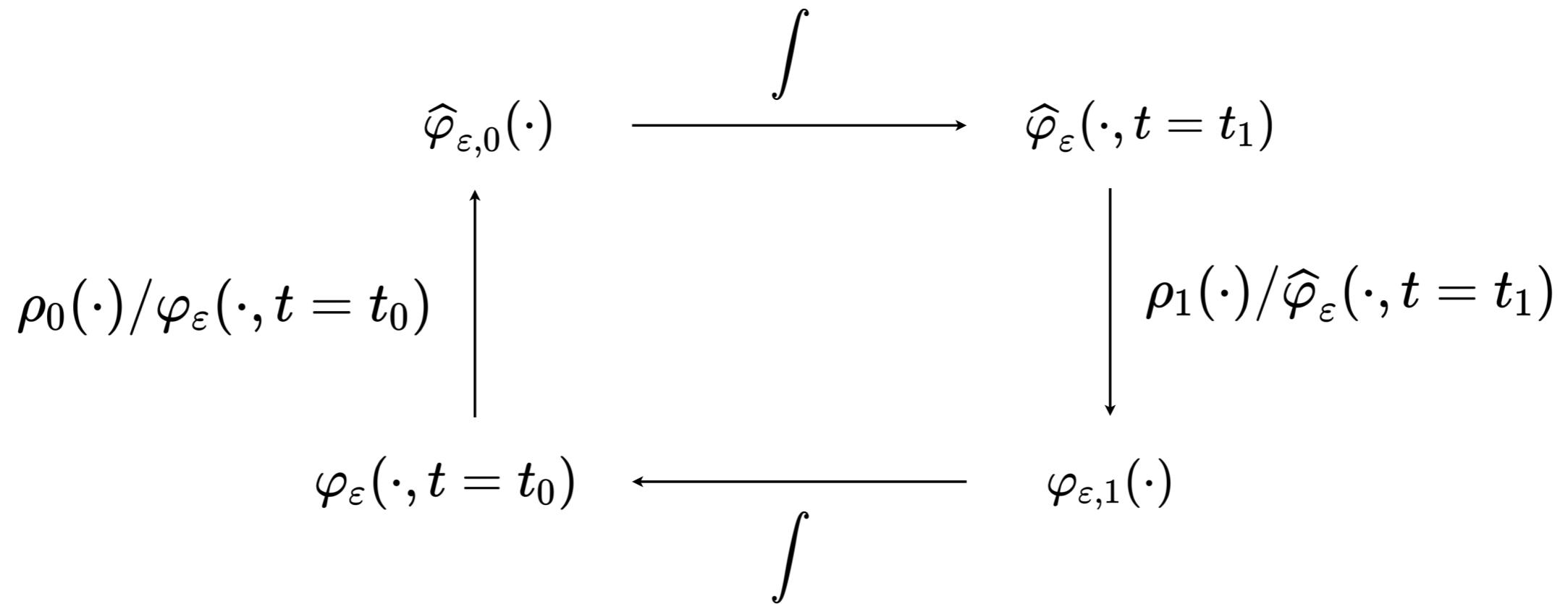
where

$$\mu_0 = \begin{pmatrix} 5000 \\ 10000 \\ 2100 \end{pmatrix}, \quad \mu_1 = \begin{pmatrix} -14600 \\ 2500 \\ 7000 \end{pmatrix}$$

$$\Sigma_0 = \frac{1}{100} \text{diag}(\mu_0^2), \quad \Sigma_1 = \frac{1}{100} \text{diag}(\mu_1^2),$$

