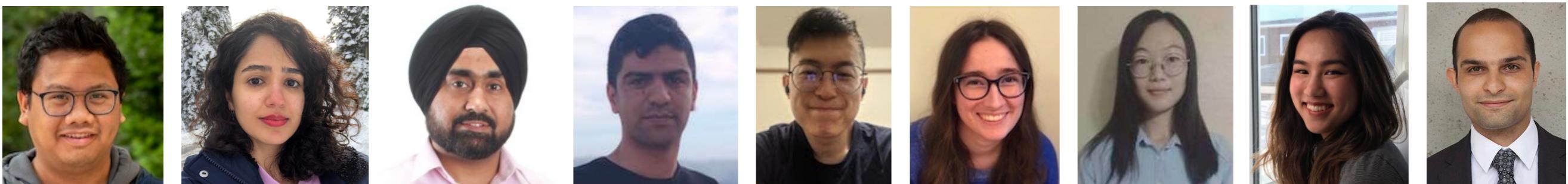


New Developments in Schrödinger Bridge: A Stochastic Control Viewpoint

Abhishek Halder

Department of Aerospace Engineering
Iowa State University

Joint work with students and collaborators



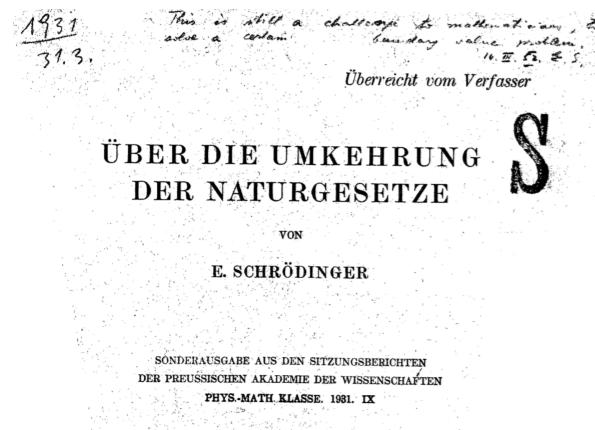
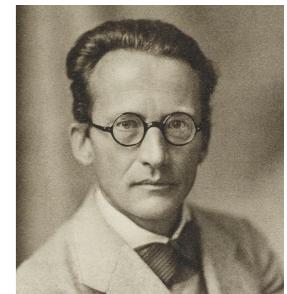
Learning, Computation, and Control Seminar
Department of Mathematics, Imperial College London

June 06, 2024



What is a Schrödinger bridge

Prior physics = Brownian motion



[1931]

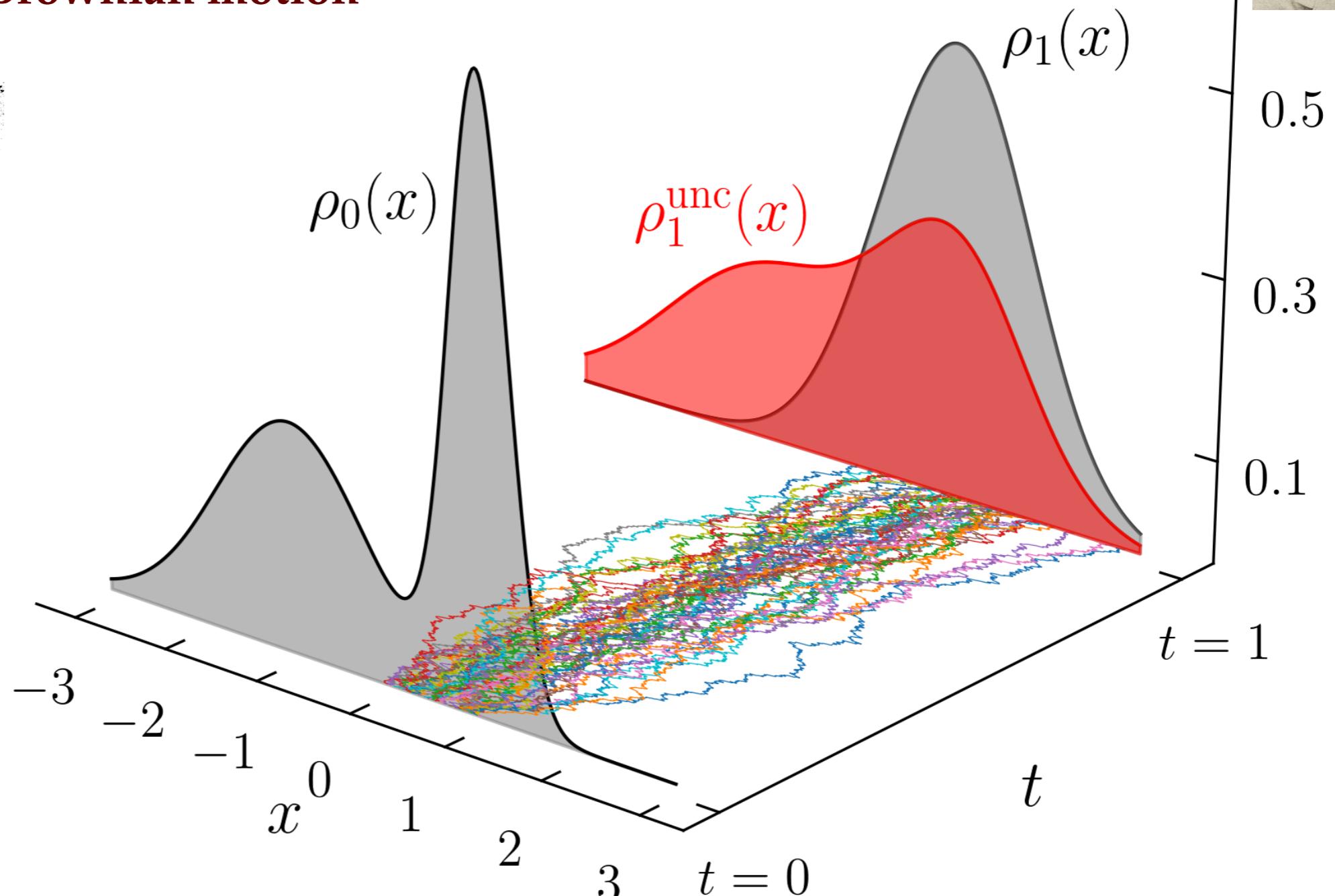
Sur la théorie relativiste de l'électron
et l'interprétation de la mécanique quantique

PAR
E. SCHRÖDINGER

I. — Introduction

J'ai l'intention d'exposer dans ces conférences diverses idées concernant la mécanique quantique et l'interprétation qu'en donne généralement à l'heure actuelle ; je parlerai principalement de la théorie quantique relativiste du mouvement de l'électron. Autant que nous pouvons nous en rendre compte aujourd'hui, il semble à peu près sûr que la mécanique quantique de l'électron, sous sa forme idéale, que nous ne possédons pas encore, doit former un jour la base de toute la physique. A cet intérêt tout à fait général, s'ajoute, ici à Paris, un intérêt particulier : vous savez tous que les bases de la théorie moderne de l'électron ont été posées à Paris par votre célèbre compatriote Louis de BROGLIE.

[1932]



Find the most likely explanation of observation vs prior physics mismatch

What is a Schrödinger bridge

Path space $\Omega := C([t_0, t_1]; \mathbb{R}^n)$



Denote the collection of all probability measures on Ω as $\mathcal{M}(\Omega)$

$\Pi_{01} := \{\mathbb{M} \in \mathcal{M}(\Omega) \mid \mathbb{M} \text{ has marginal } \rho_i \text{ } d\mathbf{x} \text{ at time } t_i \forall i \in \{0, 1\}, \rho_0, \rho_1 \in \mathcal{P}_2(\mathbb{R}^n)\}$

Schrödinger bridge = $\arg \inf_{\mathbb{P} \in \Pi_{01}} D_{\text{KL}}(\mathbb{P} \parallel \mathbb{W})$

Generated by Itô diffusion

Wiener measure

$$d\mathbf{x} = \mathbf{u}(t, \mathbf{x})dt + d\mathbf{w}(t)$$

Most parsimonious correction of prior physics

Constrained maximum likelihood problem on measure-valued paths

What is a Schrödinger bridge

Schrödinger bridge as large deviation principle: **Sanov's theorem [1957]**

$$\lim_{N \uparrow \infty} \log(\text{empirical prob}_N \text{ under } W \in \Pi_{01}) \asymp - \inf_{P \in \Pi_{01}} D_{\text{KL}}(P \parallel W)$$

KL div as rate function

Schrödinger bridge as stochastic optimal control: **[1990s]**

$$\underset{u \in \mathcal{U}}{\text{minimize}} \mathbb{E} \left[\int_{t_0}^{t_1} \frac{1}{2} \| \mathbf{u}(t, \mathbf{x}_t^u) \|_2^2 dt \right]$$

subject to

$$d\mathbf{x}_t^u = \mathbf{u}(t, \mathbf{x}_t^u) dt + d\mathbf{w}_t$$

$$\mathbf{x}_t^u(t = t_0) \sim \rho_0, \quad \mathbf{x}_t^u(t = t_1) \sim \rho_1$$

What is a Schrödinger bridge

Schrödinger bridge as large deviation principle: Sanov's theorem [1957]

$$\lim_{N \uparrow \infty} \log(\text{empirical prob}_N \text{ under } W \in \Pi_{01}) \asymp - \inf_{P \in \Pi_{01}} D_{\text{KL}}(P \parallel W)$$

KL div as rate function

Schrödinger bridge as stochastic optimal control: [1990s]

$$\underset{u \in \mathcal{U}}{\text{minimize}} \mathbb{E} \left[\int_{t_0}^{t_1} \frac{1}{2} \| \mathbf{u}(t, \mathbf{x}_t^u) \|_2^2 dt \right]$$

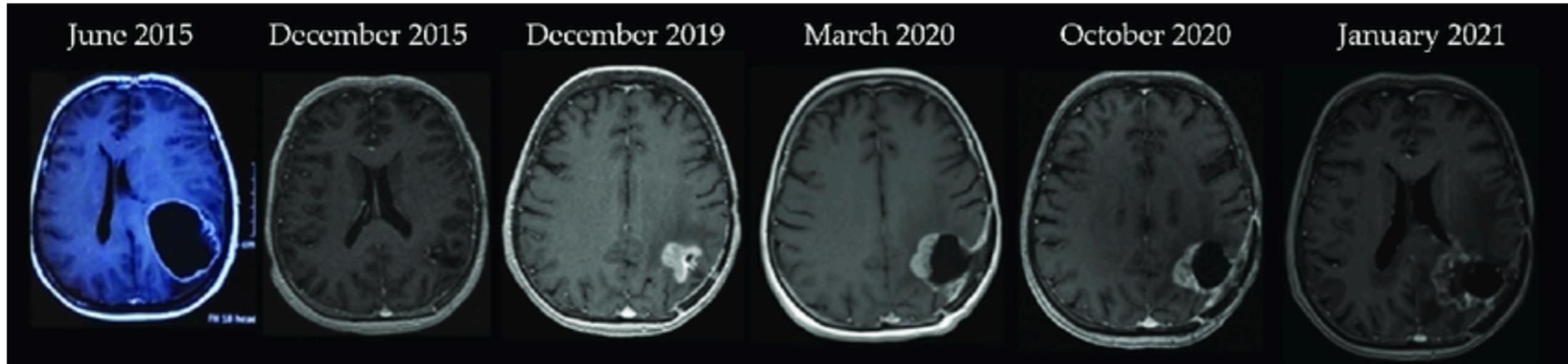
subject to

$$d\mathbf{x}_t^u = \mathbf{u}(t, \mathbf{x}_t^u) dt + d\omega_t \xrightarrow{0} \text{Benamou-Brenier OMT [1999]}$$