# Solution: Computation

IDEA: Fixed point recursion over pair  $(\varphi_1, \hat{\varphi}_0)$



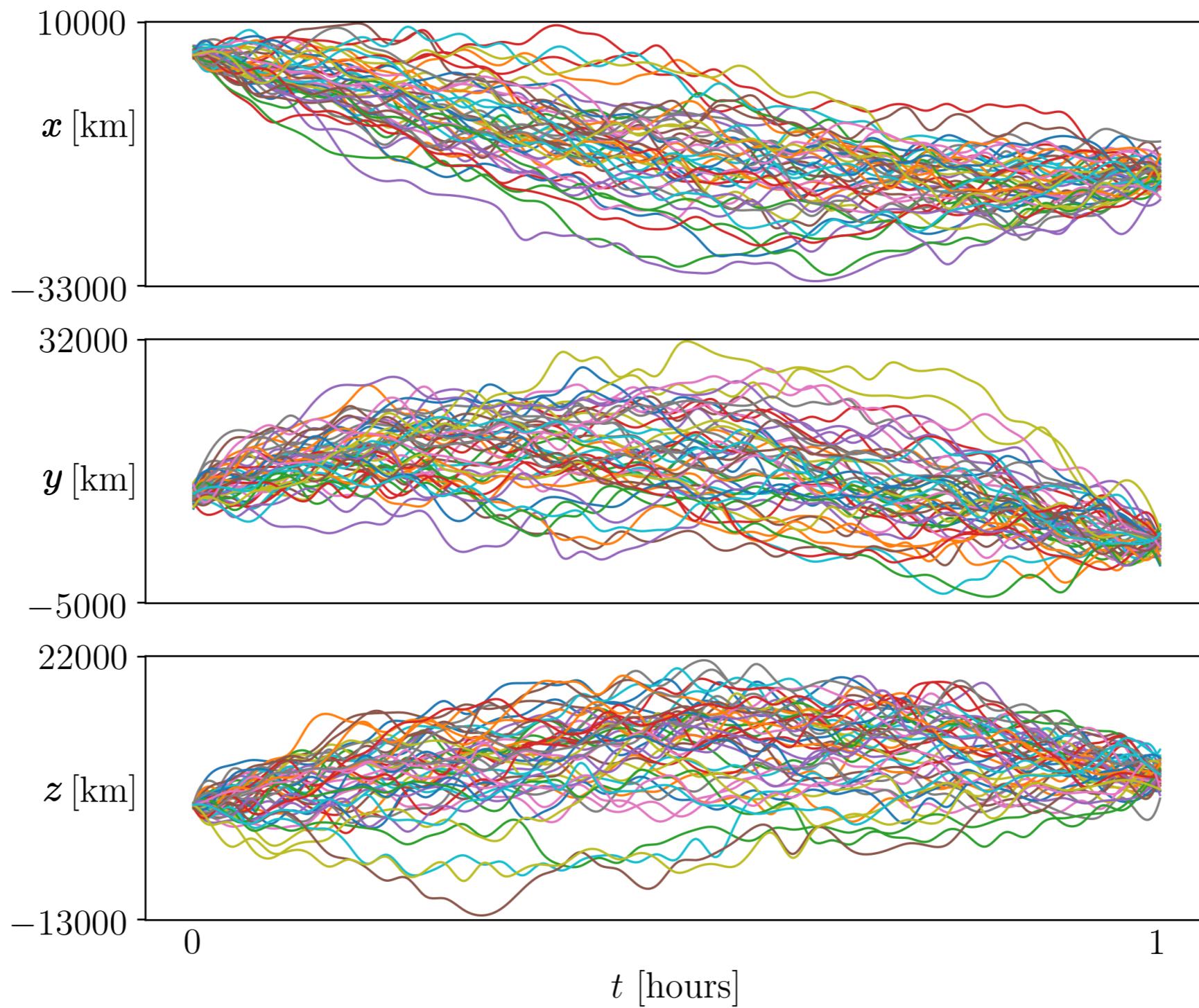
Idea:  
Left Riemann  
Approximation  
of Second Term

$$\begin{aligned} & \int_{t_0}^{t_1} \int_{\mathbb{R}^n} f(\tilde{\boldsymbol{x}}, \boldsymbol{x}, \tau, t) d\tilde{\boldsymbol{x}} d\tau \\ & \approx \sum_{q=0}^{k-1} \sum_{m=0}^{N_x} \sum_{n=0}^{N_y} \sum_{j=0}^{N_z} f(\tilde{\boldsymbol{x}}_{(m,n,j)}, \boldsymbol{x}, t_0 + k\Delta t, t) \Delta z \Delta y \Delta x \Delta t \end{aligned}$$

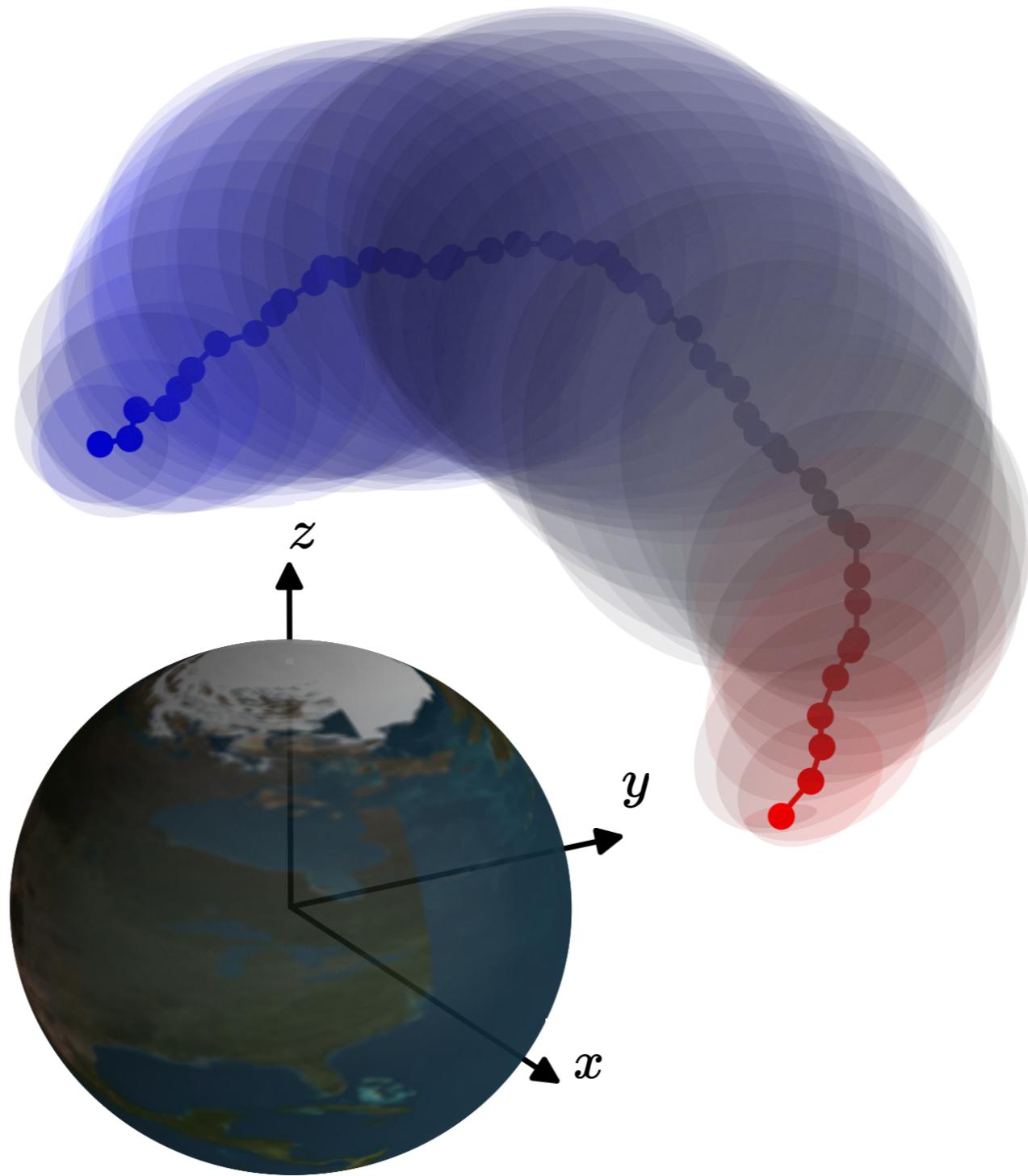
where  $\tilde{\boldsymbol{x}}_{(m,n,j)} = (x_0 + \Delta x, y_0 + \Delta y, z_0 + \Delta z)$