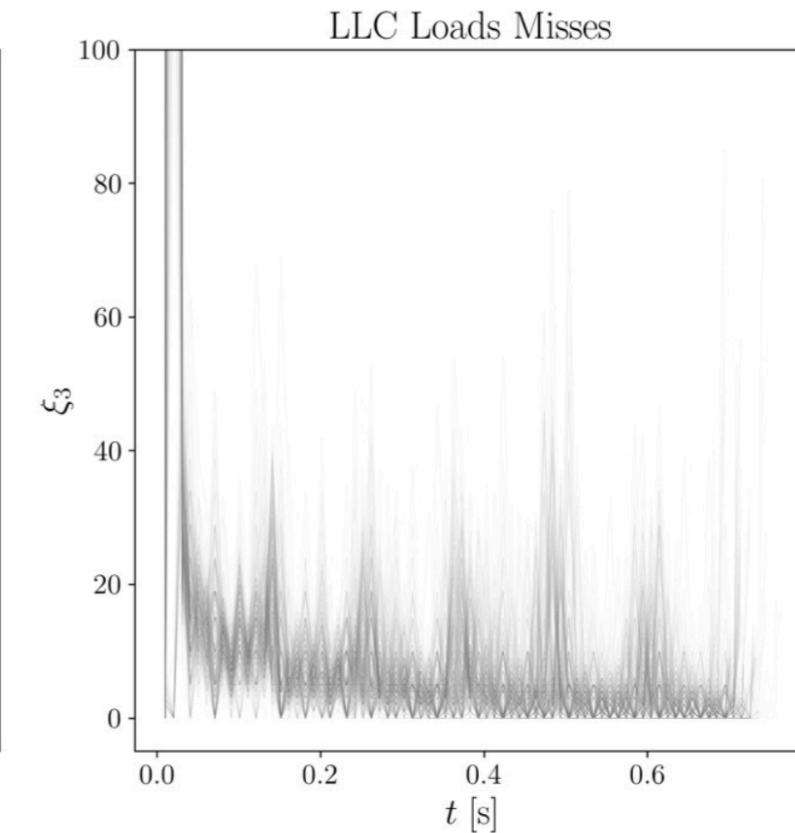
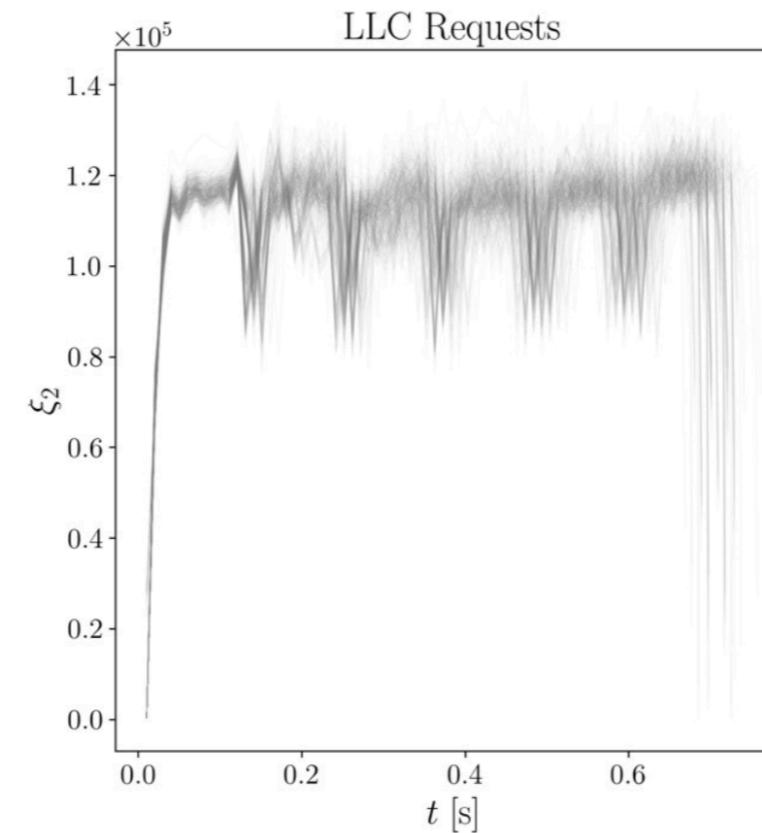
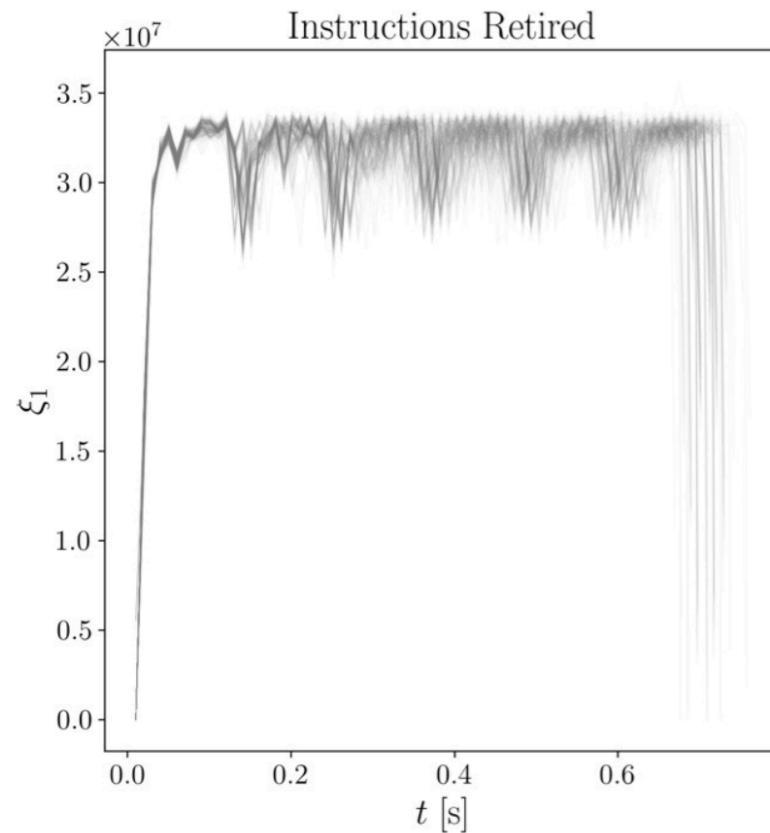
$$\mathbf{x}_t^u(t = t_0) \sim \rho_0, \quad \mathbf{x}_t^u(t = t_1) \sim \rho_1$$

Resurgence of Schrödinger bridge in ML/AI

Learn most likely progression of medical condition



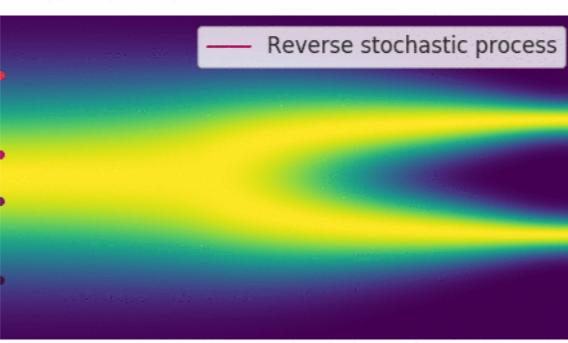
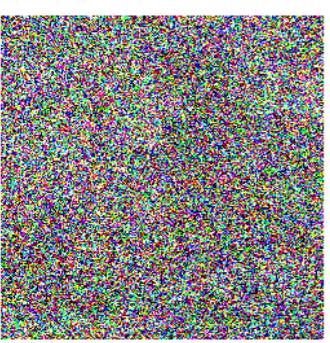
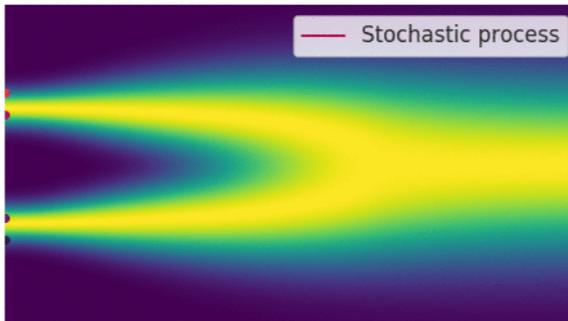
Learn joint stochastic time-varying hardware resource availability



Resurgence of Schrödinger bridge in ML/AI

Diffusion models for generative AI

Source: <https://yang-song.net/blog/2021/score/>



UAI 2023

Aligned Diffusion Schrödinger Bridges

Vignesh Ram Somnath^{*1,2}
Maria Rodriguez Martinez²

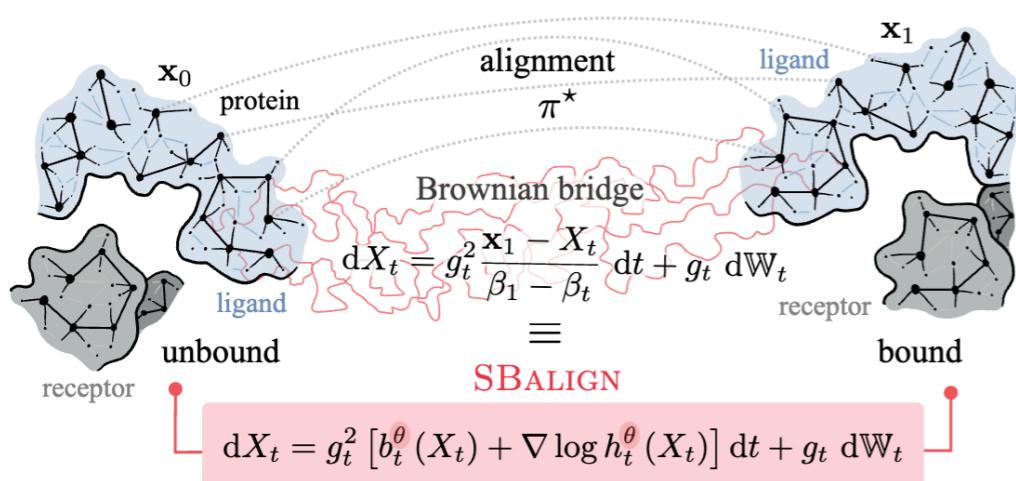
Matteo Pariset^{*1,3}
Andreas Krause¹

Ya-Ping Hsieh¹
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¹Department of Computer Science, ETH Zürich

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NeurIPS 2021

Diffusion Schrödinger Bridge with Applications to Score-Based Generative Modeling

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University of Oxford, UK

Jeremy Heng
ESSEC Business School,
Singapore

Arnaud Doucet
Department of Statistics,
University of Oxford, UK

NeurIPS 2024

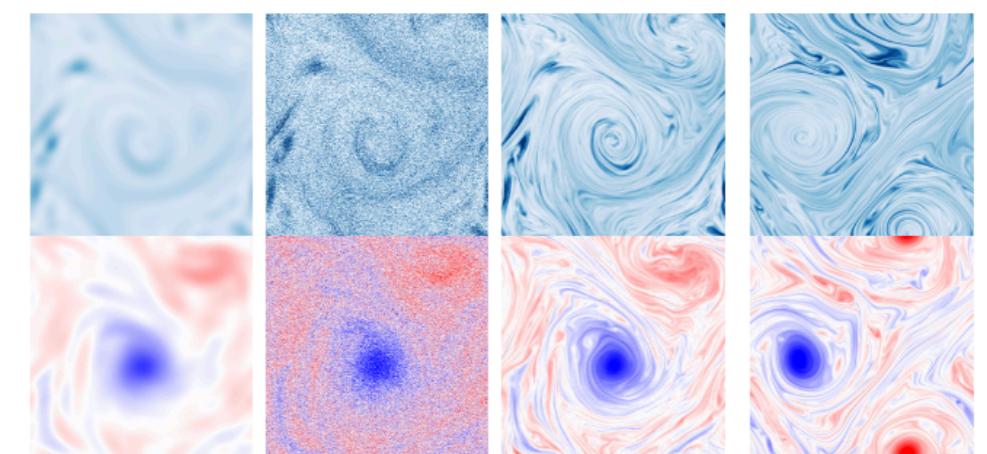
Diffusion Schrödinger Bridge Matching

Yuyang Shi*
University of Oxford

Valentin De Bortoli*
ENS ULM

Andrew Campbell
University of Oxford

Arnaud Doucet
University of Oxford



Low res

High res

This talk: generalized Schrödinger bridges

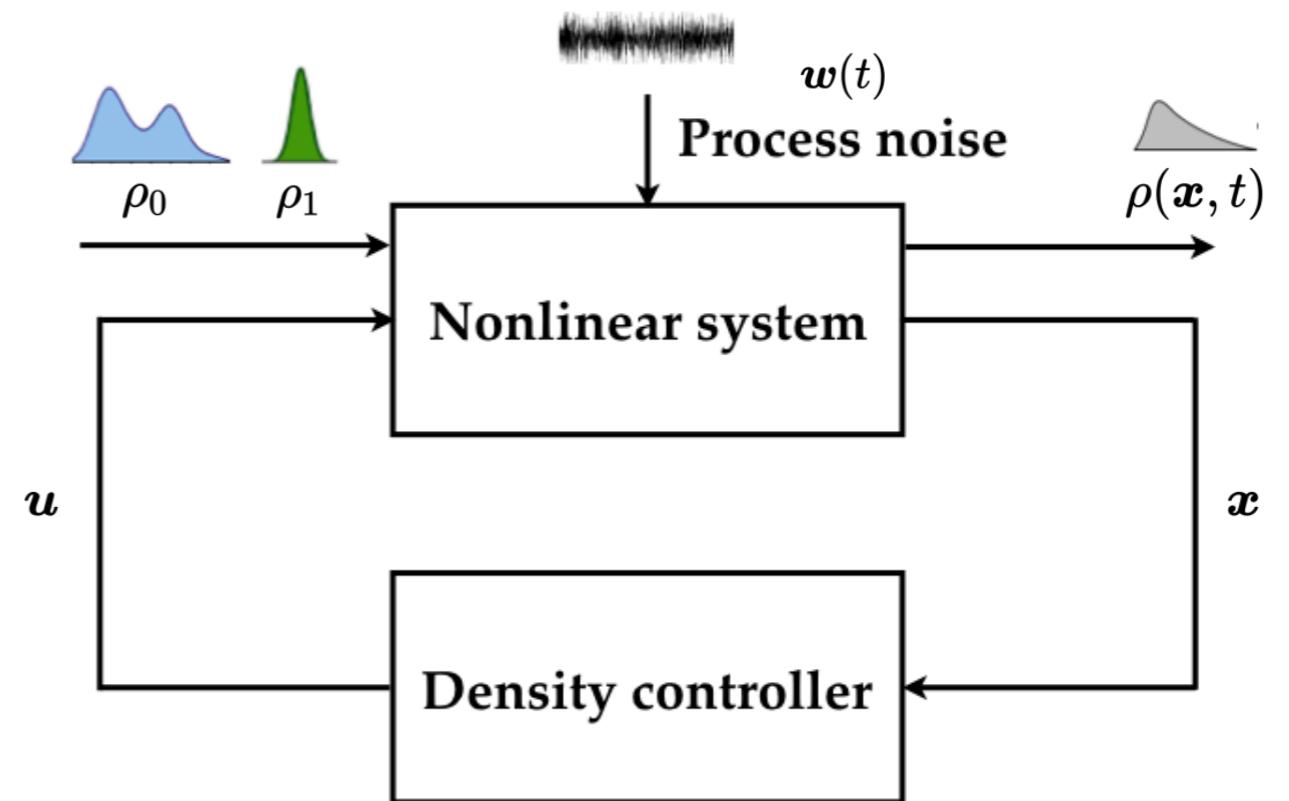
1. general controlled dynamics

2. extra sample path constraints

3. additive state cost

Generalization #1: more general controlled dyn.