# Numerical Case Study (cont.)

Optimally controlled closed loop state sample paths

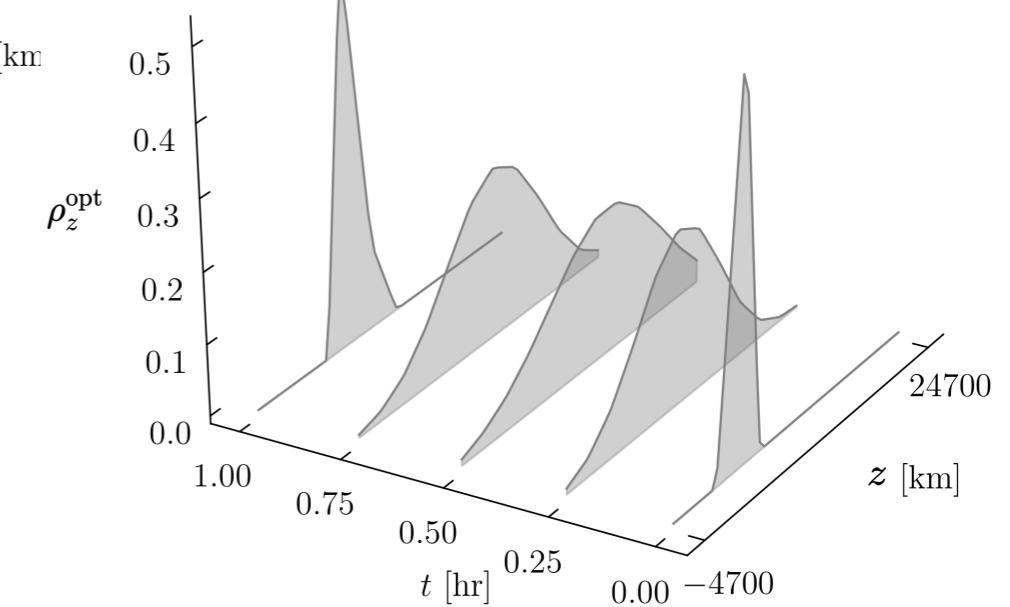
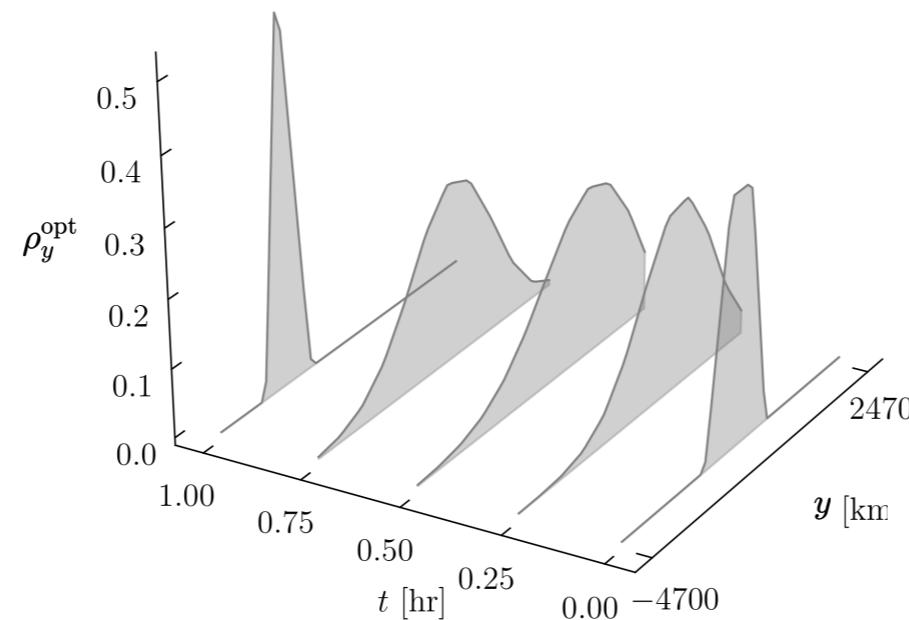
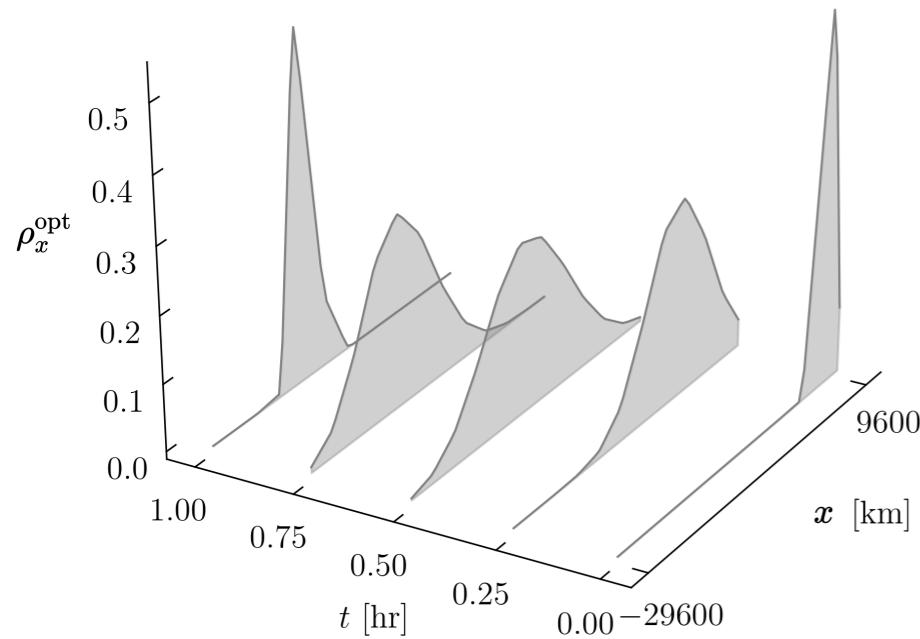


# Numerical Case Study (cont.)



# Numerical Case Study (cont.)

Univariate marginals for optimally controlled joint PDFs



# Tentative Timeline for Research

**Winter-Spring 2024:** Further investigation of convergence guarantees for reaction-diffusion PDEs associated with SBPs with additive state costs.

**Summer-Fall 2024:** Deriving conditions for optimality of generalized SBPs.

**Winter-Spring 2025:** Publishing results, writing my dissertation.

**Summer 2025:** Ph.D. defense.

# Publications

**Alexis M.H. Teter, Yongxin Chen, Abhishek Halder**

“On the contraction coefficient of the Schrödinger bridge for stochastic linear systems”

*IEEE Control Systems Letters*, Vol. 7, pp. 3325–3330, 2023

doi: 10.1109/LCSYS.2023.3326836

(also accepted for presentation at the 2024 American Control Conference)

**Alexis M.H. Teter, Iman Nodizi, Abhishek Halder**

“Probabilistic Lambert Problem: Connections with Optimal Transport, Schrödinger Bridge and Reaction-Diffusion PDEs”

under review

arXiv:2401.07961, 2024

**Alexis M.H. Teter, Iman Nodizi, Abhishek Halder**

“Proximal mean field learning in shallow neural networks”

*Transactions on Machine Learning Research*, 2024

URL: <https://openreview.net/forum?id=vyRBsqj5iG>

**Thank You**

# Backup Slides

# $\gamma$ in Linear SBP

Thm. (informal)

$$\begin{aligned}\tilde{\alpha}_L &= \left\{ \max_{\mathbf{y} \in \mathcal{S}^{n-1}} (h_{\mathcal{X}_0}(\Phi_{t_1 t_0}^\top \mathbf{M}_{10}^{-1/2} \mathbf{y}) + h_{\mathcal{X}_1}(-\mathbf{M}_{10}^{-1/2} \mathbf{y})) \right\}^2 \\ \tilde{\beta}_L &= \left\{ \min_{\mathbf{y} \in \mathcal{S}^{n-1}} (h_{\mathcal{X}_0}(\Phi_{t_1 t_0}^\top \mathbf{M}_{10}^{-1/2} \mathbf{y}) + h_{\mathcal{X}_1}(-\mathbf{M}_{10}^{-1/2} \mathbf{y})) \right\}^2\end{aligned}$$