Steer joint state PDF via feedback control over finite time horizon



Common scenario: $G \equiv B$

$$\underset{u \in \mathcal{U}}{\text{minimize}} \quad \mathbb{E} \left[\int_0^1 \left(\frac{1}{2} \|u(t, x_t^u)\|_2^2 + q(t, x_t^u) \right) dt \right]$$

subject to

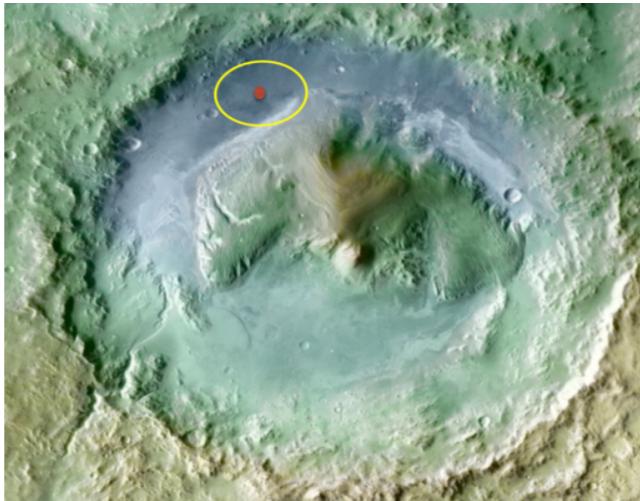
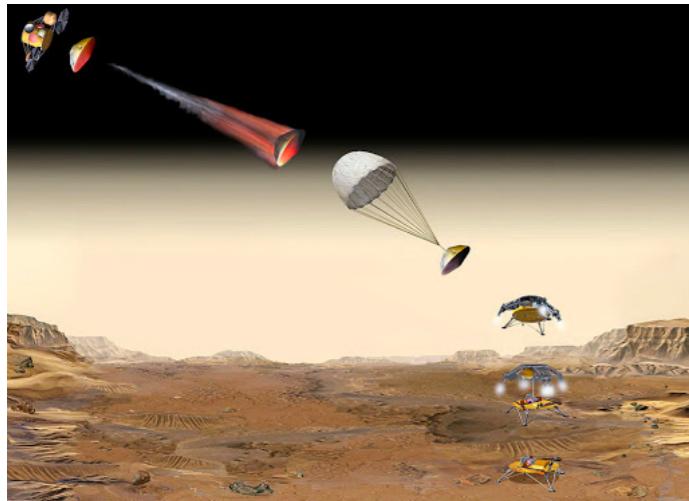
$$dx_t^u = \{f(t, x_t^u) + B(t, x_t^u)u\}dt + \sqrt{2}G(t, x_t^u)dw_t$$

$$x_0^u := x_t^u(t=0) \sim \rho_0, \quad x_1^u := x_t^u(t=1) \sim \rho_1$$

Motivating applications

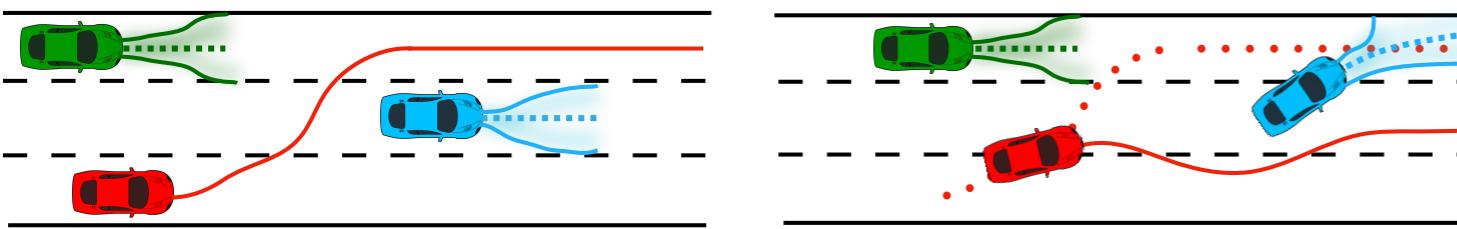
Distribution ~ Probability

Spacecraft landing with desired statistical accuracy



Gale Crater (4.49S, 137.42E)

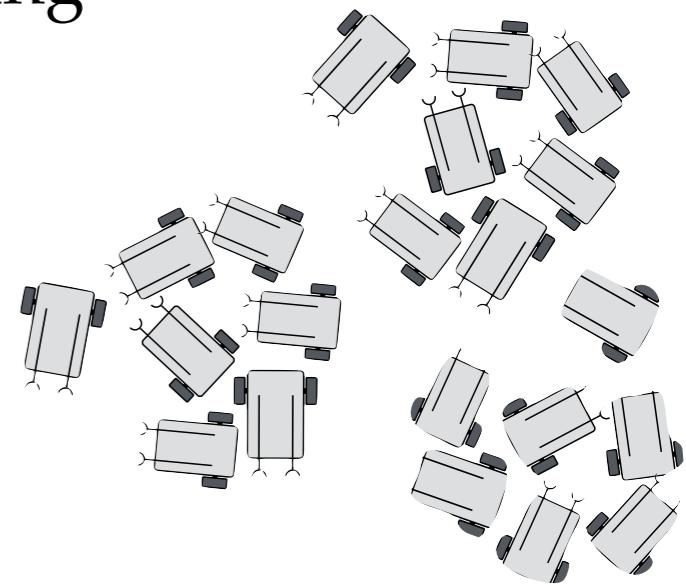
Risk management for automated driving in multi-lane highways



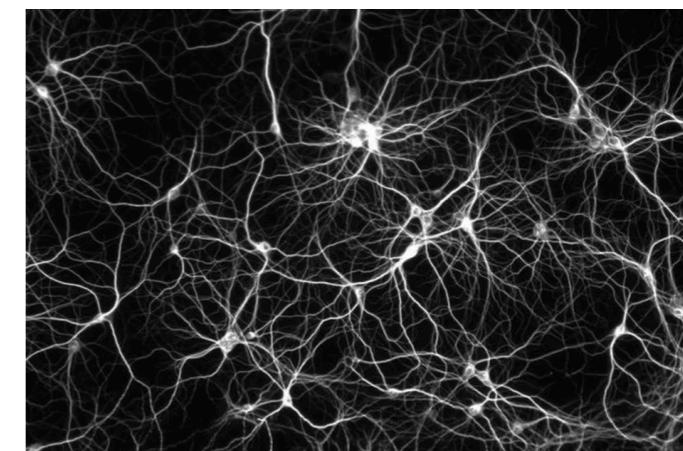
Control of uncertainties

Distribution ~ Population

Dynamic shaping of swarms



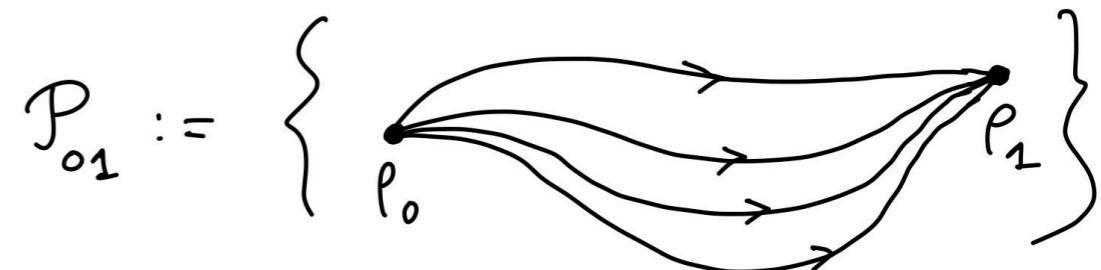
Feedback sync. and desync. of neuronal population



Control of ensemble

Generalized Schrödinger bridge

Diffusion tensor: $D := GG^\top$



Hessian operator w.r.t. state: Hess

$$\inf_{(\rho, \mathbf{u}) \in \mathcal{P}_{01} \times \mathcal{U}} \int_{\mathbb{R}^n} \int_0^1 \left(\frac{1}{2} \|\mathbf{u}(t, \mathbf{x}_t^u)\|_2^2 + q(t, \mathbf{x}_t^u) \right) \rho(t, \mathbf{x}_t^u) dt d\mathbf{x}_t^u$$

subject to

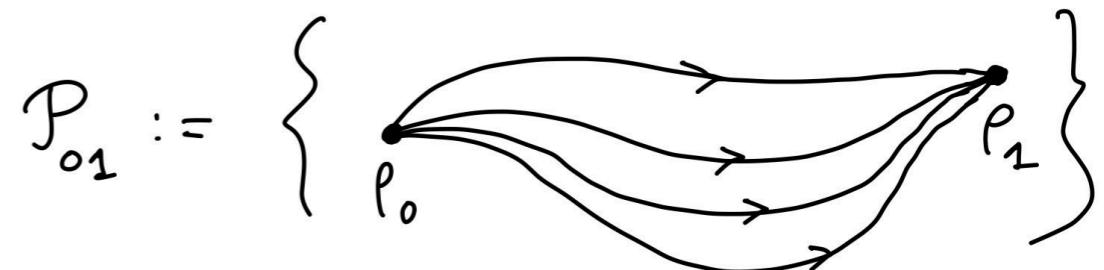
$$\frac{\partial \rho}{\partial t} + \nabla \cdot ((\mathbf{f} + \mathbf{B}\mathbf{u})\rho) = \Delta_D \rho$$

$$\rho(t=0, \mathbf{x}_0^u) = \rho_0, \quad \rho(t=1, \mathbf{x}_1^u) = \rho_1$$

Controlled Fokker-Planck or Kolmogorov's forward PDE

Zero process noise \rightsquigarrow Generalized OMT

Diffusion tensor: $D := GG^\top$



Hessian operator w.r.t. state: Hess

$$\inf_{(\rho, \mathbf{u}) \in \mathcal{P}_{01} \times \mathcal{U}} \int_{\mathbb{R}^n} \int_0^1 \left(\frac{1}{2} \|\mathbf{u}(t, \mathbf{x}_t^u)\|_2^2 + q(t, \mathbf{x}_t^u) \right) \rho(t, \mathbf{x}_t^u) dt d\mathbf{x}_t^u$$

subject to

$$\begin{aligned} \frac{\partial \rho}{\partial t} + \nabla \cdot ((\mathbf{f} + \mathbf{B}\mathbf{u})\rho) &= \Delta_D \rho \xrightarrow{0} \\ \rho(t = 0, \mathbf{x}_0^u) &= \rho_0, \quad \rho(t = 1, \mathbf{x}_1^u) = \rho_1 \end{aligned}$$

Controlled Liouville PDE

Necessary Conditions of Optimality (Assuming $G \equiv B$)

Coupled nonlinear PDEs + linear boundary conditions

Controlled Fokker-Planck or Kolmogorov's forward PDE

$$\frac{\partial \rho^{\text{opt}}}{\partial t} + \nabla \cdot ((f + D\nabla\psi) \rho^{\text{opt}}) = \Delta_D \rho^{\text{opt}}$$

Hamilton-Jacobi-Bellman-like PDE

$$\frac{\partial \psi}{\partial t} + \langle \nabla \psi, f \rangle + \langle D, \text{Hess}(\psi) \rangle + \frac{1}{2} \langle \nabla \psi, D \nabla \psi \rangle = q$$

Boundary conditions:

$$\rho^{\text{opt}}(\cdot, t=0) = \rho_0, \quad \rho^{\text{opt}}(\cdot, t=1) = \rho_1$$

Optimal control: $u^{\text{opt}} = B^\top \nabla \psi$

Feedback synthesis via the Schrödinger factors

Hopf-Cole a.k.a. Fleming's logarithmic transform:

$$(\rho^{\text{opt}}, \psi) \mapsto (\hat{\varphi}, \varphi) \quad \text{— Schrödinger factors} \quad \hat{\varphi}(x, t) = \rho^{\text{opt}}(x, t) \exp(-\psi(x, t))$$

$$\varphi(x, t) = \exp(\psi(x, t))$$

2 coupled nonlinear PDEs \rightarrow boundary-coupled linear PDEs!!

Uncontrolled forward-backward advection-reaction-diffusion PDEs:

$$\begin{aligned} \frac{\partial \hat{\varphi}}{\partial t} &= \boxed{-\nabla \cdot (\hat{\varphi} \mathbf{f}) + \Delta_D \hat{\varphi} - q \hat{\varphi}}, & \hat{\varphi}_0 \varphi_0 &= \rho_0 \\ \frac{\partial \varphi}{\partial t} &= \boxed{-\langle \nabla \varphi, \mathbf{f} \rangle - \Delta_D \hat{\varphi} + q \hat{\varphi}}, & \hat{\varphi}_1 \varphi_1 &= \rho_1 \end{aligned}$$

Optimal controlled joint state PDF: $\rho^{\text{opt}}(x, t) = \hat{\varphi}(x, t) \varphi(x, t)$

Optimal control: $u^{\text{opt}}(x, t) = 2B^\top \nabla_x \log \varphi(x, t)$

What exactly are Schrödinger factors?

Consider Schrödinger's original case: $f = 0, B = D = I$

Classical: $\rho^{\text{opt}}(\mathbf{x}, t) = \varphi(\mathbf{x}, t)\hat{\varphi}(\mathbf{x}, t)$

$$\left(\frac{\partial}{\partial t} + \frac{1}{2}\Delta - q \right) \varphi = 0 \quad [\text{Backward reaction-diffusion PDE}]$$

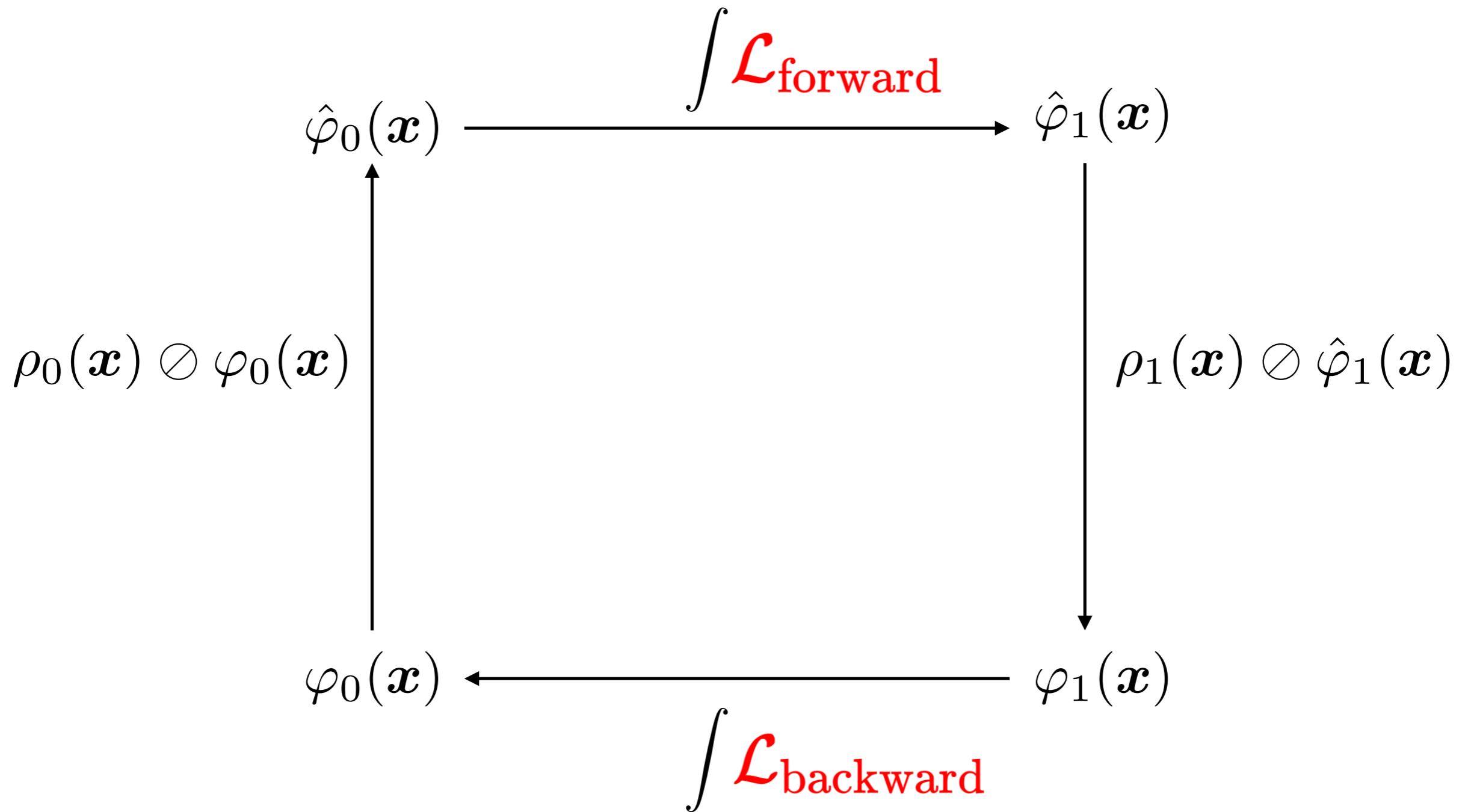
$$\left(\frac{\partial}{\partial t} - \frac{1}{2}\Delta + q \right) \hat{\varphi} = 0 \quad [\text{Forward reaction-diffusion PDE}]$$

Quantum: $\rho^{\text{opt}}(\mathbf{x}, t) = \Psi(\mathbf{x}, t)\widehat{\Psi}(\mathbf{x}, t)$ [Born's relation]
wave function

$$\left(\sqrt{-1}\frac{\partial}{\partial t} + \frac{1}{2}\Delta - q \right) \Psi = 0 \quad [\text{Schrödinger PDE}]$$

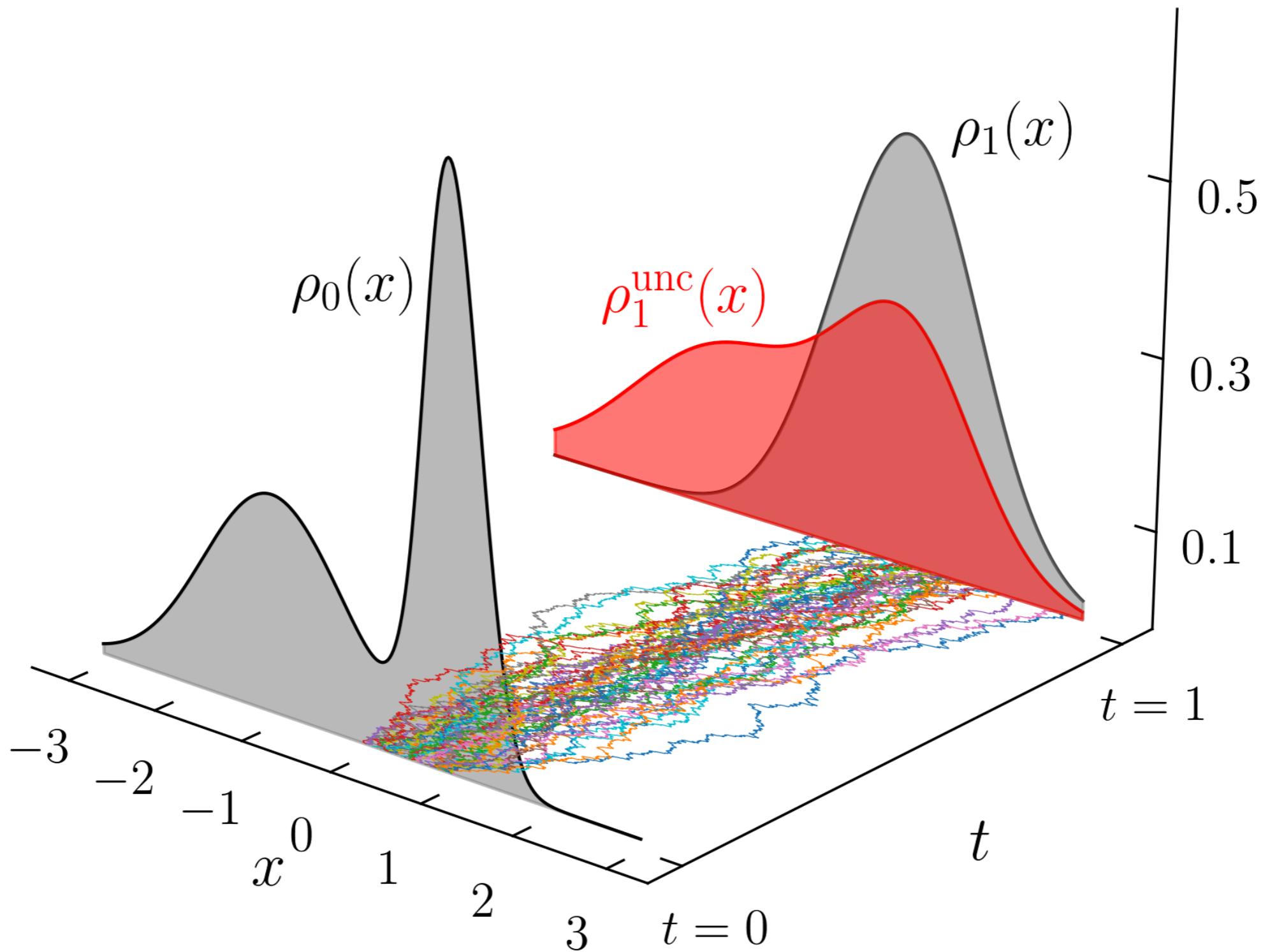
$$\left(-\sqrt{-1}\frac{\partial}{\partial t} - \frac{1}{2}\Delta + q \right) \widehat{\Psi} = 0 \quad [\text{Adjoint Schrödinger PDE}]$$

Fixed Point Recursion Over Pair $(\varphi_1, \hat{\varphi}_0)$



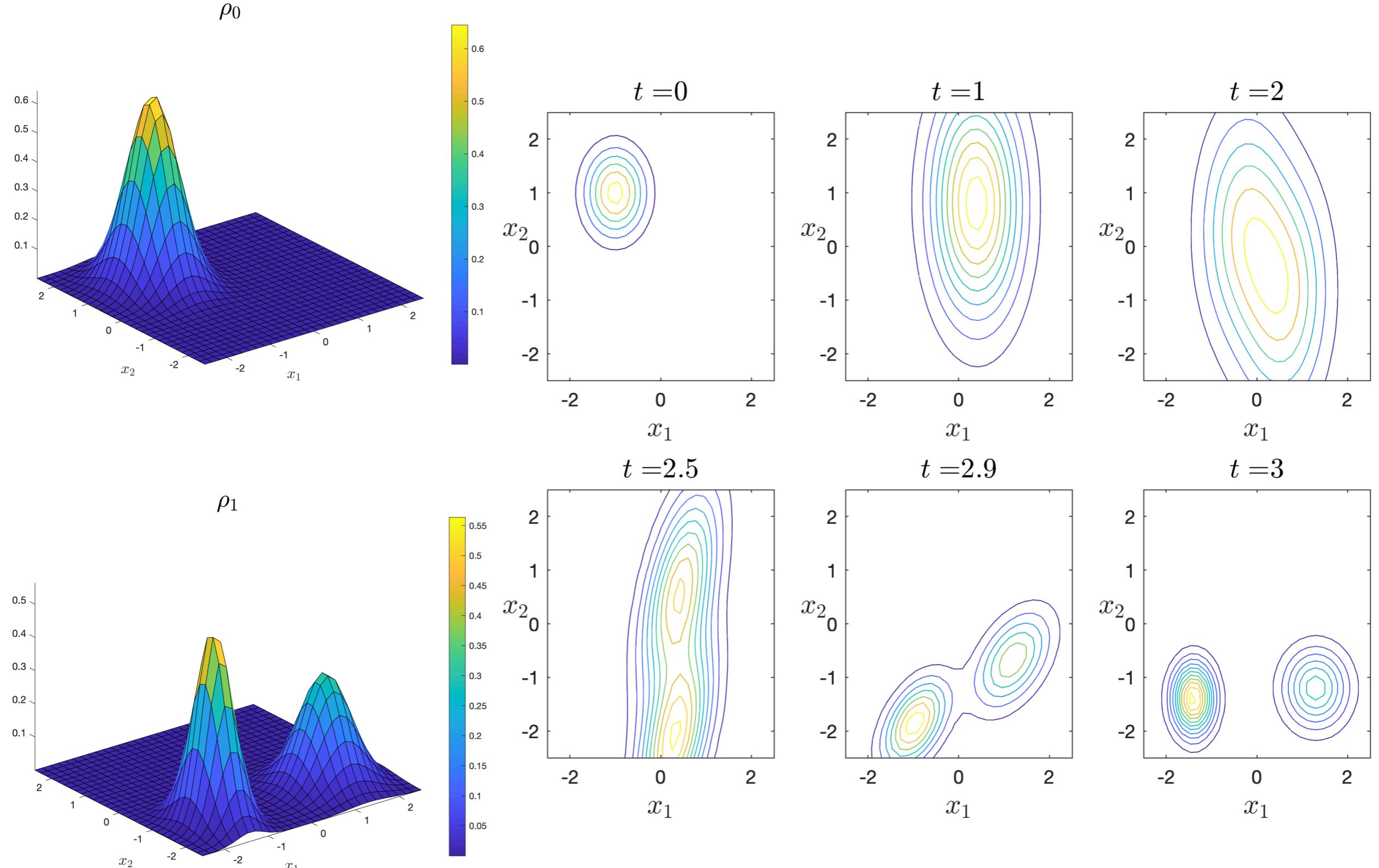
This recursion is contractive in the Hilbert's projective metric!!

Feedback Density Control: $f \equiv 0, B = G \equiv I, q \equiv 0$



Zero prior dynamics

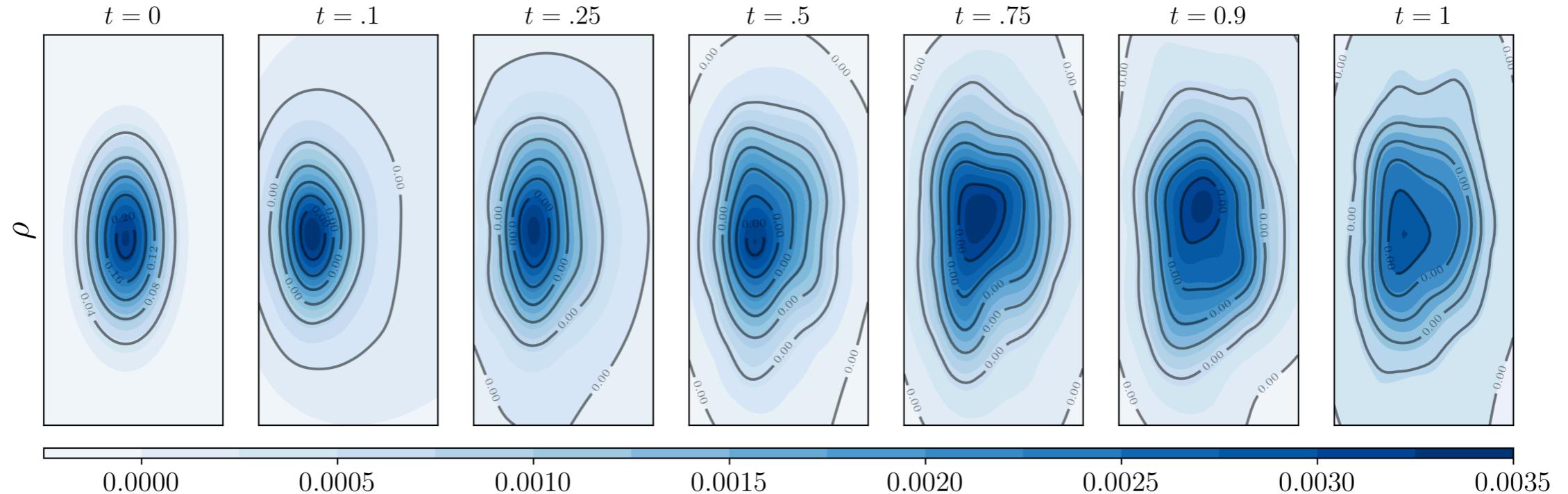
Feedback Density Control: $f \equiv Ax, B = G, q \equiv 0$



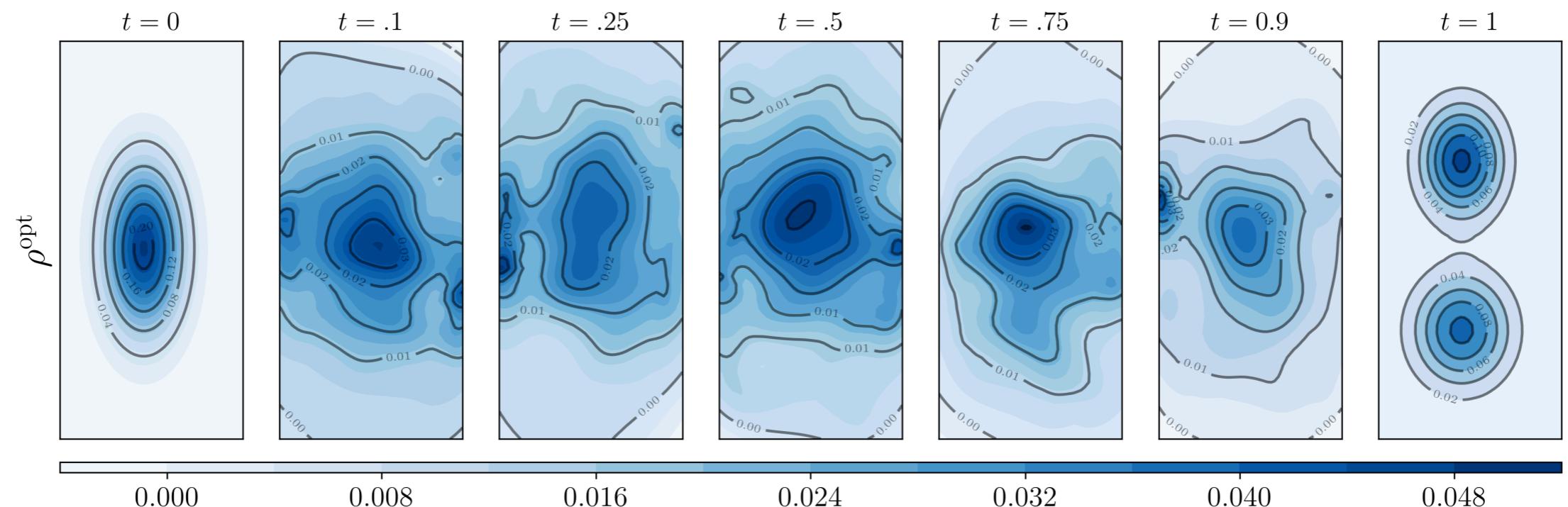
Linear prior dynamics

Feedback Density Control: Nonlinear Grad. Drift

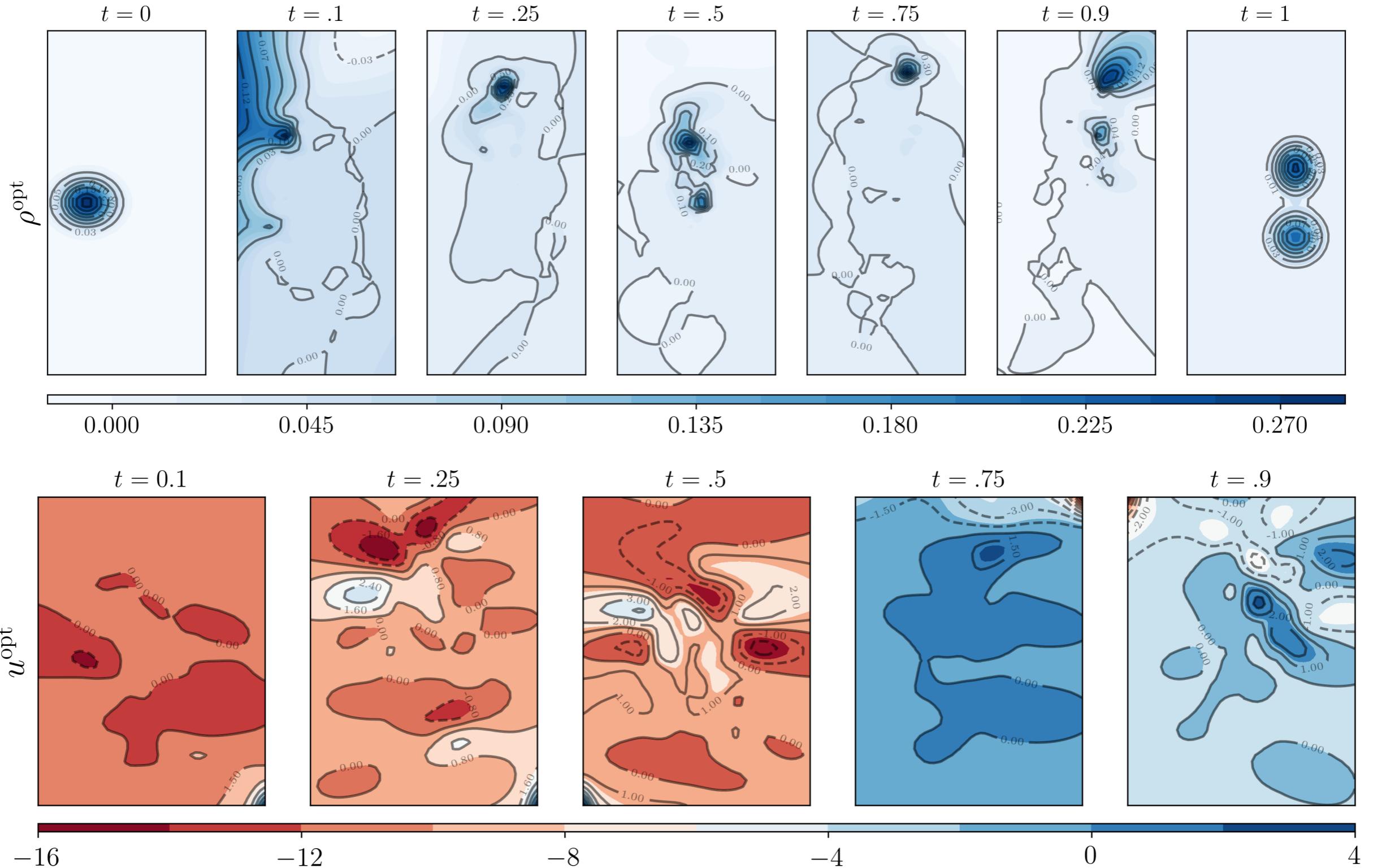
Uncontrolled joint PDF evolution:



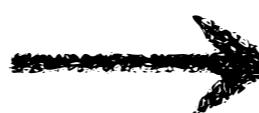
Optimal controlled joint PDF evolution:



Feedback Density Control: Mixed Conservative-Dissipative Drift



Application: Multi-lane Automated Driving

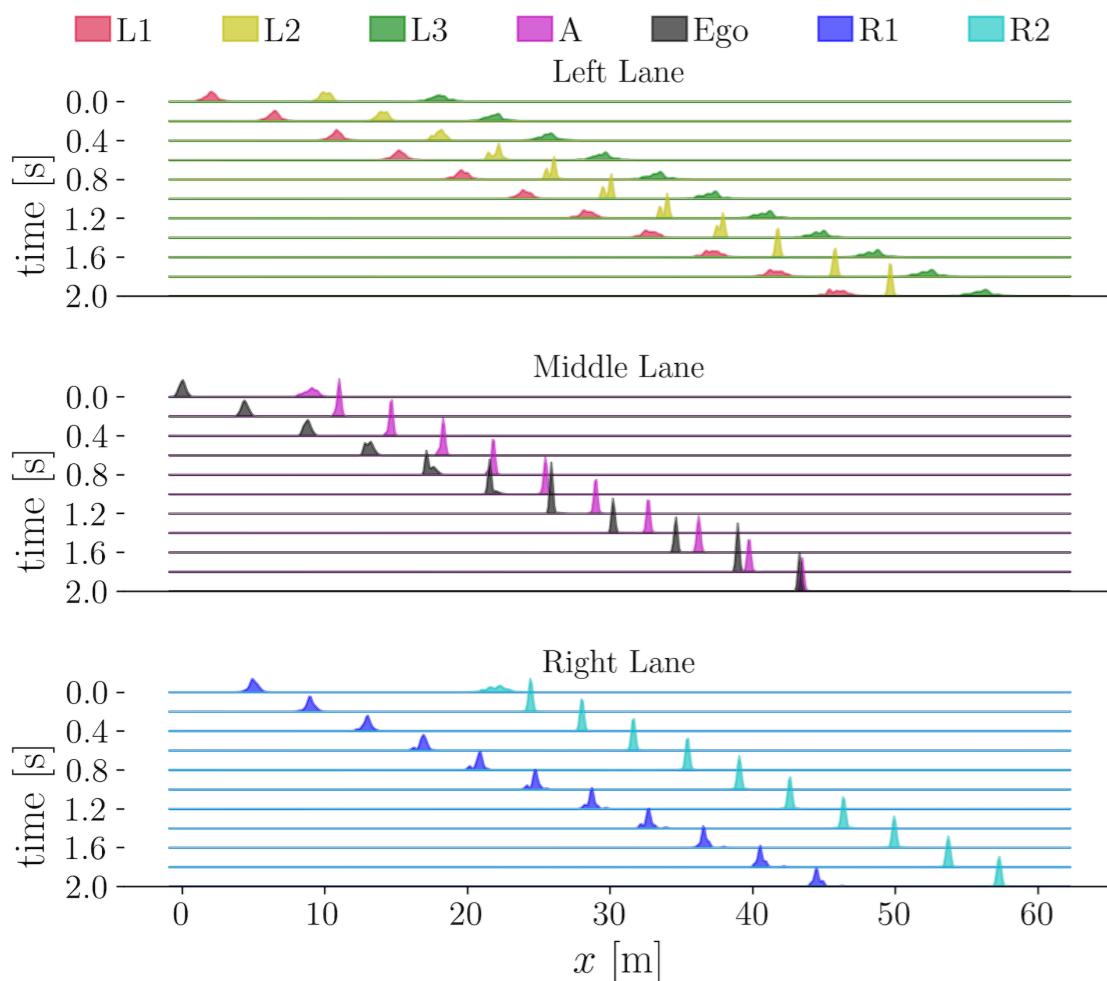


t_0

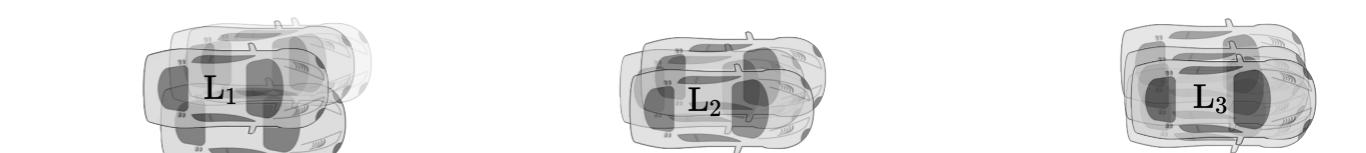
t_1

x marginals

y marginals

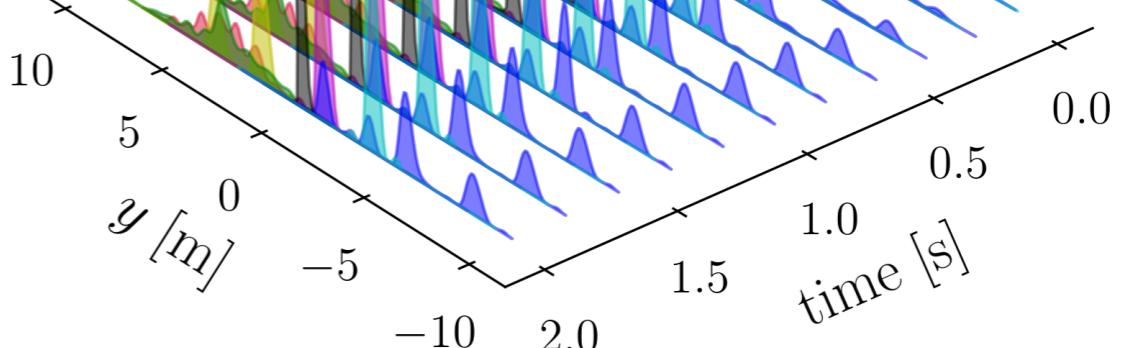


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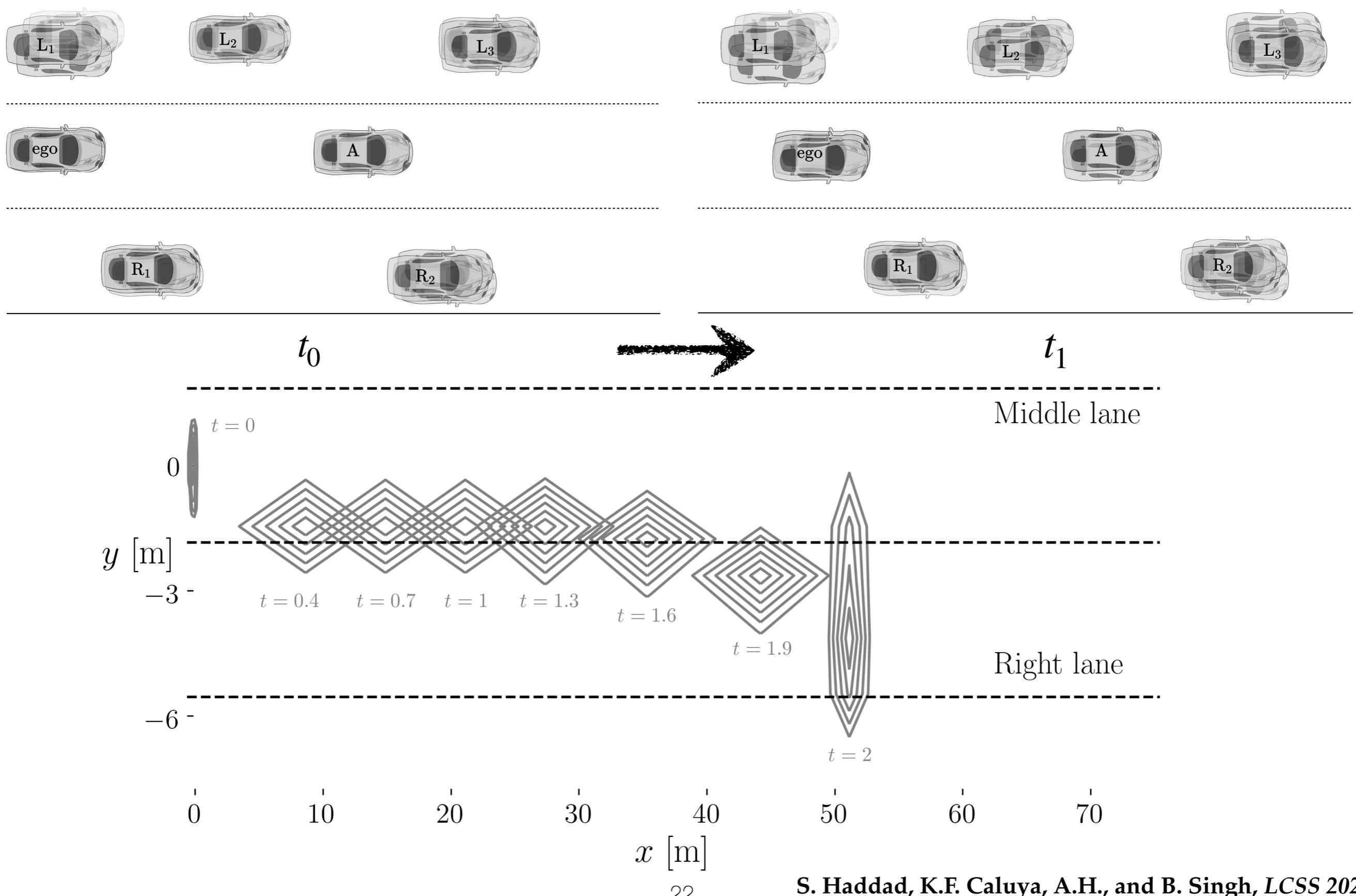


t_0

t_1



Application: Multi-lane Automated Driving

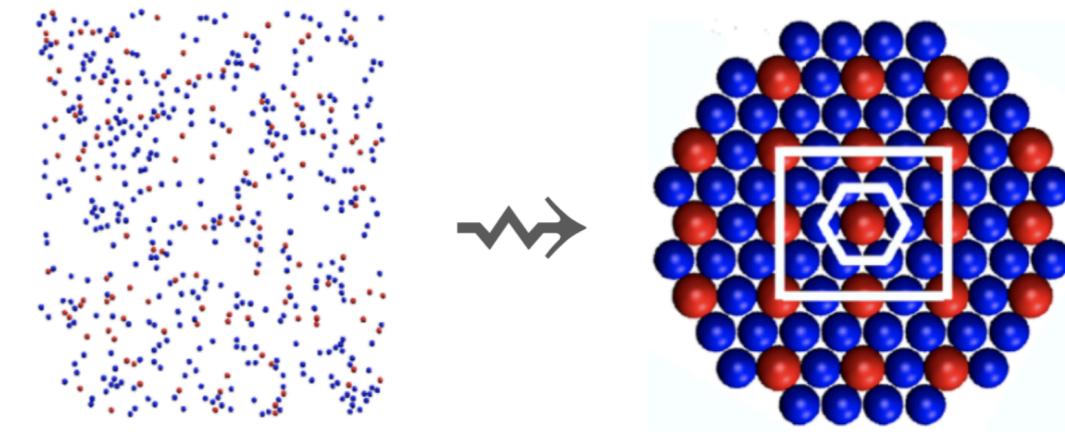


Control non-affine generalized Schrödinger bridge

No state cost: $q = 0$

Controlled SDE:

$$dx_t^u = f(t, x_t^u, u)dt + \sqrt{2}g(t, x_t^u, u)d\omega_t$$



Controlled diffusion tensor: $G := gg^\top \succeq 0$

Conditions for optimality: system of $m + 2$ coupled PDEs

$$\frac{\partial \psi}{\partial t} = \frac{1}{2} \|u_{\text{opt}}\|_2^2 - \langle \nabla_x \psi, f \rangle - \langle G, \text{Hess}(\psi) \rangle$$

$$\frac{\partial \rho_{\text{opt}}^u}{\partial t} = -\nabla \cdot (\rho_{\text{opt}}^u f) + \Delta_G \rho_{\text{opt}}^u$$

$$u_{\text{opt}} = \nabla_{u_{\text{opt}}} (\langle \nabla_x \psi, f \rangle + \langle G, \text{Hess}(\psi) \rangle)$$

$$\rho_{\text{opt}}^u(0, x) = \rho_0, \quad \rho_{\text{opt}}^u(T, x) = \rho_T$$

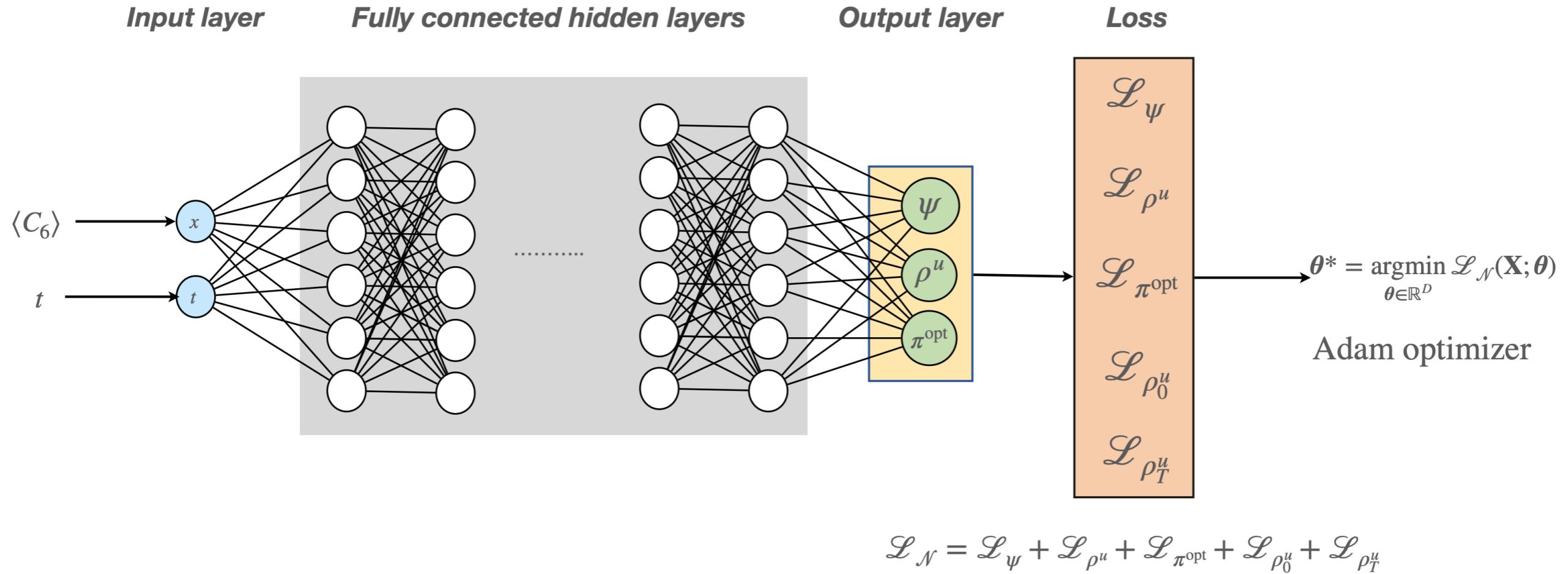
Known f, g

I. Nodozi, J.O'Leary, A. Mesbah,
and A.H., ACC 2023

Data-driven f, g

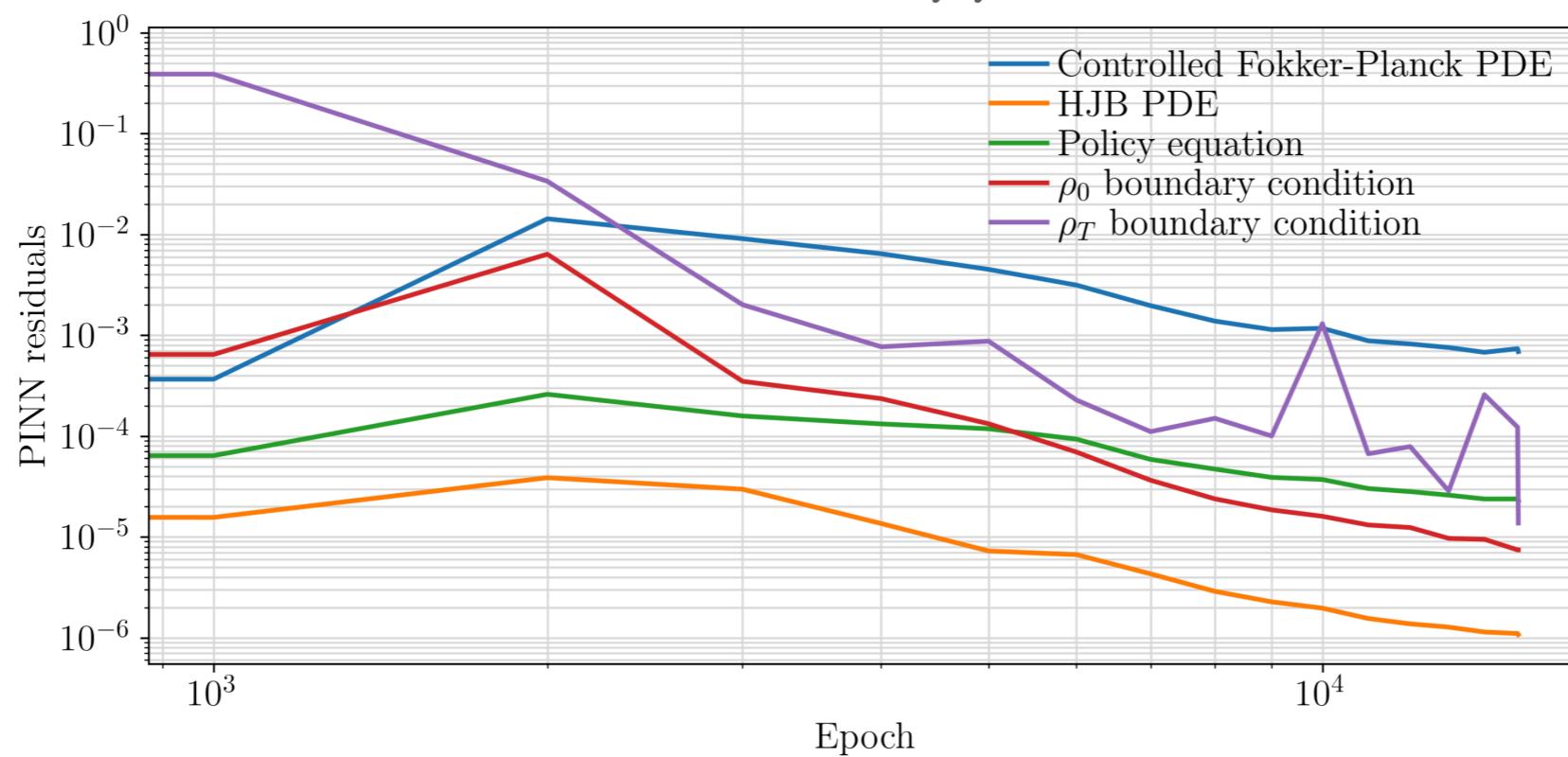
I. Nodozi, C. Yan, M. Khare, A.H.,
and A. Mesbah, TCST 2024

Control non-affine generalized Schrödinger bridge



$$\mathcal{L}_{\mathcal{N}} = \mathcal{L}_\psi + \mathcal{L}_{\rho^u} + \mathcal{L}_{\pi^{\text{opt}}} + \mathcal{L}_{\rho_0^u} + \mathcal{L}_{\rho_T^u}$$

Benchmark controlled self-assembly system: [Y Xue, et al, *IEEE Trans. Control Sys. Technology*, 2014]



Generalization #2: hard sample path constraints

Main idea: path constraints \sim reflected Itô SDEs
modify the controlled sample path dynamics to

$$dx_t^u = \{f(t, x_t^u) + B(t)u(t, x_t^u)\}dt + \sqrt{2\theta}G(t)d\omega_t + n(x_t^u)d\gamma_t$$

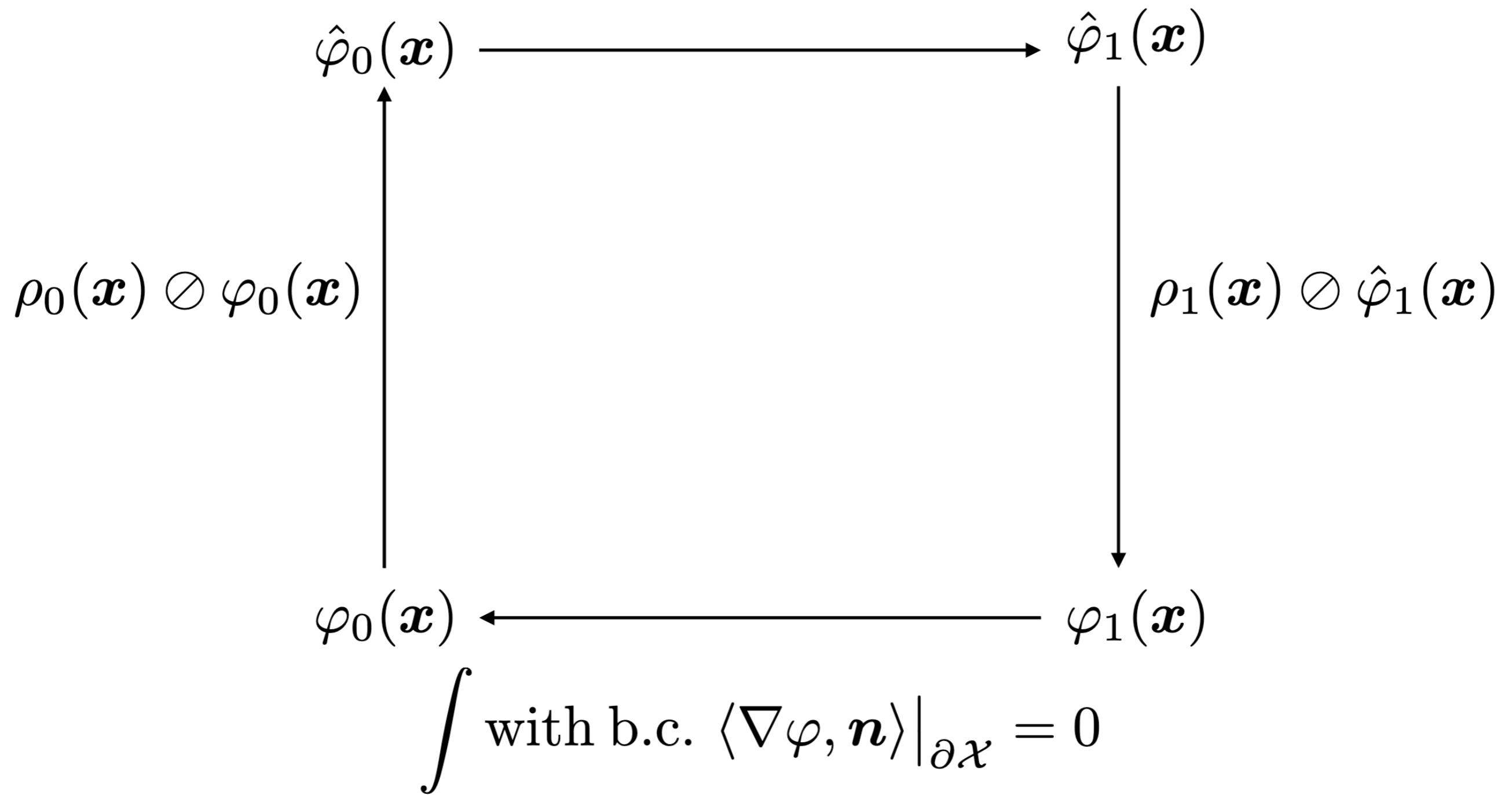
$x_t^u \in \overline{\mathcal{X}} := \mathcal{X} \cup \partial\mathcal{X}$, closure of connected smooth \mathcal{X}

n is inward unit normal to the boundary $\partial\mathcal{X}$

γ_t is minimal local time stochastic process

Reflected bridge: Schrödinger factor recursion

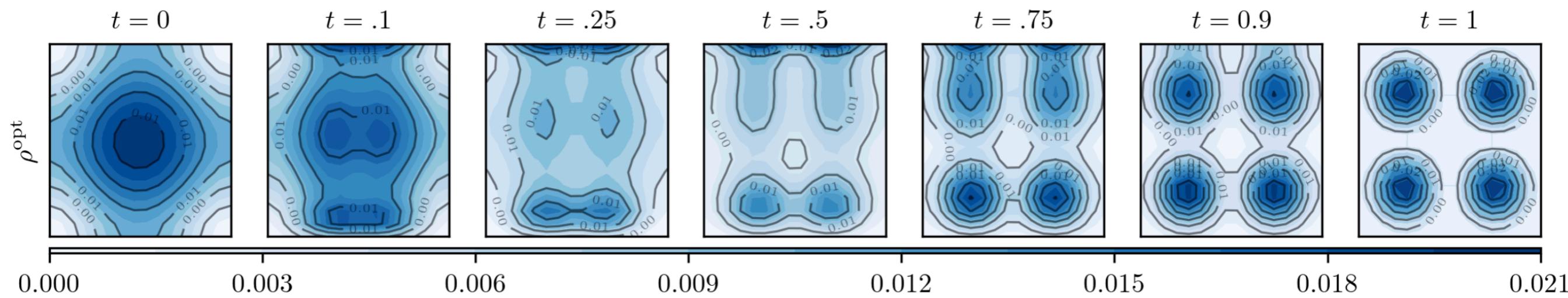
$$\int \text{with b.c. } \langle f\hat{\varphi} - \theta\nabla\hat{\varphi}, \mathbf{n} \rangle|_{\partial\mathcal{X}} = 0$$



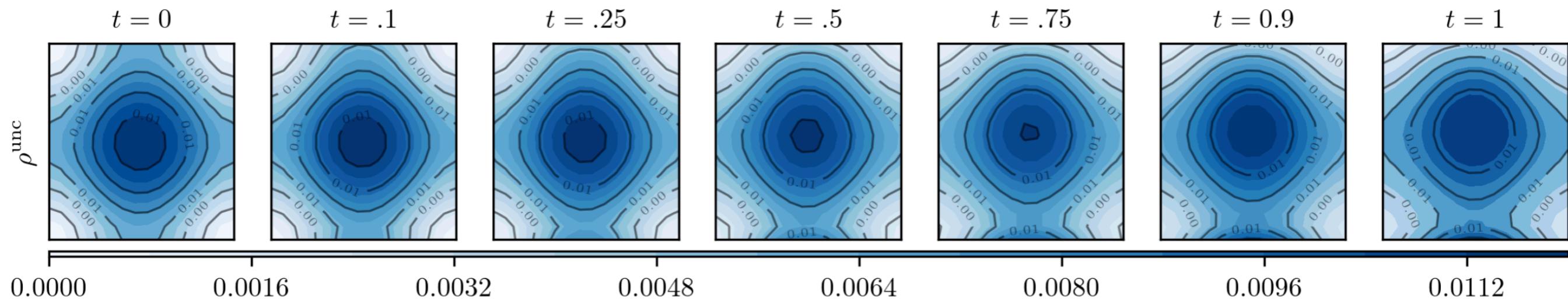
Reflected bridge: numerics with ∇V drift

$$V(x_1, x_2) = (x_1^2 + x_2^3)/5, \quad \overline{\mathcal{X}} = [-4, 4]^2$$

Optimal controlled state PDFs:



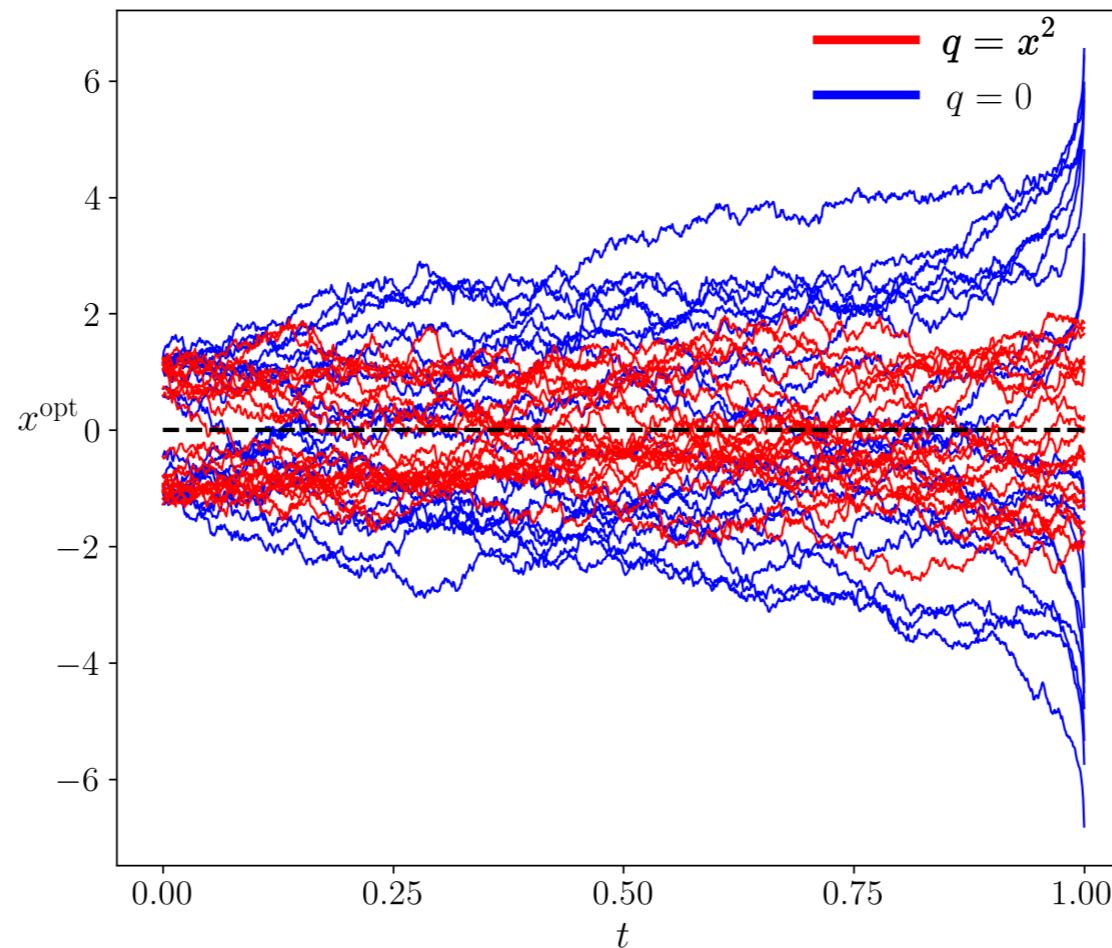
Uncontrolled state PDFs:



Generalization #3: additive state cost ($q \neq 0$)

Question. Where does state cost come from?

Answer 1. From extra regularization (e.g., classical LQ optimal control)



Answer 2. Problem reformulation (push dynamical nonlinearity to Lagrangian)

[Probabilistic Lambert Problem: Connections with Optimal Mass Transport, Schrödinger Bridge and Reaction-Diffusion PDEs*](#)

Alexis M.H. Teter[†], Iman Nodozi[‡], and Abhishek Halder[§]

A.M. Teter, I. Nodozi, and A.H.,
arXiv:2401.07961

Schrödinger bridge with quadratic state cost:

$$q(\boldsymbol{x}) = \boldsymbol{x}^\top Q \boldsymbol{x}, Q \succeq 0$$

Solution: $\rho^{\text{opt}}(\boldsymbol{x}, t) = \varphi(\boldsymbol{x}, t)\hat{\varphi}(\boldsymbol{x}, t)$

$$\left(\frac{\partial}{\partial t} + \frac{1}{2}\Delta - q \right) \varphi = 0 \quad [\text{Backward reaction-diffusion PDE}]$$

$$\left(\frac{\partial}{\partial t} - \frac{1}{2}\Delta + q \right) \hat{\varphi} = 0 \quad [\text{Forward reaction-diffusion PDE}]$$

Schrödinger bridge with quadratic state cost:

$$q(\mathbf{x}) = \mathbf{x}^\top Q \mathbf{x}, Q \succeq 0$$

We know: $\rho^{\text{opt}}(\mathbf{x}, t) = \varphi(\mathbf{x}, t)\hat{\varphi}(\mathbf{x}, t)$

$$\left(\frac{\partial}{\partial t} + \frac{1}{2}\Delta - q \right) \varphi = 0 \quad [\text{Backward reaction-diffusion PDE}]$$

$$\boxed{\left(\frac{\partial}{\partial t} - \frac{1}{2}\Delta + q \right) \hat{\varphi} = 0} \quad [\text{Forward reaction-diffusion PDE}]$$

Need kernel/Green's function $\kappa(0, \mathbf{x}; t, \mathbf{y})$

for IVP solutions to use in Schrödinger factor recursion:

$$\frac{\partial \hat{\varphi}}{\partial t} = \underbrace{\mathcal{L}_{\text{forward}}}_{(\Delta - \mathbf{x}^\top Q \mathbf{x})} \hat{\varphi}, \quad \hat{\varphi}(t=0, \mathbf{x}) = \hat{\varphi}_0 \quad \Leftrightarrow \quad \hat{\varphi}(\mathbf{x}, t) = \int_{\mathbb{R}^n} \boxed{\kappa(0, \mathbf{x}; t, z)} \hat{\varphi}_0(z) dz$$

Schrödinger bridge with quadratic state cost:

$$q(\mathbf{x}) = \mathbf{x}^\top Q \mathbf{x}, Q > 0$$

Thm. Eig. decomposition: $\mathbf{Q} = \mathbf{V} \mathbf{D} \mathbf{V}^\top$

Then, $\widehat{\varphi}(\mathbf{x}, t) = \eta(\mathbf{y} = \mathbf{V}\mathbf{x}, t)$ where $\eta(\mathbf{y}, t) = \int_{\mathbb{R}^n} \kappa(0, \mathbf{y}; t, z) \eta_0(z) dz$

and

$$\kappa(0, \mathbf{y}; t, z) = \frac{(\det(\mathbf{D}))^{1/4}}{\sqrt{(2\pi)^n \det(\sinh(2t\sqrt{\mathbf{D}}))}} \exp\left(-\frac{1}{2}(\mathbf{y} - z)\mathbf{M}\begin{pmatrix} \mathbf{y} \\ z \end{pmatrix}\right)$$

$$\mathbf{M} := \begin{bmatrix} \mathbf{D}^{1/4} & \mathbf{0}_{n \times n} \\ \mathbf{0}_{n \times n} & \mathbf{D}^{1/4} \end{bmatrix} \mathbf{M}_1 \mathbf{M}_2 \begin{bmatrix} \mathbf{D}^{1/4} & \mathbf{0}_{n \times n} \\ \mathbf{0}_{n \times n} & \mathbf{D}^{1/4} \end{bmatrix}, \quad \mathbf{M}_1 := \begin{bmatrix} \cosh(2t\sqrt{\mathbf{D}}) & -\mathbf{I}_n \\ -\mathbf{I}_n & \cosh(2t\sqrt{\mathbf{D}}) \end{bmatrix}, \quad \mathbf{M}_2 := \begin{bmatrix} \operatorname{csch}(2t\sqrt{\mathbf{D}}) & \mathbf{0} \\ \mathbf{0} & \operatorname{csch}(2t\sqrt{\mathbf{D}}) \end{bmatrix}$$

$$\eta_0(\mathbf{y}) = \widehat{\varphi}_0(\mathbf{V}^\top \mathbf{x})$$

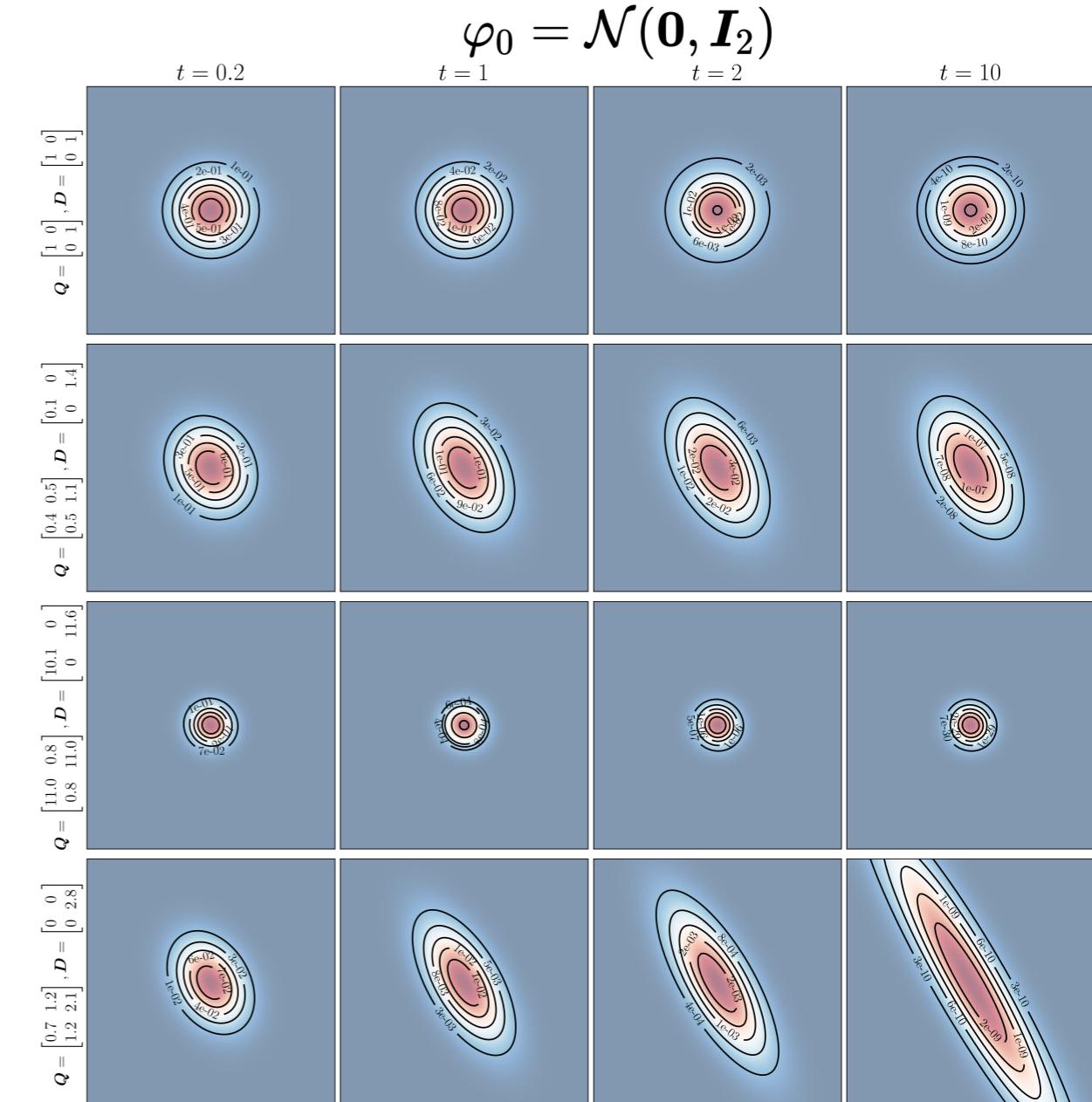
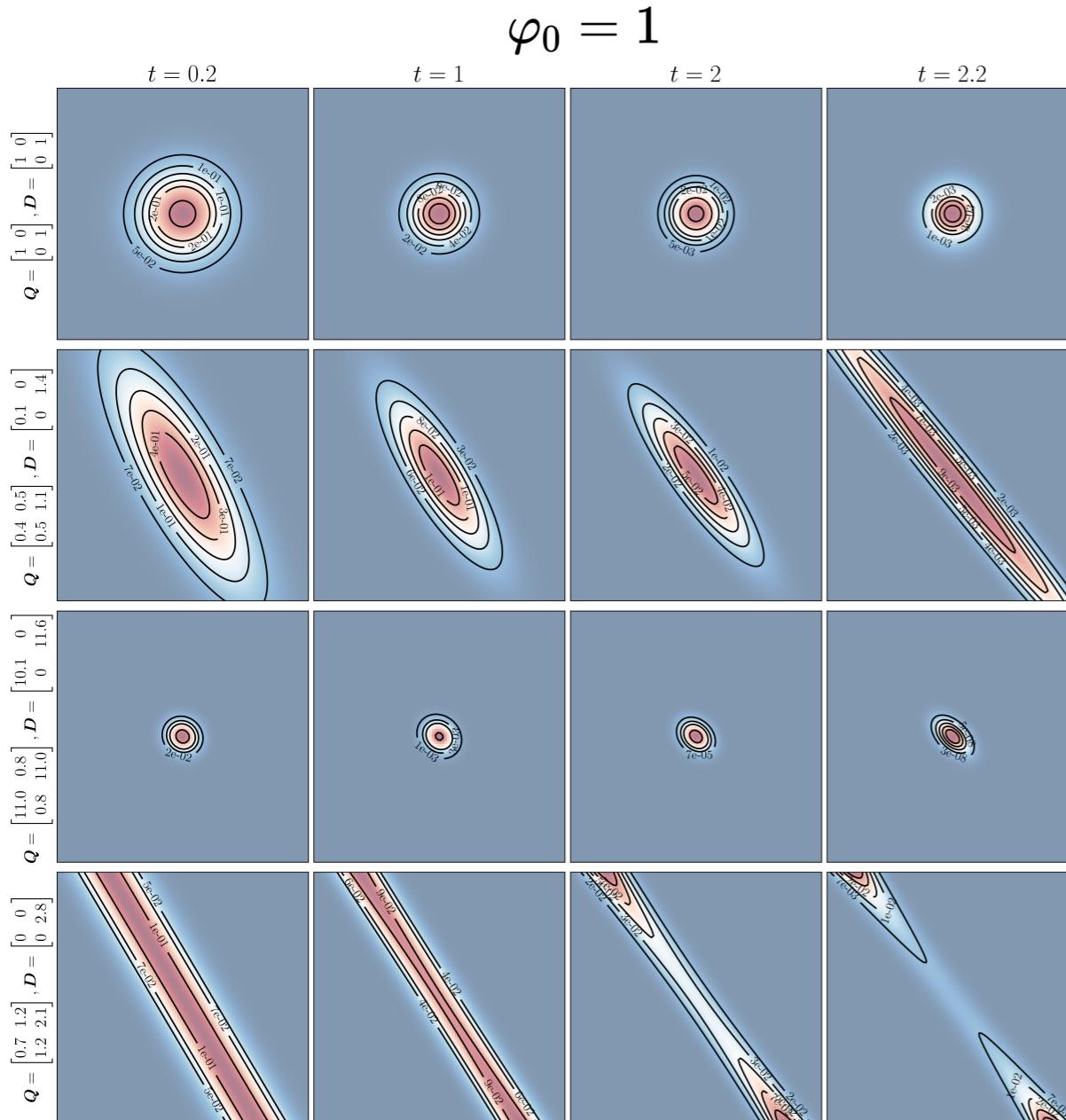
$\mathbf{Q} = \mathbf{I}$ recovers the multivariate Mehler kernel in quantum harmonic oscillator

Schrödinger bridge with quadratic state cost:

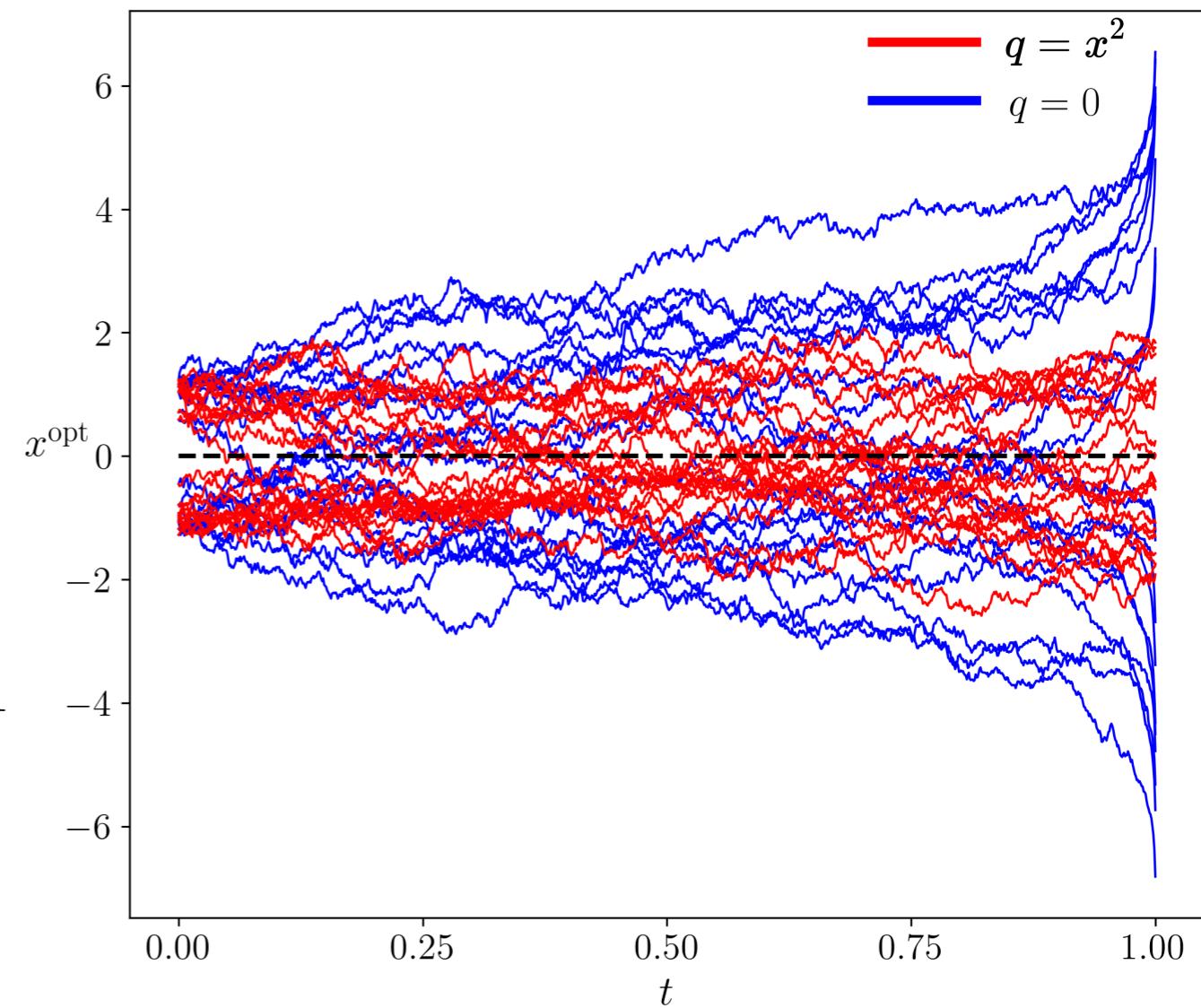
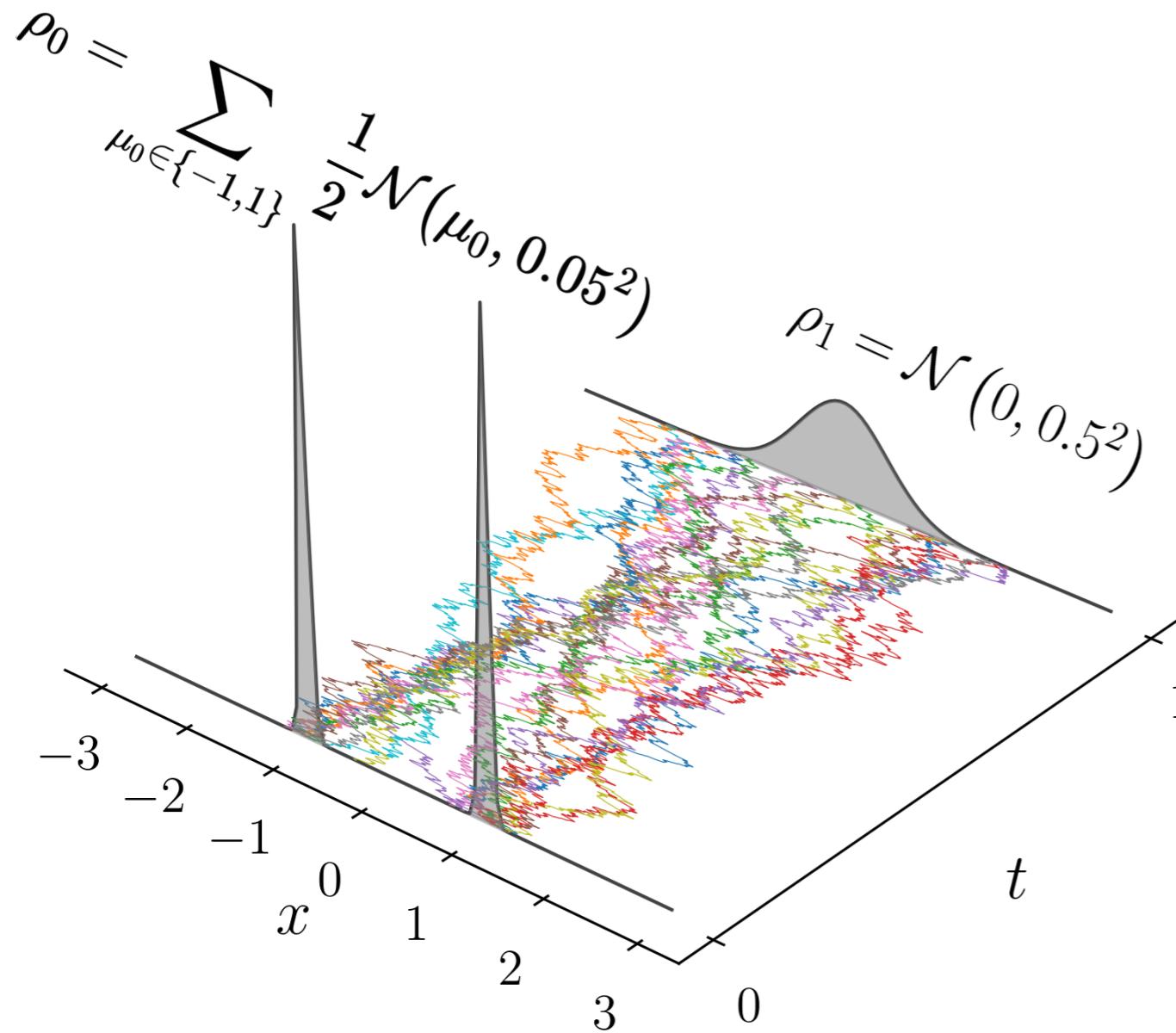
$$q(x) = x^\top Q x, Q \succeq 0$$

Thm. $\kappa(0, \mathbf{y}; t, \mathbf{z}) = \underbrace{\kappa_+(0, \mathbf{y}_{[i_1:i_{n-p}]}; t, \mathbf{z}_{[i_1:i_{n-p}]})}_{\text{derived pos def kernel in } n-p \text{ variables}} + \underbrace{\kappa_0(0, \mathbf{y}_{[i_{n-p+1}:i_n]}; t, \mathbf{z}_{[i_{n-p+1}:i_n]})}_{\text{heat kernel in } p \text{ variables}}$

Action of kernel in x coordinates



Schrödinger bridge in 1D: with vs without quadratic state cost



A.M. Teter, W. Wang, and A.H.,
arXiv:2406.00503

Outlook

- Theory and applications of Schrödinger bridge are undergoing rapid developments
- Lots of mathematics, algorithms, and applications to be done
- Growing interdisciplinary community
- Strong intersections with many areas: control, statistics, scientific computing, differential geometry, analysis, AI/ML, information theory, robotics, biology

Thank You

Support:



CITRIS
PEOPLE AND
ROBOTS