Proof idea:

$$\tilde{\alpha}_L = \max_{\mathbf{x}_0 \in \mathcal{X}_0, \mathbf{x}_1 \in \mathcal{X}_1} (\Phi_{t_1 t_0} \mathbf{x}_0 - \mathbf{x}_1)^\top \mathbf{M}_{10}^{-1} (\Phi_{t_1 t_0} \mathbf{x}_0 - \mathbf{x}_1)$$

$$\tilde{\alpha}_L = \max_{\mathbf{x} \in \mathbf{M}_{10}^{-1/2} \Phi_{10} \mathcal{X}_0 - \mathbf{M}_{10}^{-1/2} \mathcal{X}_1} |\mathbf{x}|^2 = \left\{ \max_{\mathbf{x} \in \mathbf{M}_{10}^{-1/2} \Phi_{10} \mathcal{X}_0 - \mathbf{M}_{10}^{-1/2} \mathcal{X}_1} \left\langle \frac{\mathbf{x}}{|\mathbf{x}|}, \mathbf{x} \right\rangle \right\}^2$$

$$\tilde{\alpha}_L = \left\{ \max_{\mathbf{y} \in \mathbb{S}^{n-1}} h_{\mathbf{M}_{10}^{-1/2} \Phi_{10} \mathcal{X}_0 - \mathbf{M}_{10}^{-1/2} \mathcal{X}_1}(\mathbf{y}) \right\}^2$$

# Solution to the Classical SBP

**Thm. (Necessary conditions of optimality for the classical SBP):**

The pair  $(\rho_\varepsilon^{\text{opt}}, \mathbf{v}_\varepsilon^{\text{opt}})$  solves the coupled PDEs

## Value function

$$\frac{\partial \psi_\varepsilon}{\partial t} + \frac{1}{2} |\nabla_x \psi_\varepsilon|^2 + \varepsilon \Delta_x \psi_\varepsilon = 0,$$

$$\frac{\partial \rho_\varepsilon^{\text{opt}}}{\partial t} + \nabla_x \cdot (\rho_\varepsilon^{\text{opt}} \nabla_x \psi_\varepsilon) = \varepsilon \Delta_x \rho_\varepsilon^{\text{opt}}$$

with boundary conditions

$$\rho_\varepsilon^{\text{opt}}(\mathbf{x}, t = t_0) = \rho_0(\mathbf{x})$$

$$\rho_\varepsilon^{\text{opt}}(\mathbf{x}, t = t_1) = \rho_1(\mathbf{x})$$

# Solution to the Classical SBP

Hopf-Cole transform

$$\varphi_\varepsilon := \exp\left(\frac{\psi_\varepsilon}{2\varepsilon}\right), \quad \hat{\varphi}_\varepsilon := \rho_\varepsilon^{\text{opt}} \exp\left(-\frac{\psi_\varepsilon}{2\varepsilon}\right)$$

Schrödinger factors

results in

$$\begin{aligned} \frac{\partial \hat{\varphi}_\varepsilon}{\partial t} &= \varepsilon \Delta_x \hat{\varphi}_\varepsilon \\ \frac{\partial \varphi_\varepsilon}{\partial t} &= -\varepsilon \Delta_x \varphi_\varepsilon \\ \hat{\varphi}_\varepsilon(\mathbf{x}, t = t_0) \varphi_\varepsilon(\mathbf{x}, t = t_0) &= \rho_0(\mathbf{x}), \\ \hat{\varphi}_\varepsilon(\mathbf{x}, t = t_1) \varphi_\varepsilon(\mathbf{x}, t = t_1) &= \rho_1(\mathbf{x}) \end{aligned}$$

# Contraction Coefficient for Linear SBP

Thm. (informal)

$$\gamma_L = \tanh^2 \left( \frac{\tilde{\alpha}_L - \tilde{\beta}_L}{8\varepsilon} \right)$$

Proof Idea: