

Generalized Schrödinger Bridges

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Joint work with students and collaborators



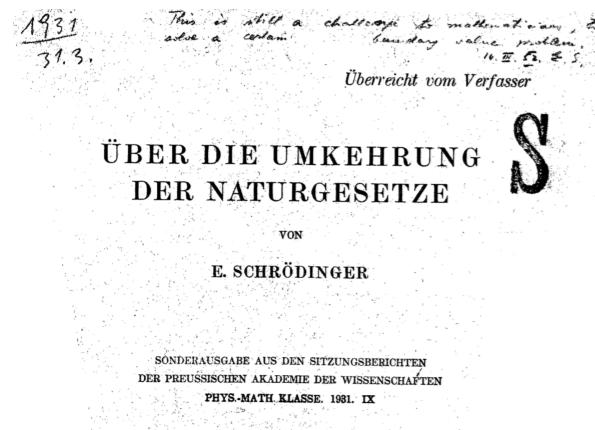
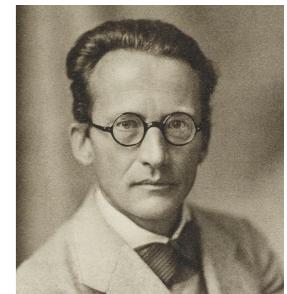
Level Set Seminar, Department of Mathematics, University of California Los Angeles

May 13, 2024



What is a Schrödinger bridge

Prior physics = Brownian motion



[1931]

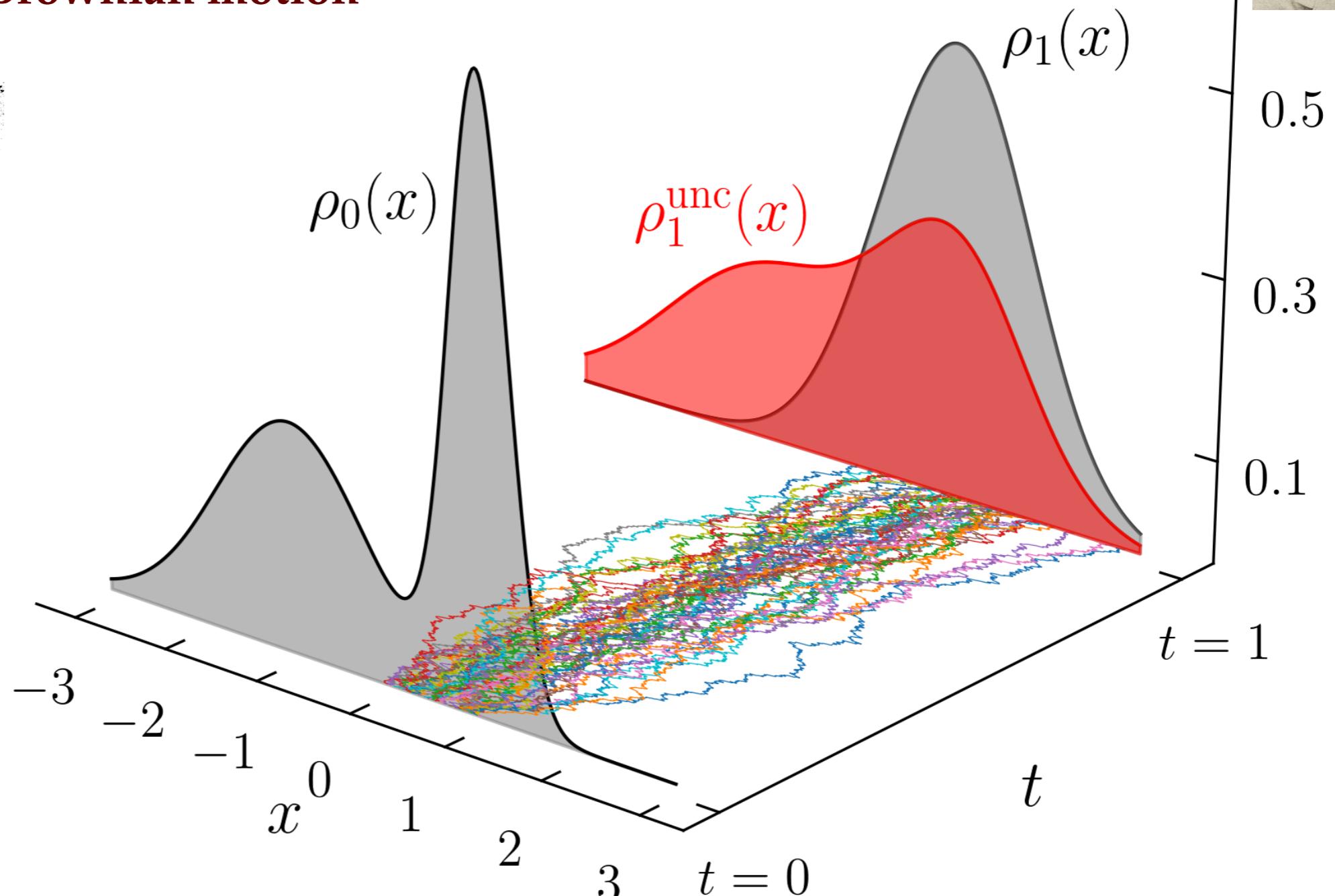
Sur la théorie relativiste de l'électron
et l'interprétation de la mécanique quantique

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]

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

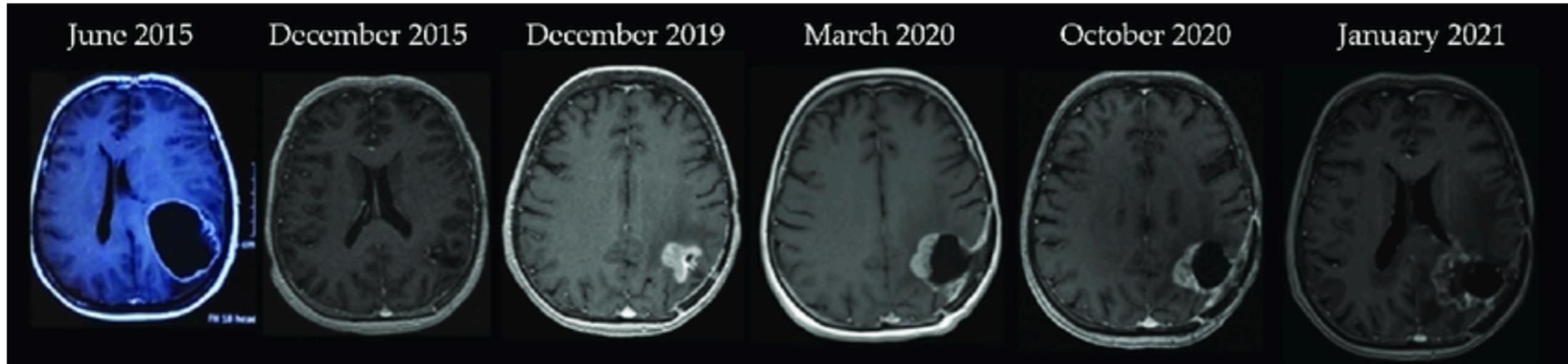
subject to

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

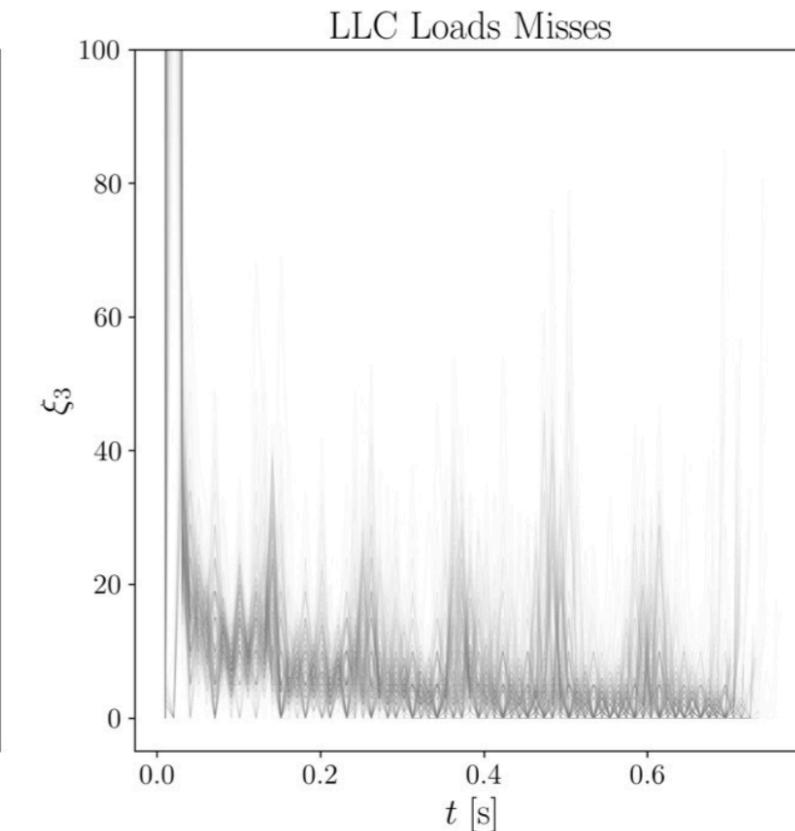
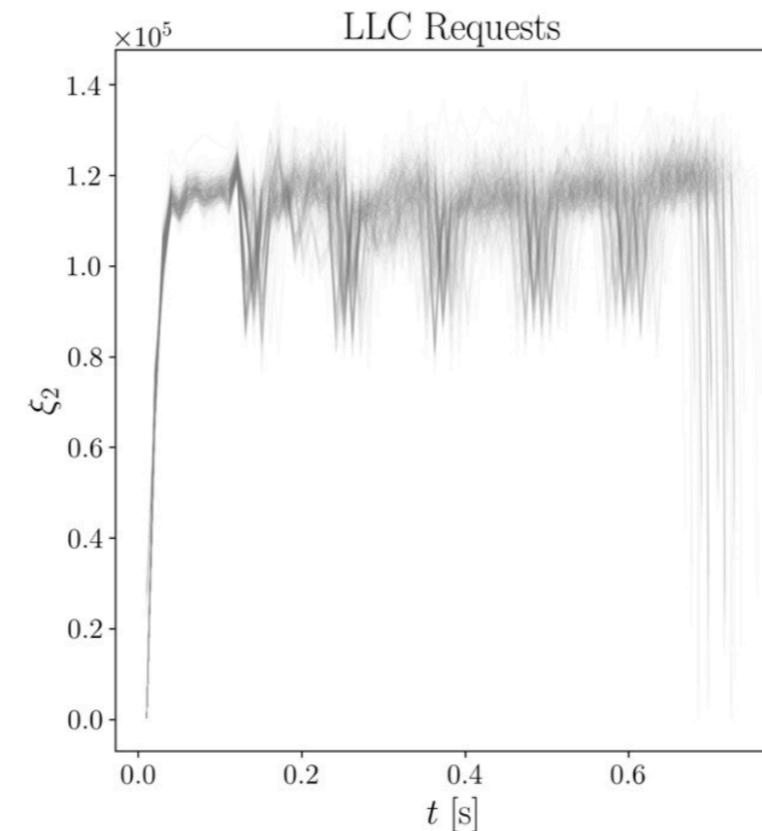
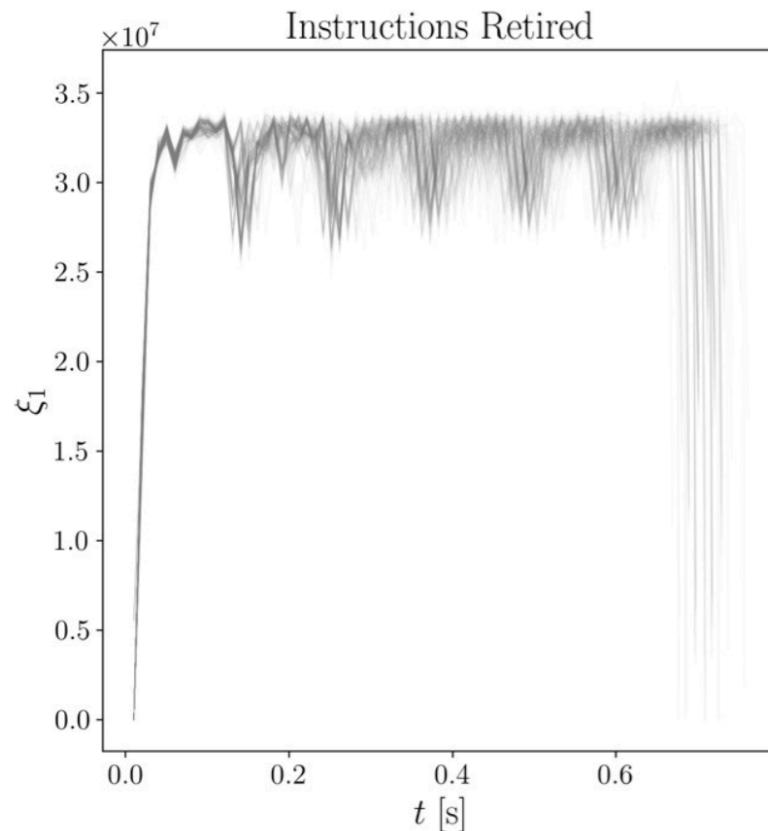
$$\mathbf{x}_t^u(t = t_0) \sim \rho_0, \quad \mathbf{x}_t^u(t = t_1) \sim \rho_1$$

Resurgence of Schrödinger bridge in ML/AI

Learn most likely progression of medical condition



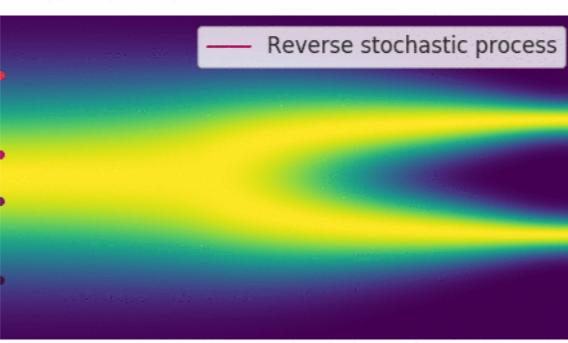
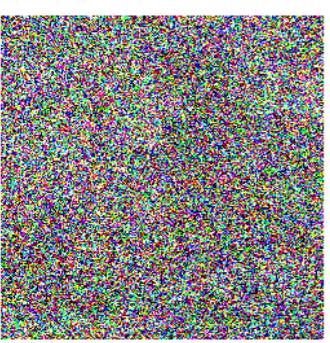
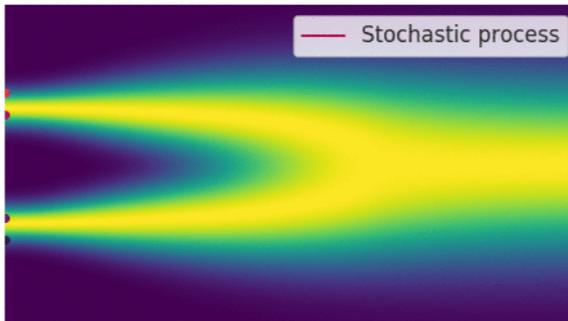
Learn joint stochastic time-varying hardware resource availability



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

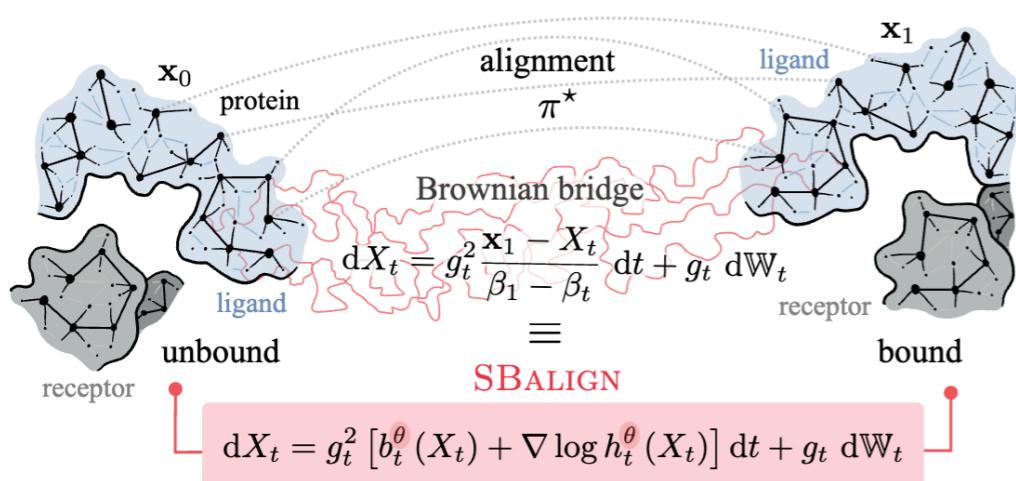
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Ya-Ping Hsieh¹
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NeurIPS 2021

Diffusion Schrödinger Bridge with Applications to Score-Based Generative Modeling

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Department of Statistics,
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James Thornton
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University of Oxford, UK

Jeremy Heng
ESSEC Business School,
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Arnaud Doucet
Department of Statistics,
University of Oxford, UK

NeurIPS 2024

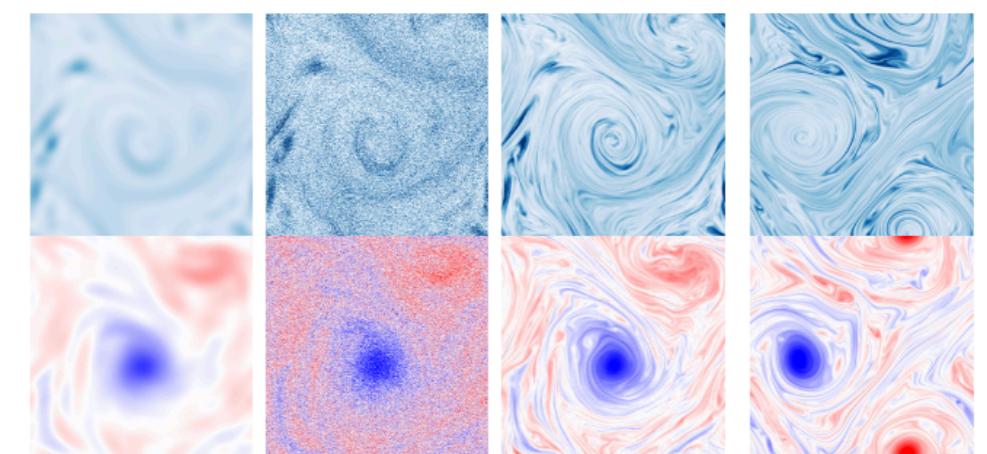
Diffusion Schrödinger Bridge Matching

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

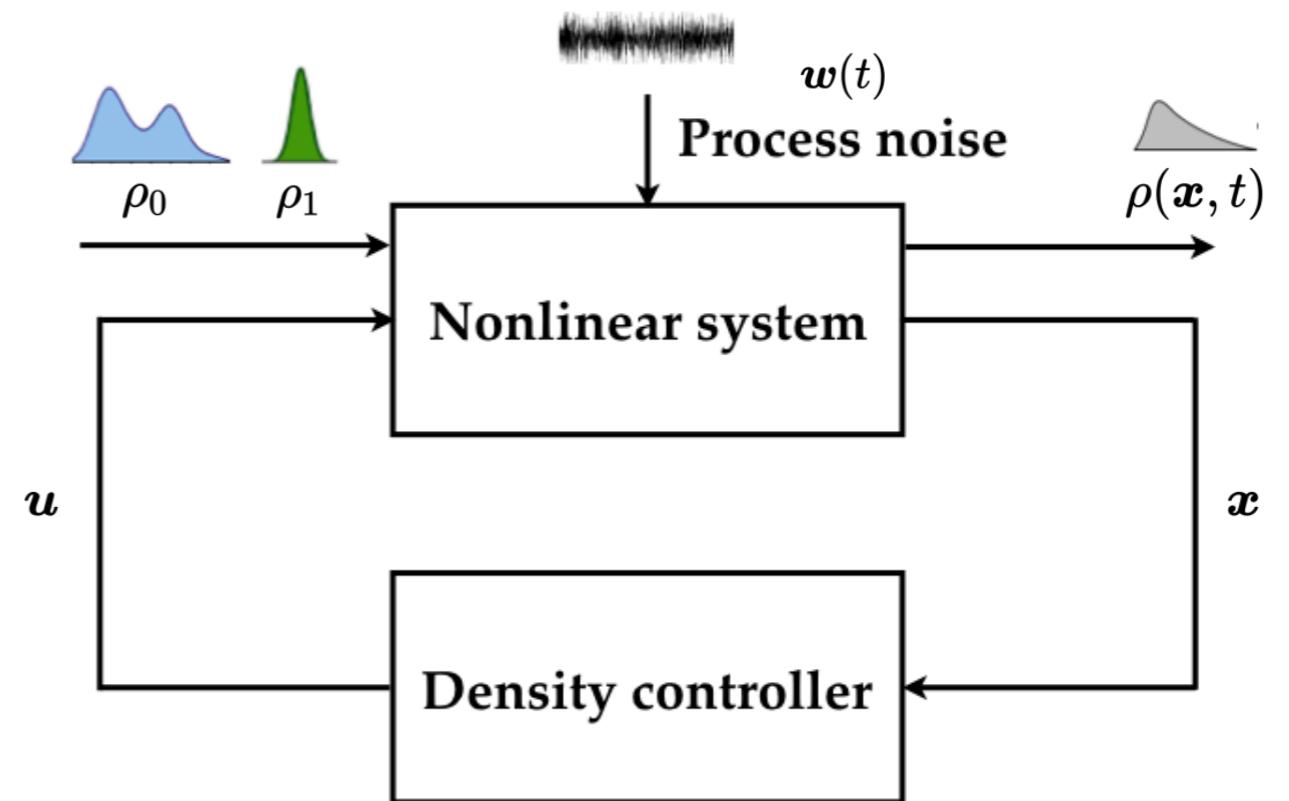
1. general controlled dynamics

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

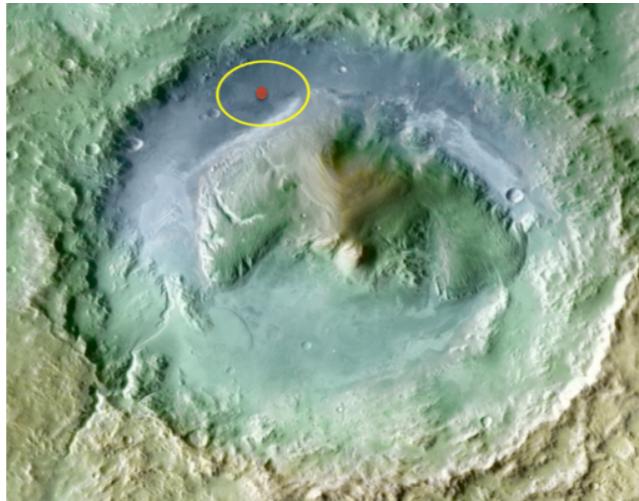
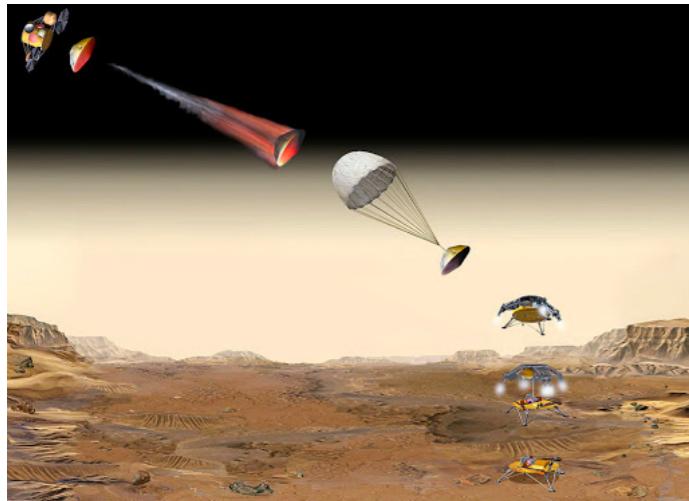
$$dx_t^u = \{f(t, x_t^u) + B(t, x_t^u)u\}dt + \sqrt{2}G(t, x_t^u)dw_t$$

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

Motivating applications

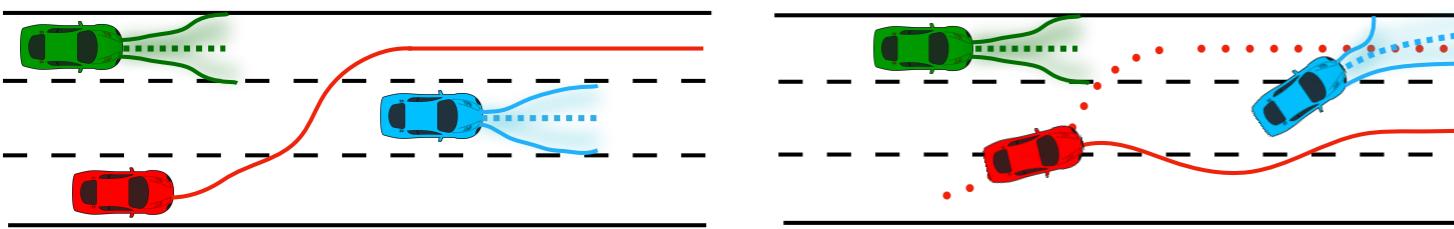
Distribution ~ Probability

Spacecraft landing with desired statistical accuracy



Gale Crater (4.49S, 137.42E)

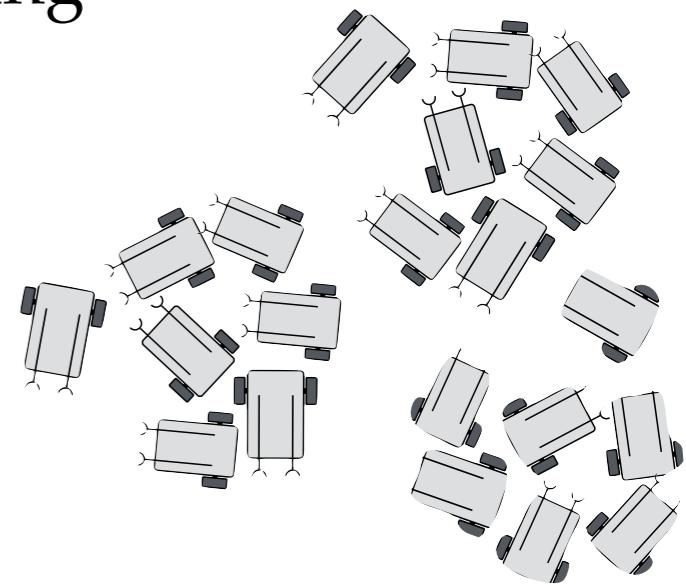
Risk management for automated driving in multi-lane highways



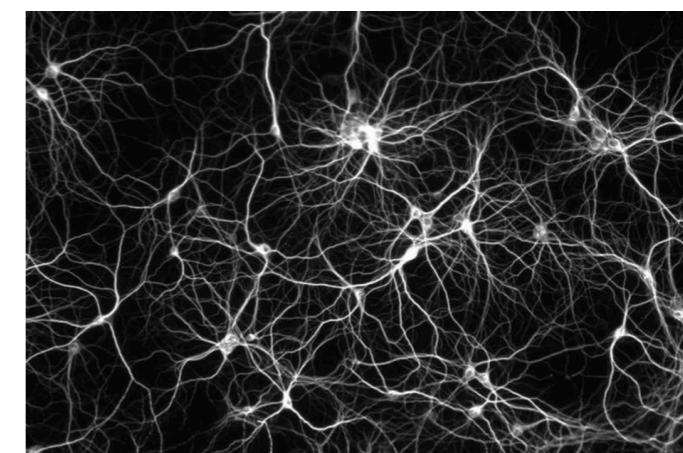
Control of uncertainties

Distribution ~ Population

Dynamic shaping of swarms



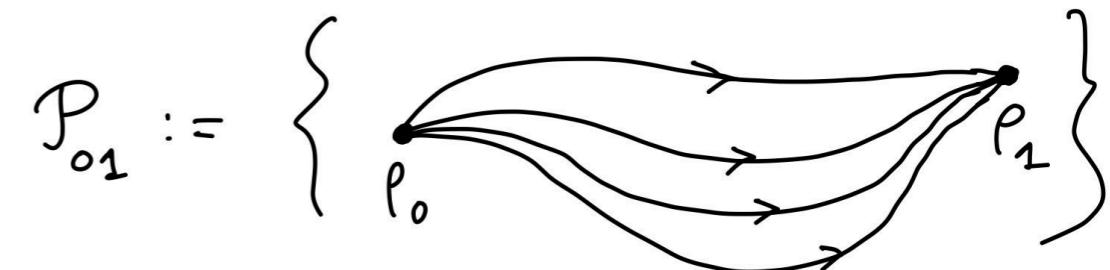
Feedback sync. and desync. of neuronal population



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

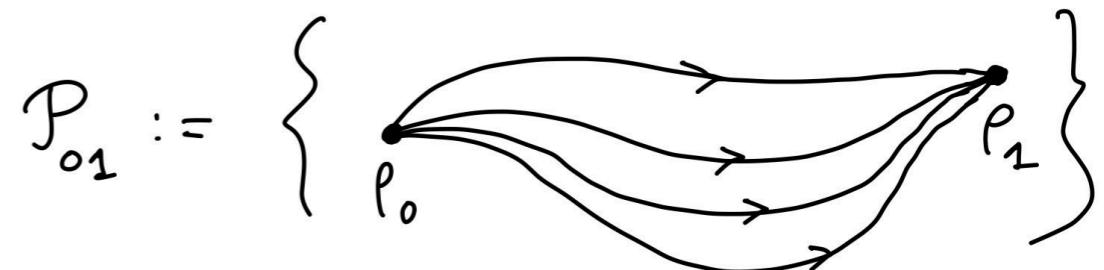
$$\frac{\partial \rho}{\partial t} + \nabla \cdot ((\mathbf{f} + \mathbf{B}\mathbf{u})\rho) = \Delta_D \rho$$

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

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

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

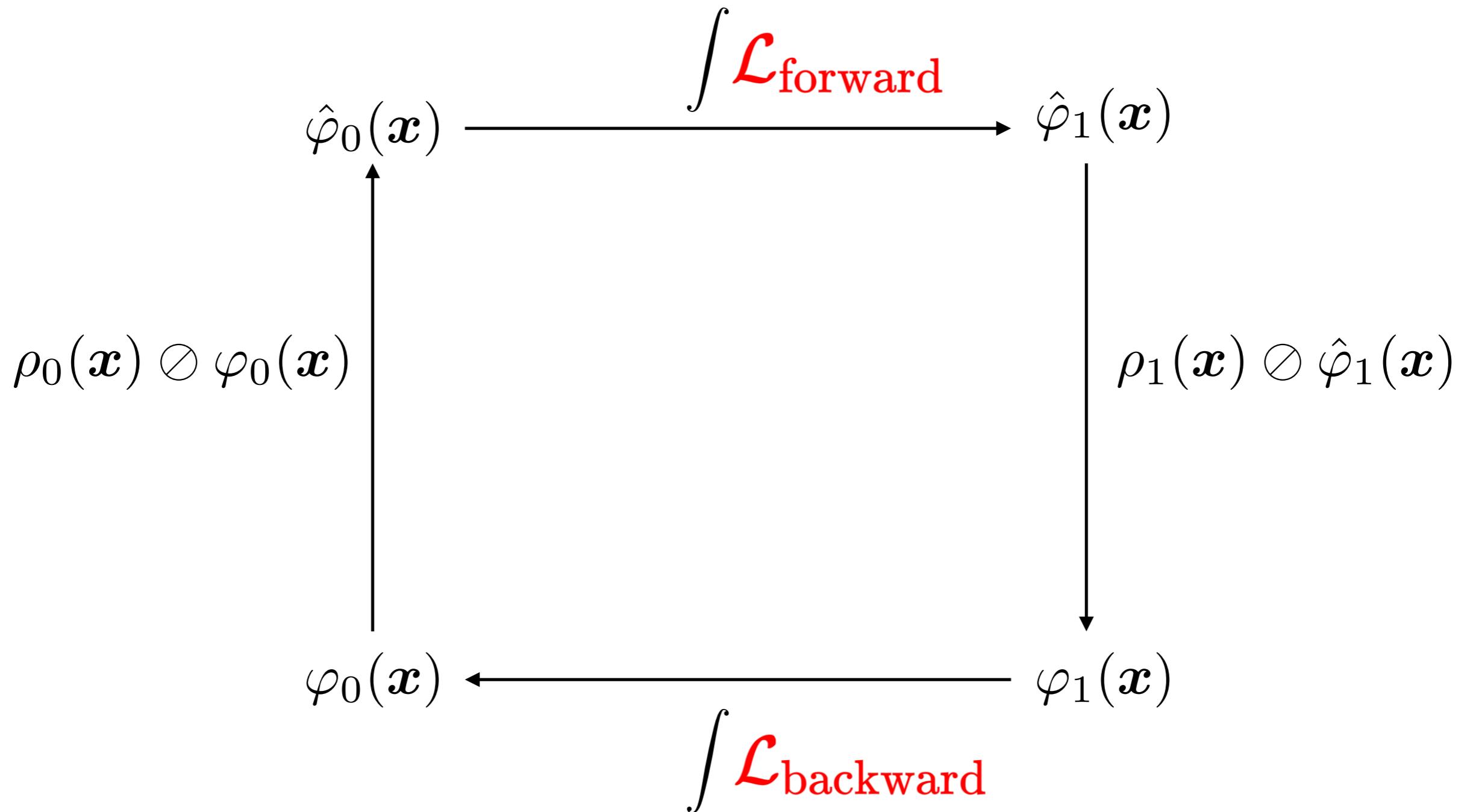
$$\left(\frac{\partial}{\partial t} - \frac{1}{2}\Delta + q \right) \hat{\varphi} = 0 \quad [\text{Forward reaction-diffusion PDE}]$$

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

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

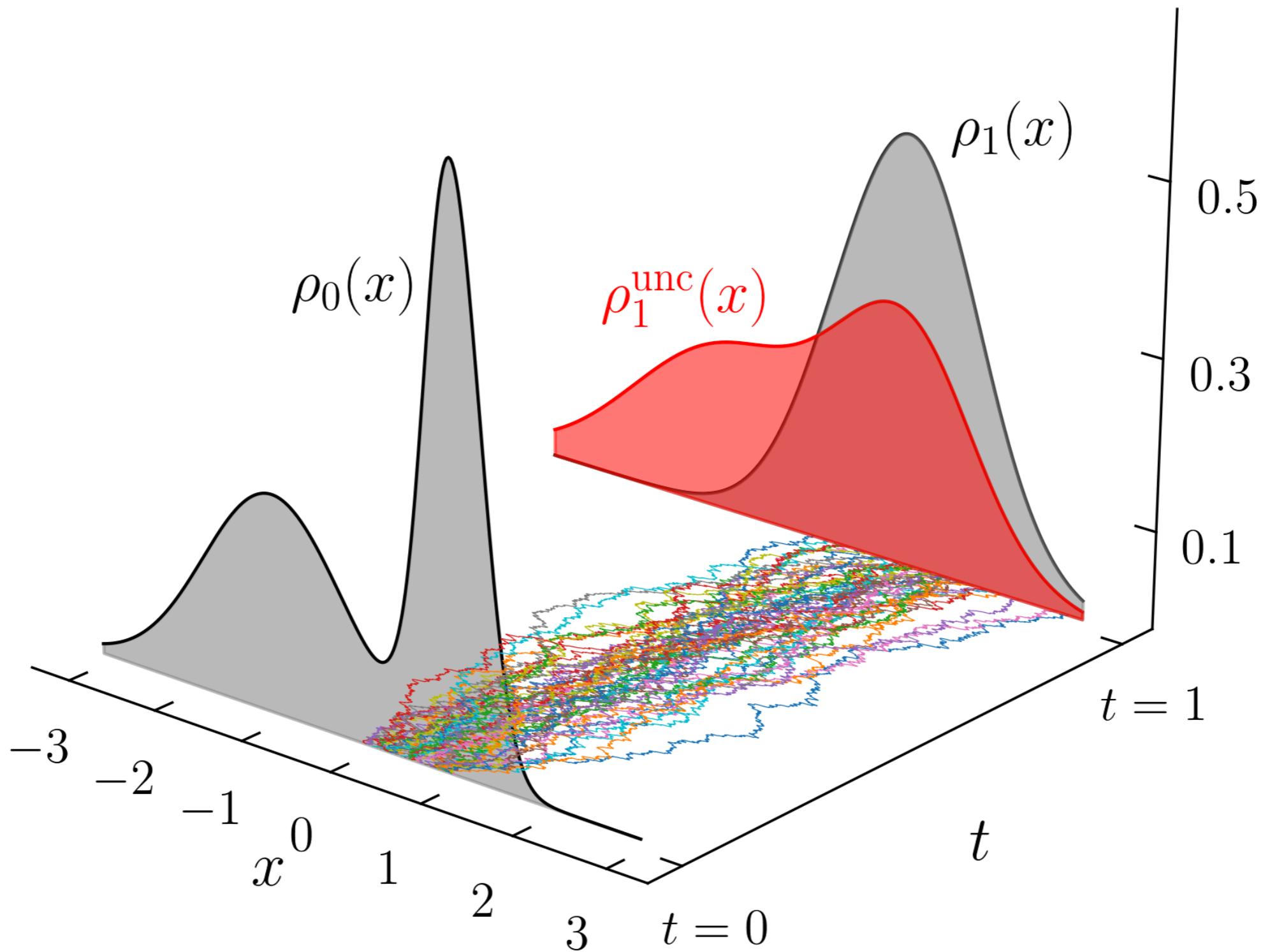
$$\left(-\sqrt{-1}\frac{\partial}{\partial t} - \frac{1}{2}\Delta + q \right) \widehat{\Psi} = 0 \quad [\text{Adjoint Schrödinger PDE}]$$

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



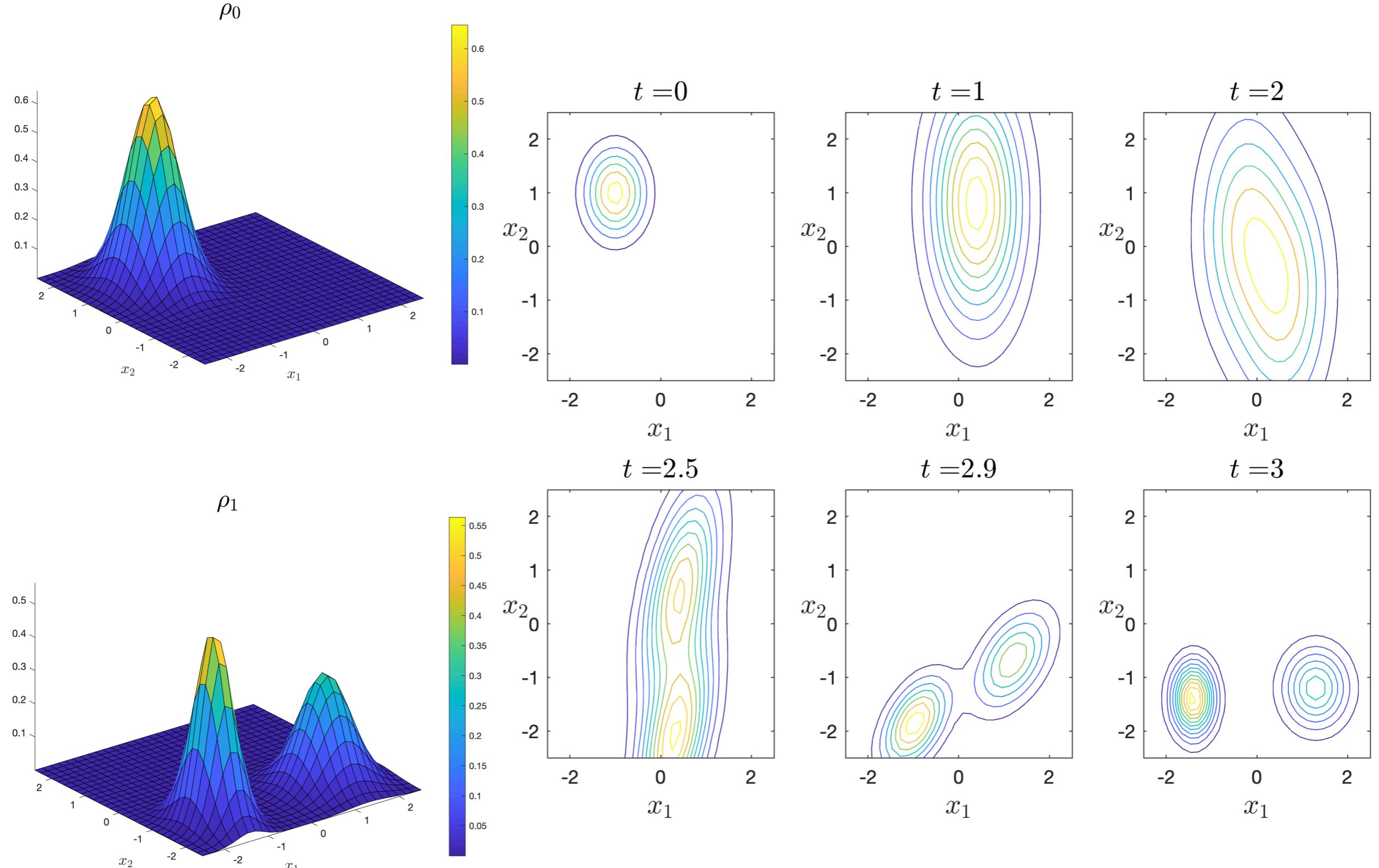
This recursion is contractive in the Hilbert's projective metric!!

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



Zero prior dynamics

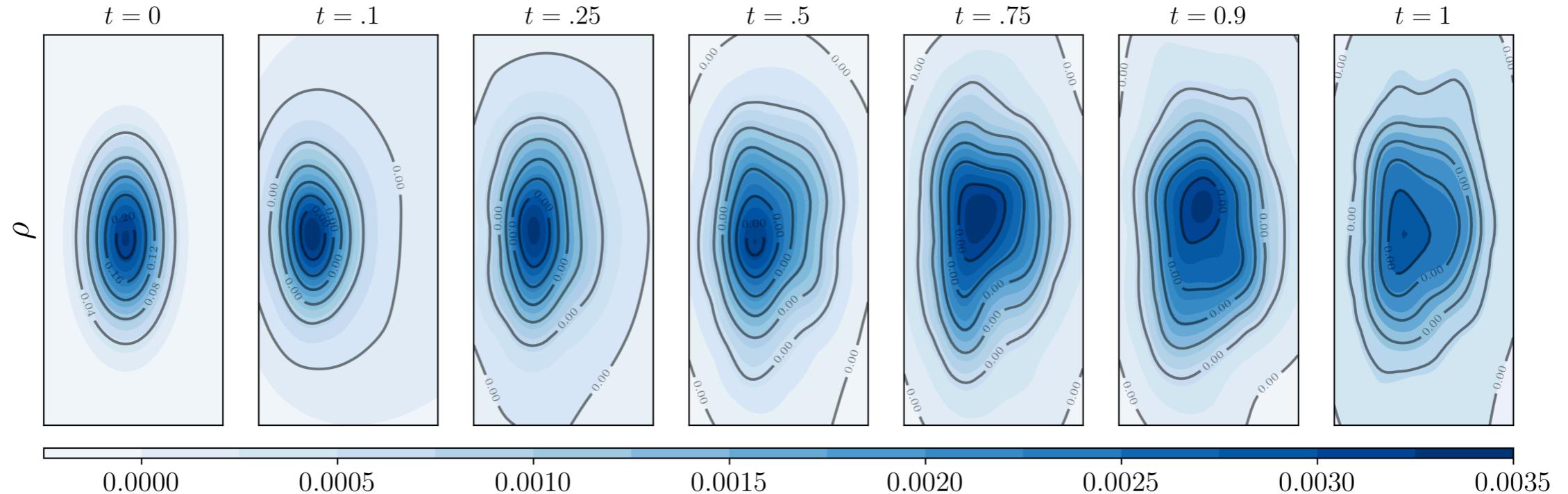
Feedback Density Control: $f \equiv Ax, B = G, q \equiv 0$



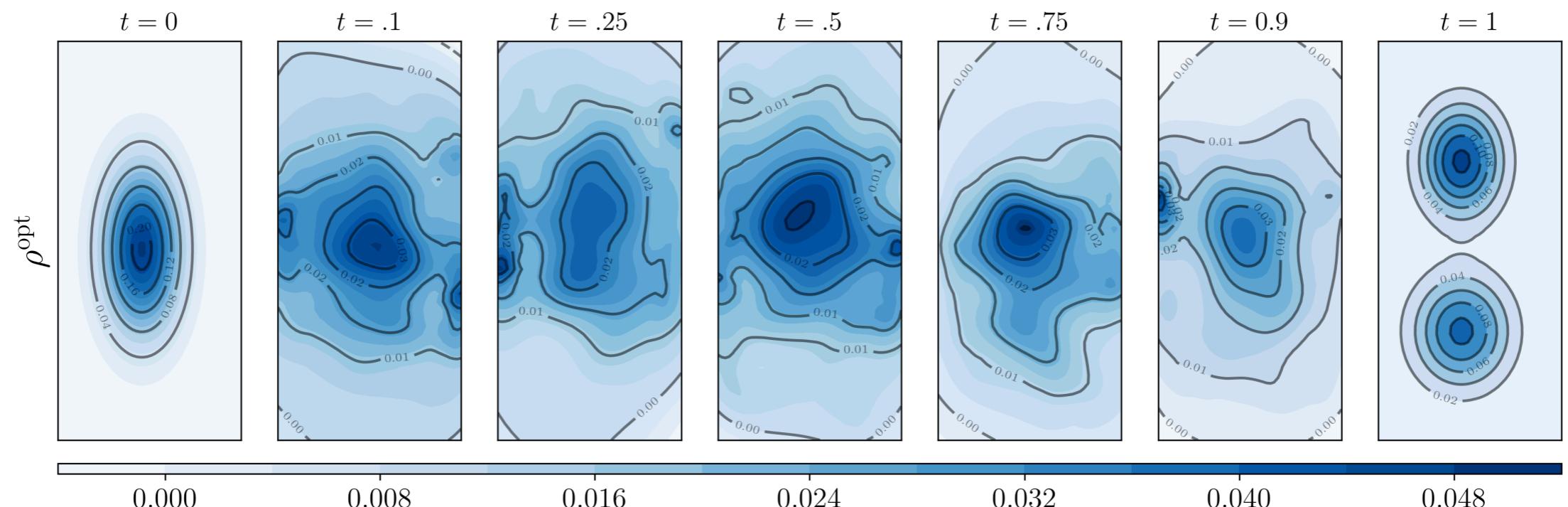
Linear prior dynamics

Feedback Density Control: Nonlinear Grad. Drift

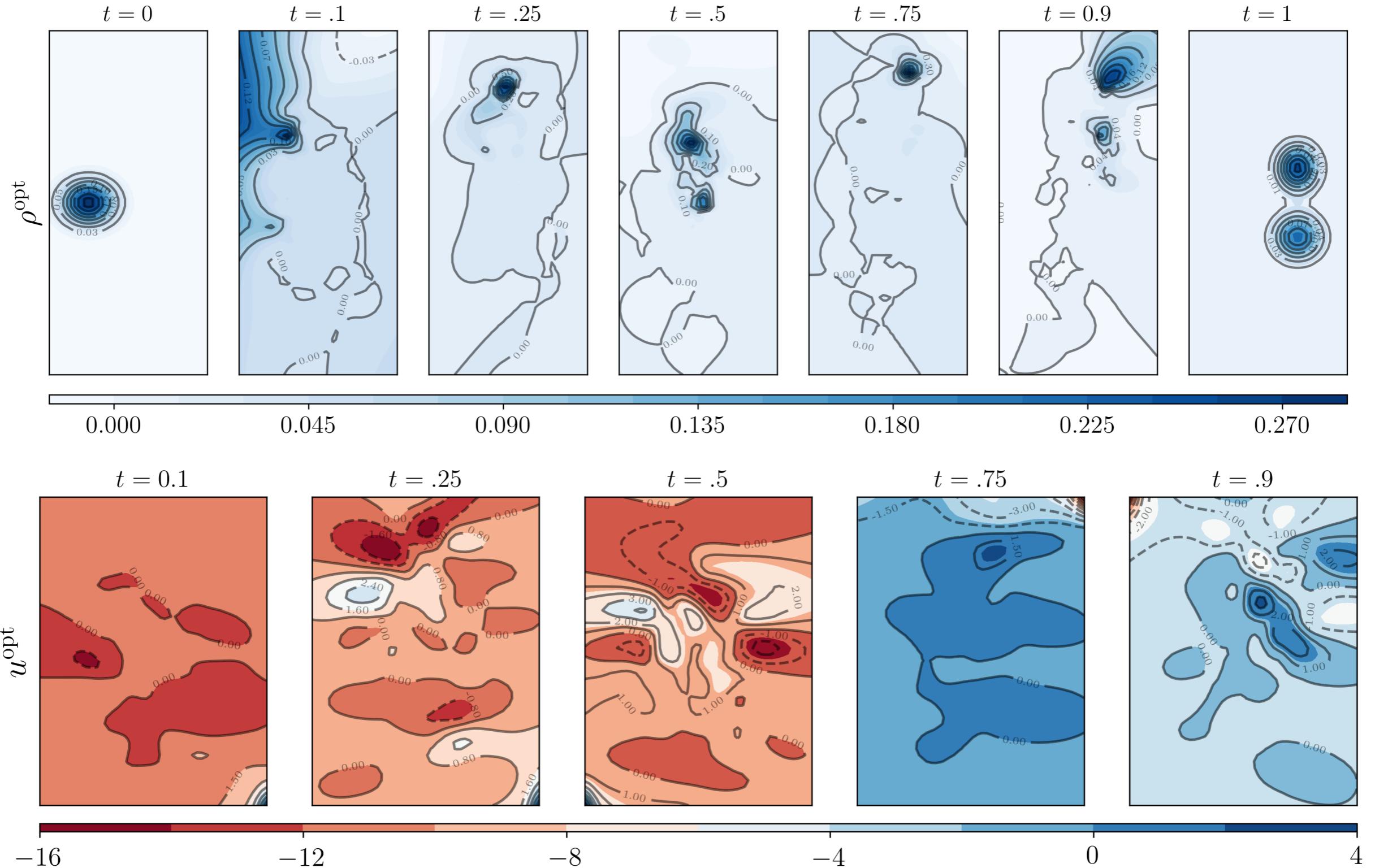
Uncontrolled joint PDF evolution:



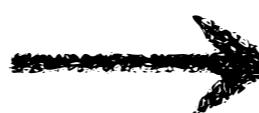
Optimal controlled joint PDF evolution:



Feedback Density Control: Mixed Conservative-Dissipative Drift



Application: Multi-lane Automated Driving

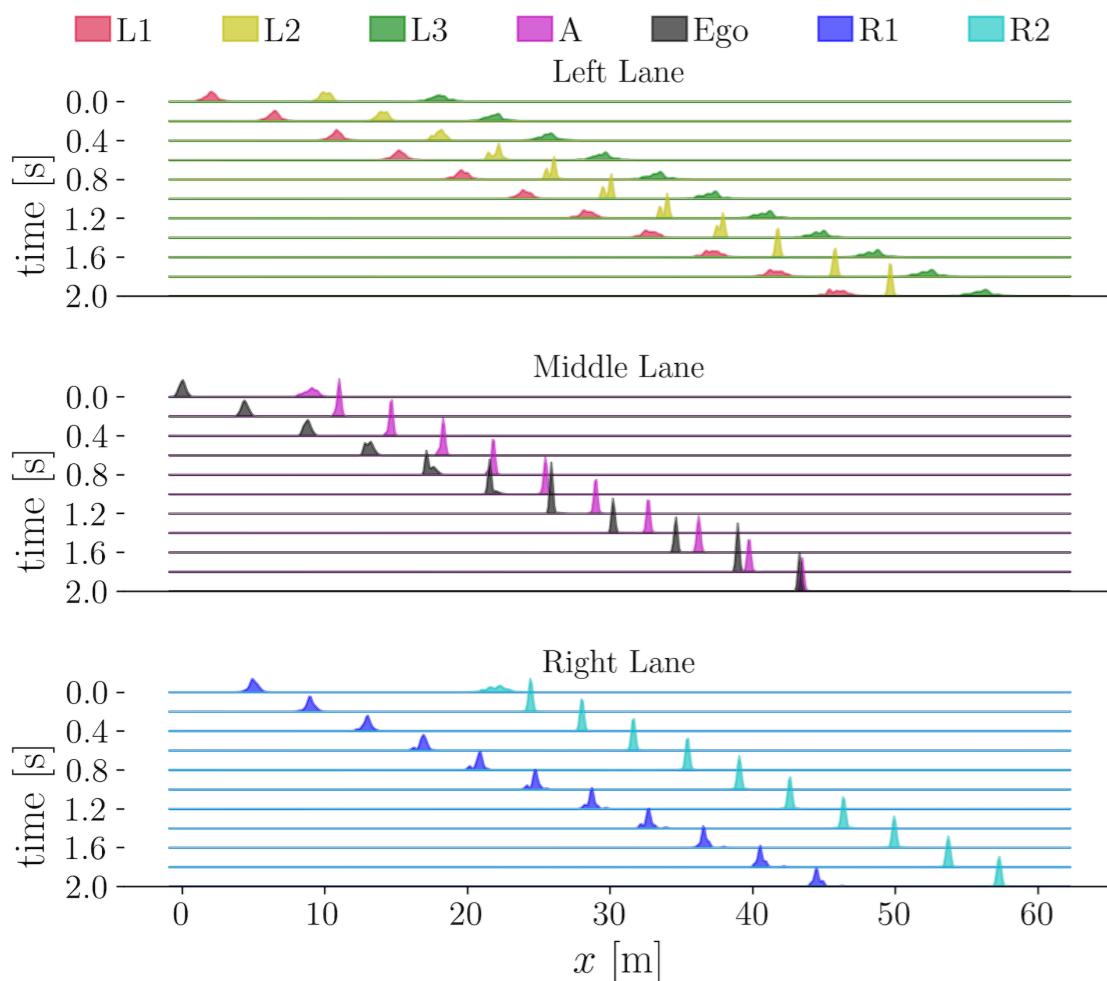


t_0

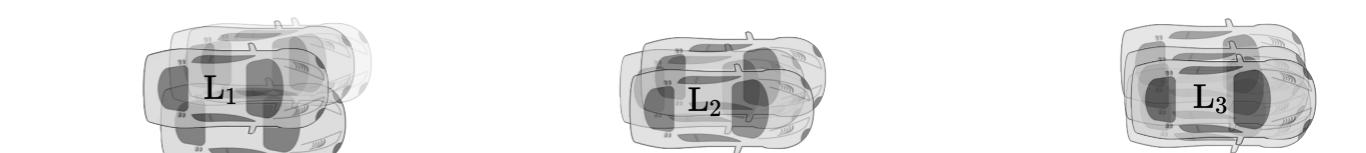
t_1

x marginals

y marginals

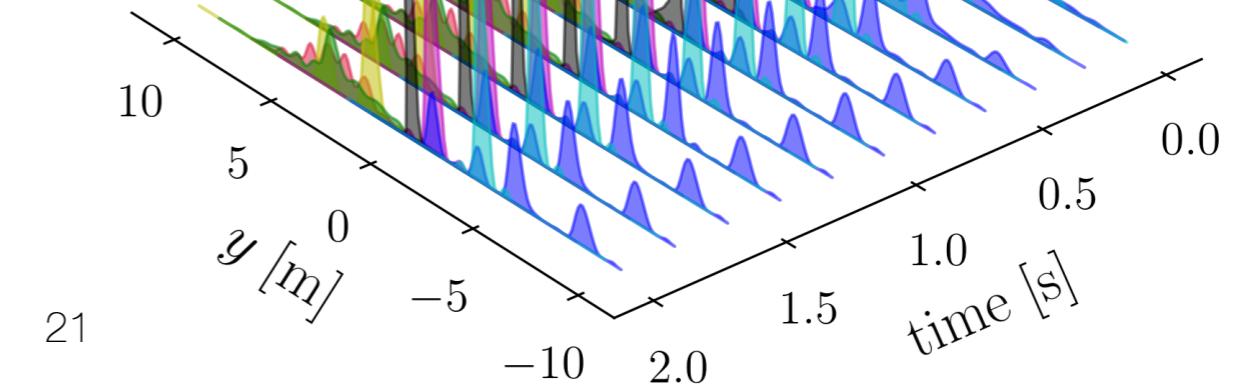


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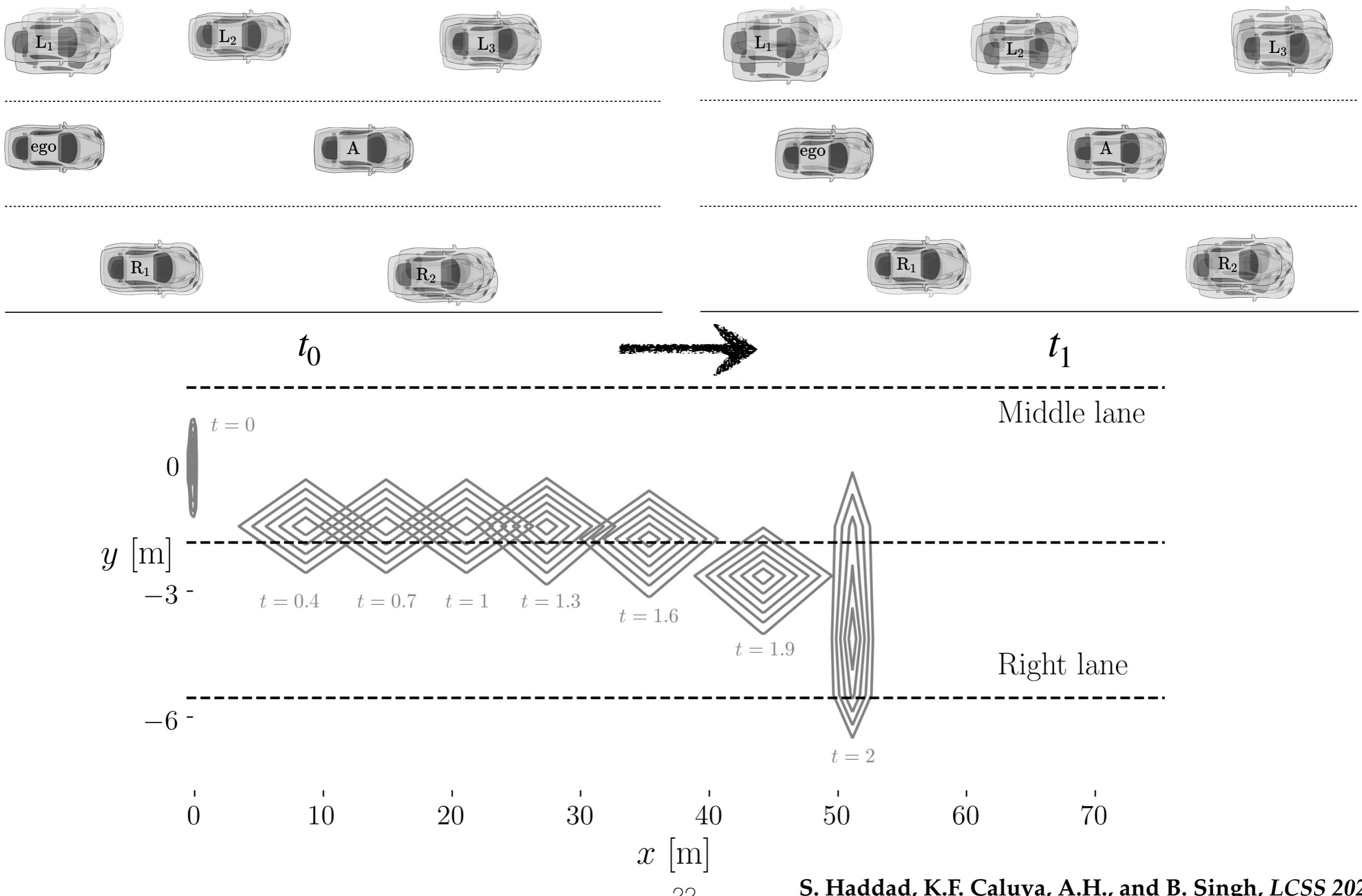


t_0

t_1



Application: Multi-lane Automated Driving

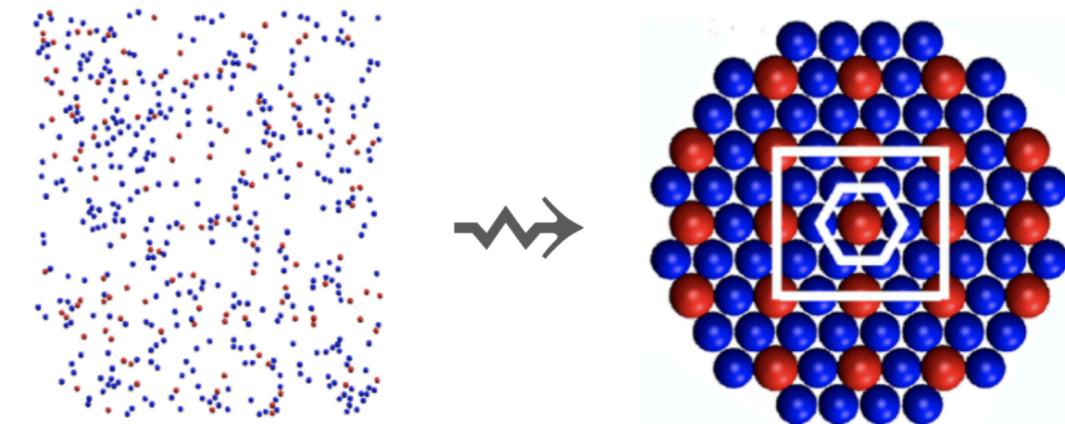


Control non-affine generalized Schrödinger bridge

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

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

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

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

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

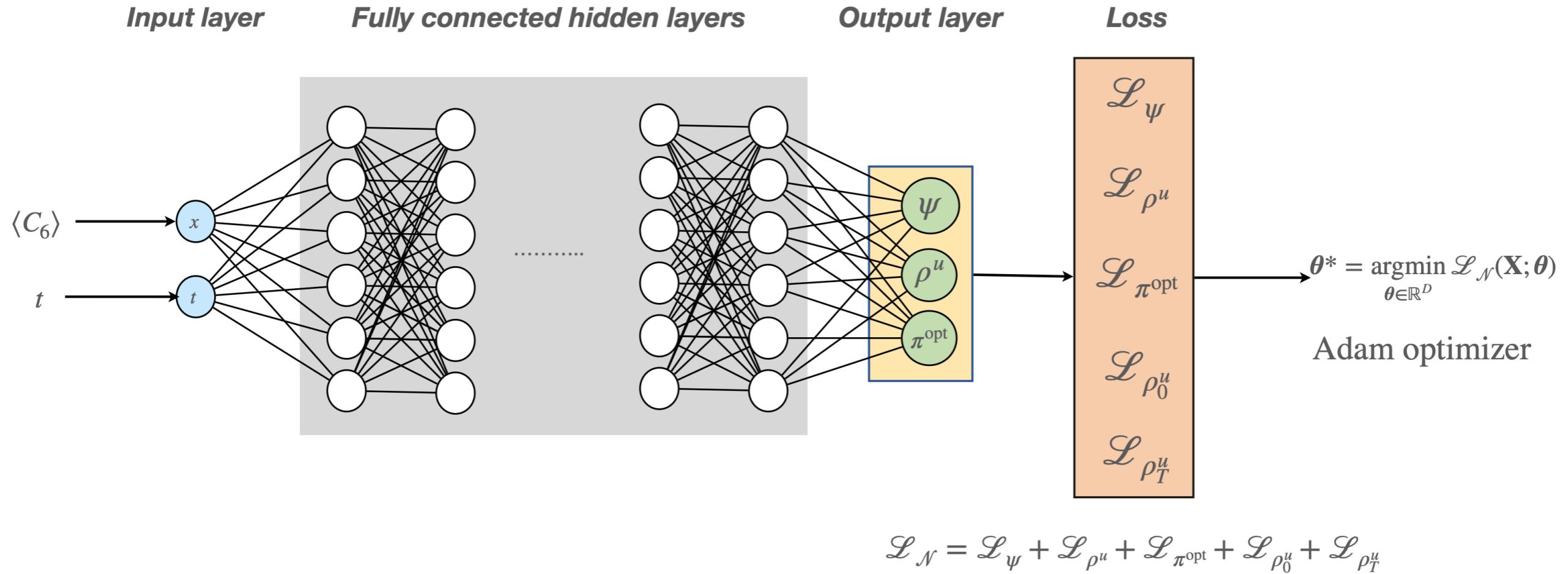
Known f, g

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

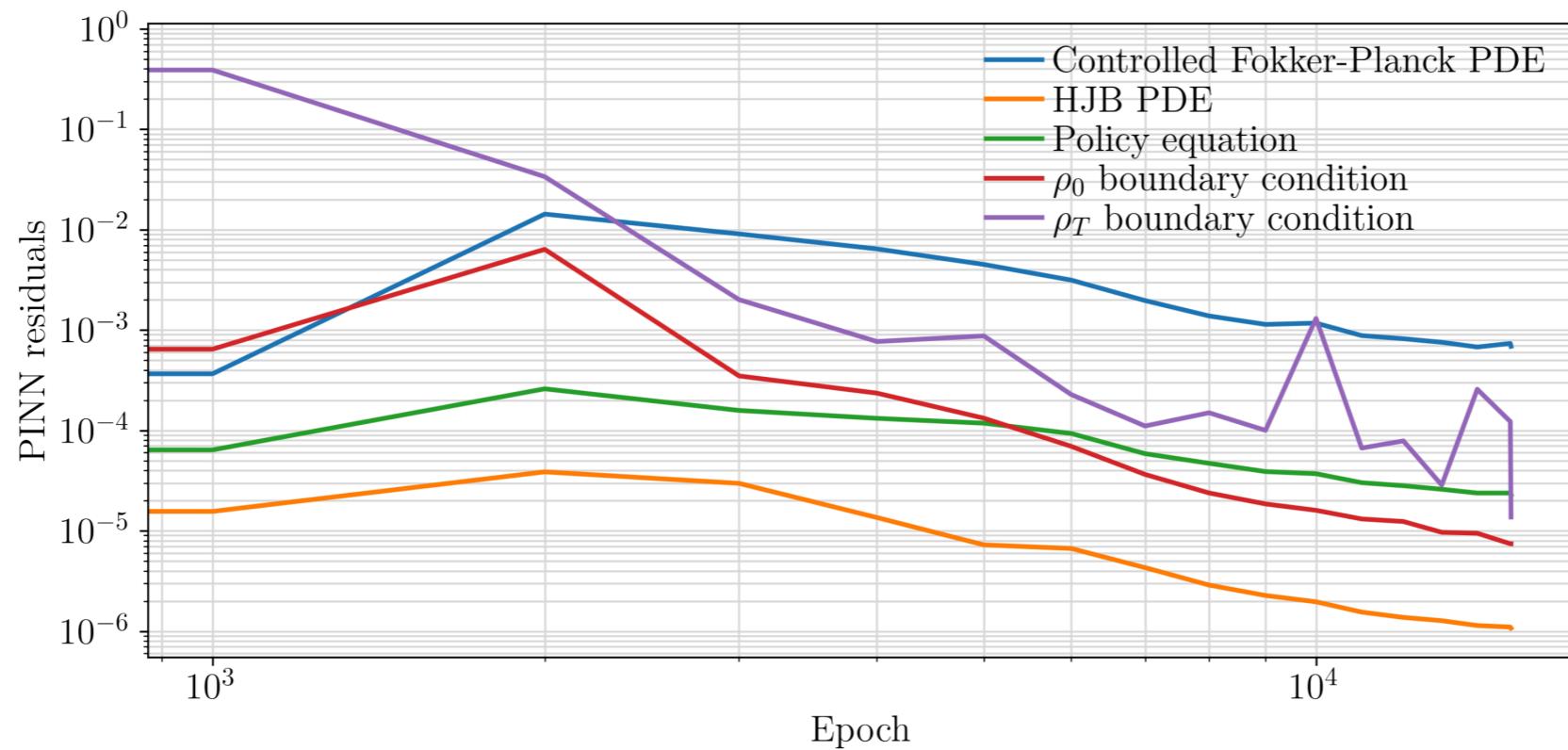
Data-driven f, g

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

Control non-affine generalized Schrödinger bridge



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

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

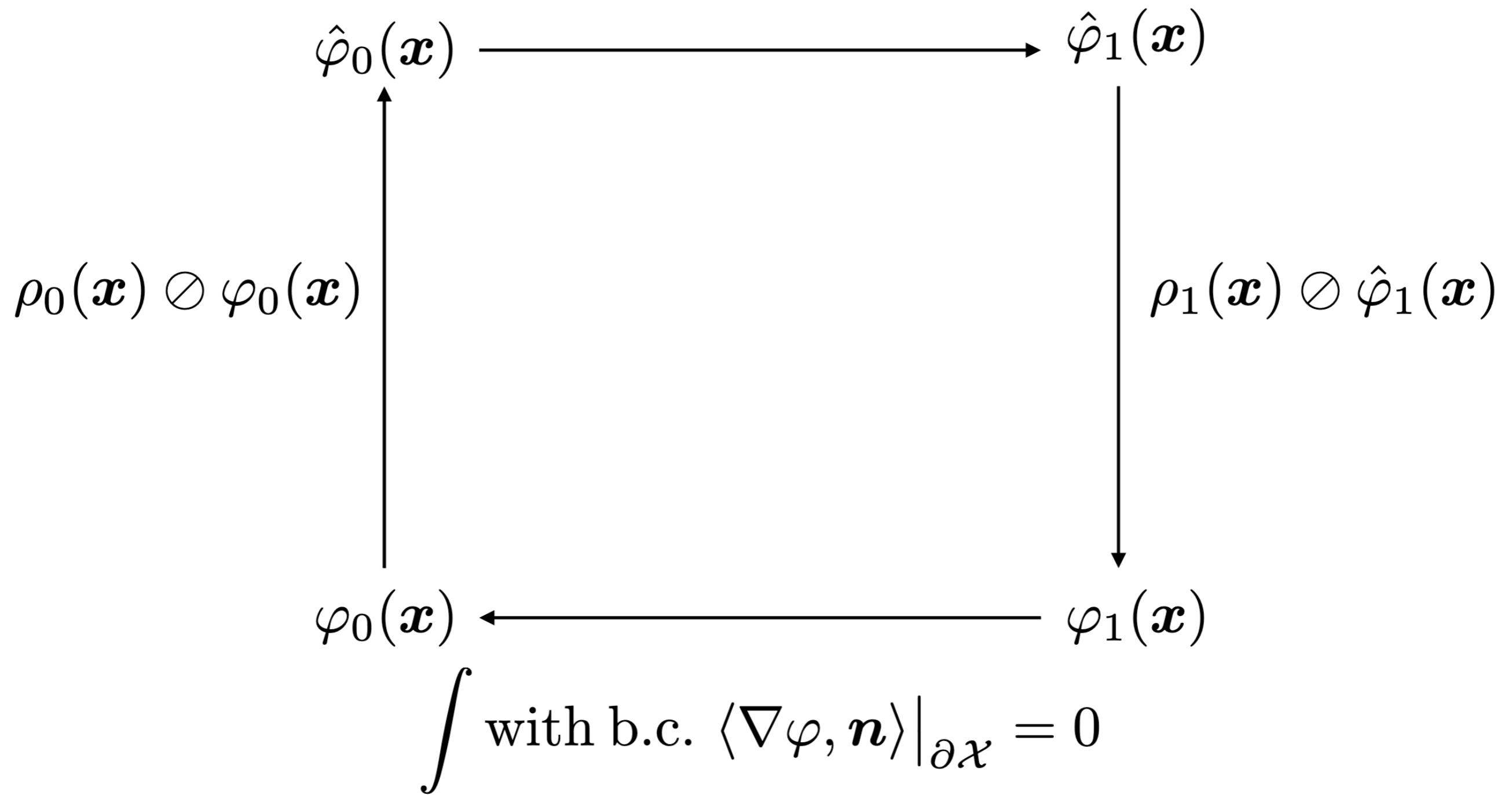
$x_t^u \in \overline{\mathcal{X}} := \mathcal{X} \cup \partial\mathcal{X}$, closure of connected smooth \mathcal{X}

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

γ_t is minimal local time stochastic process

Reflected bridge: Schrödinger factor recursion

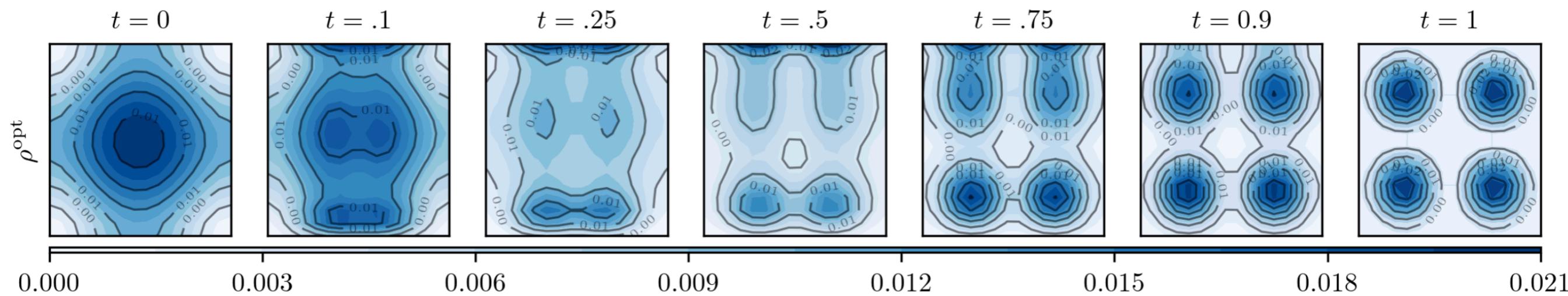
$$\int \text{with b.c. } \langle f\hat{\varphi} - \theta\nabla\hat{\varphi}, \mathbf{n} \rangle|_{\partial\mathcal{X}} = 0$$



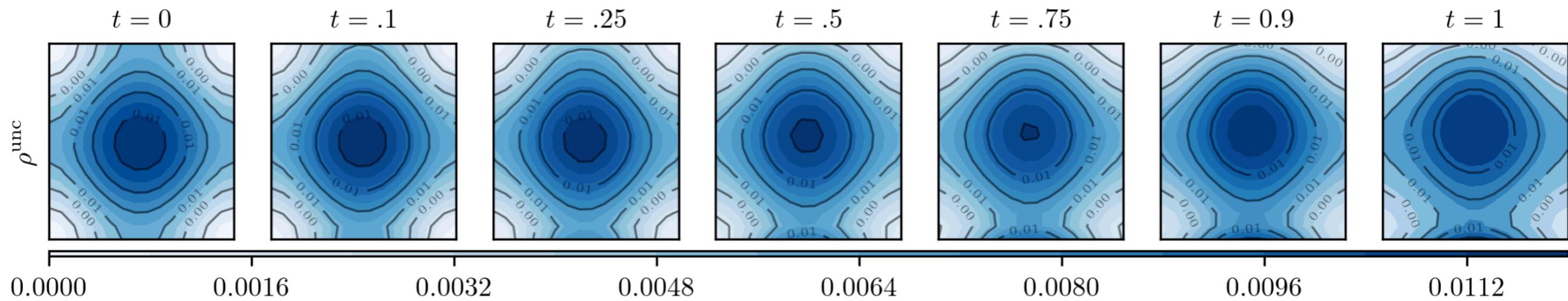
Reflected bridge: numerics with ∇V drift

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

Optimal controlled state PDFs:



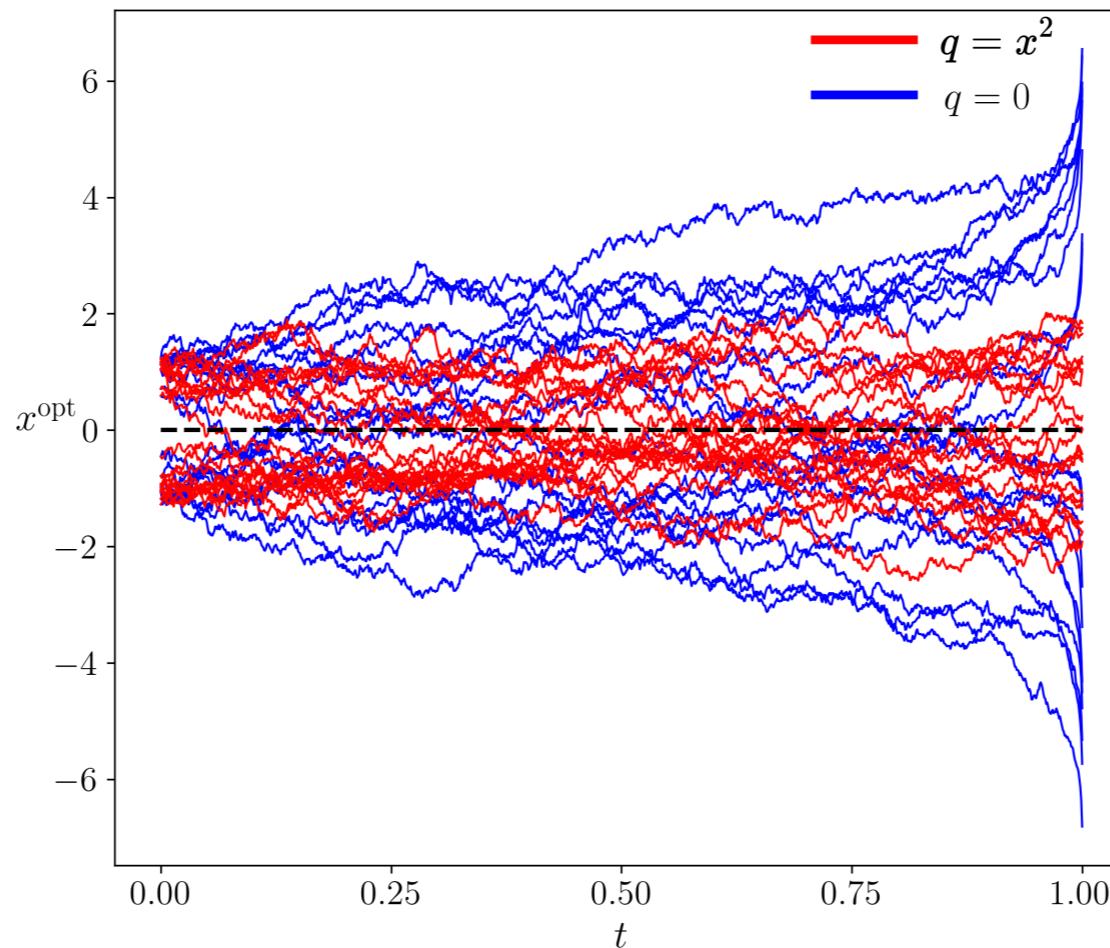
Uncontrolled state PDFs:



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 dyn. 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:

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

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

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

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

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

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

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

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

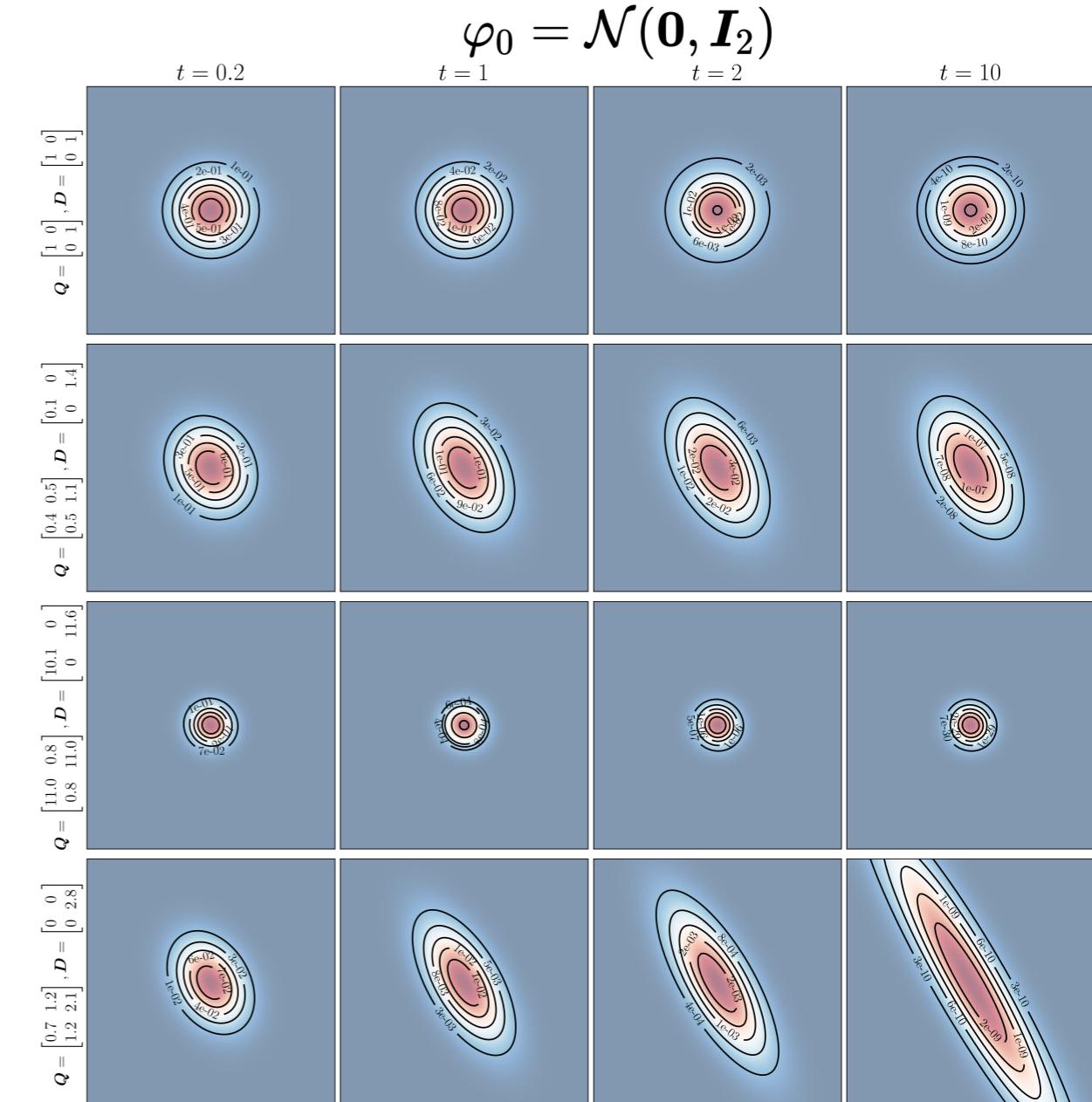
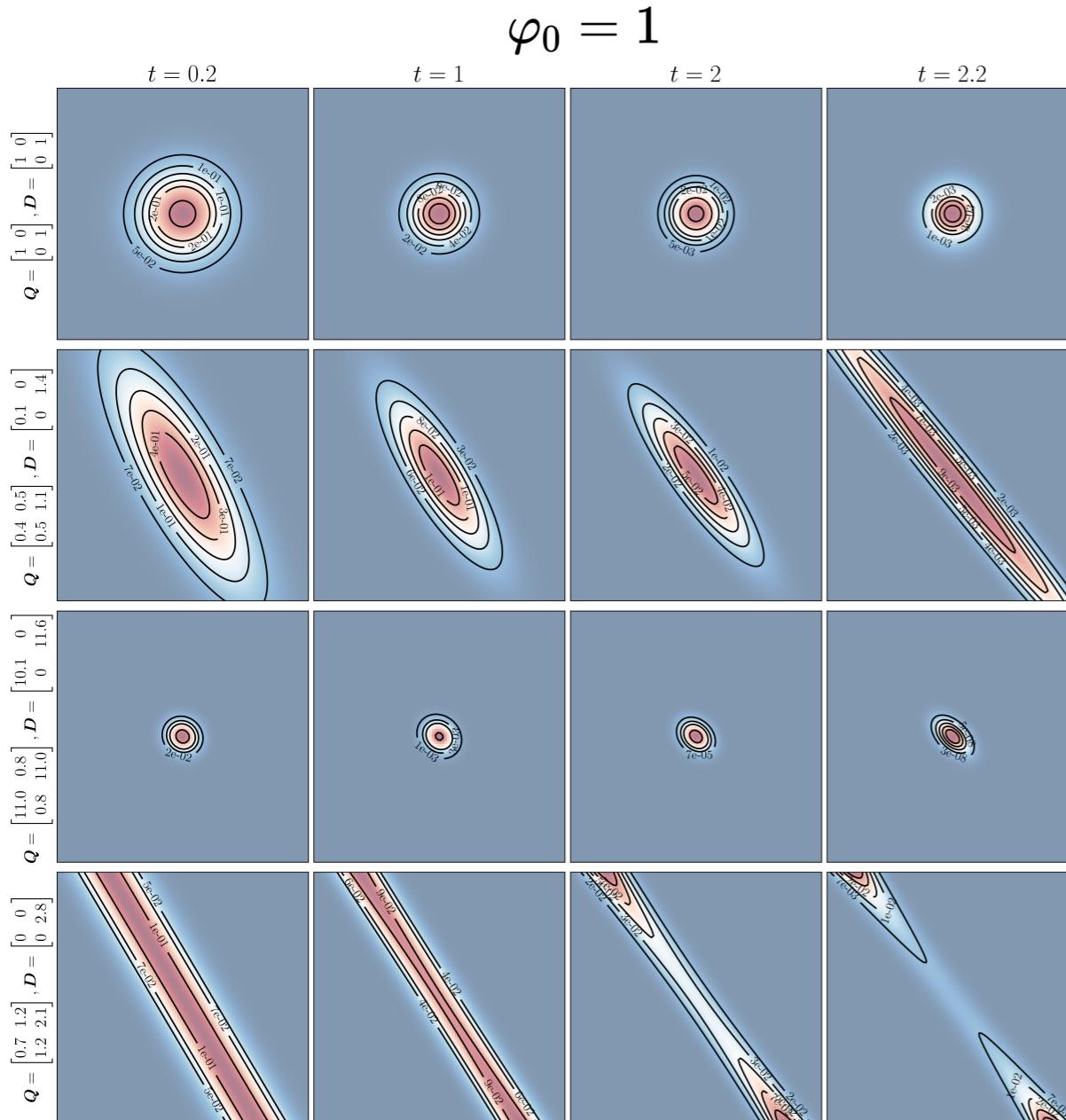
$\mathbf{Q} = \mathbf{I}$ recovers the multivariate Mehler kernel in quantum harmonic oscillator

Schrödinger bridge with quadratic state cost:

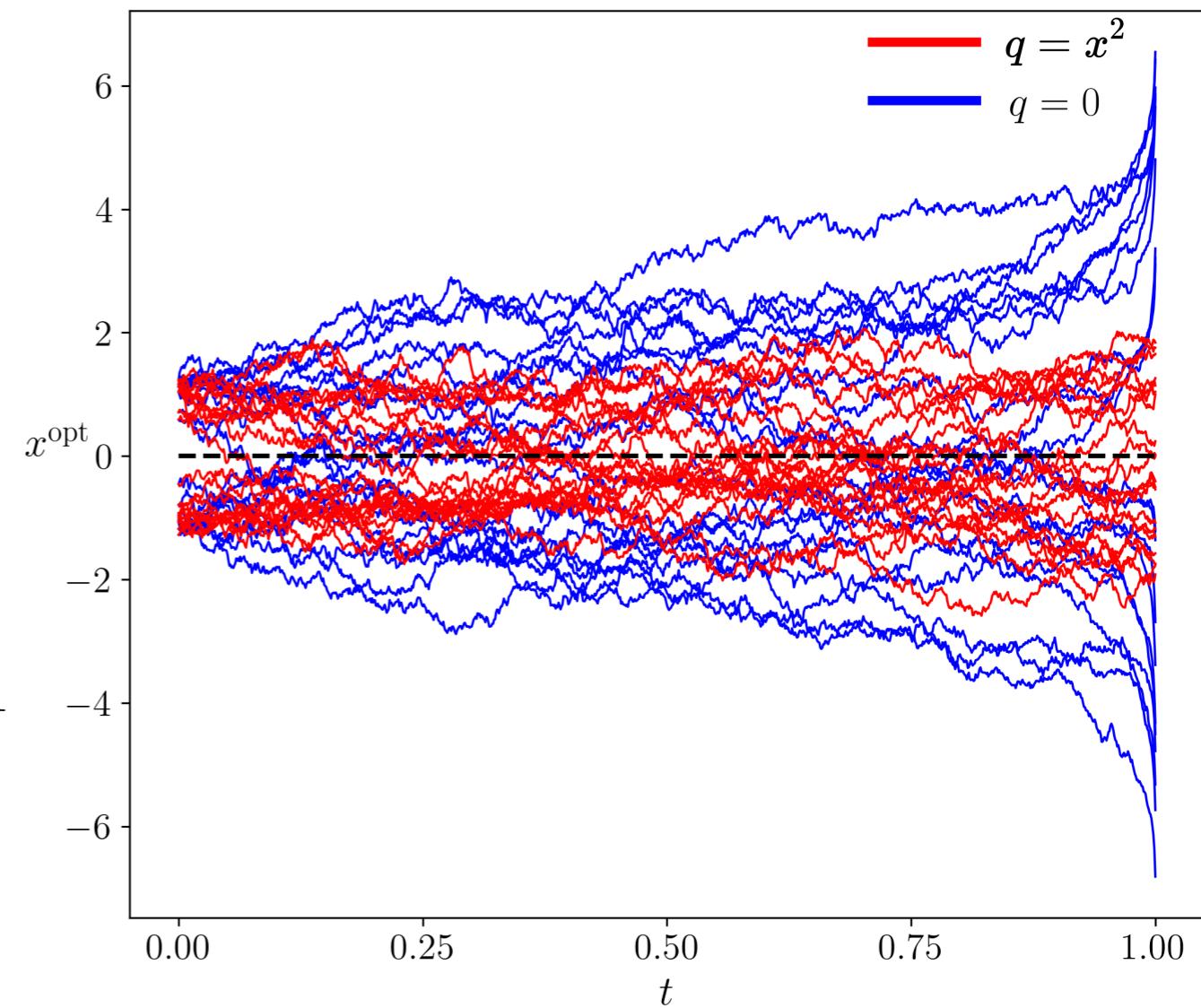
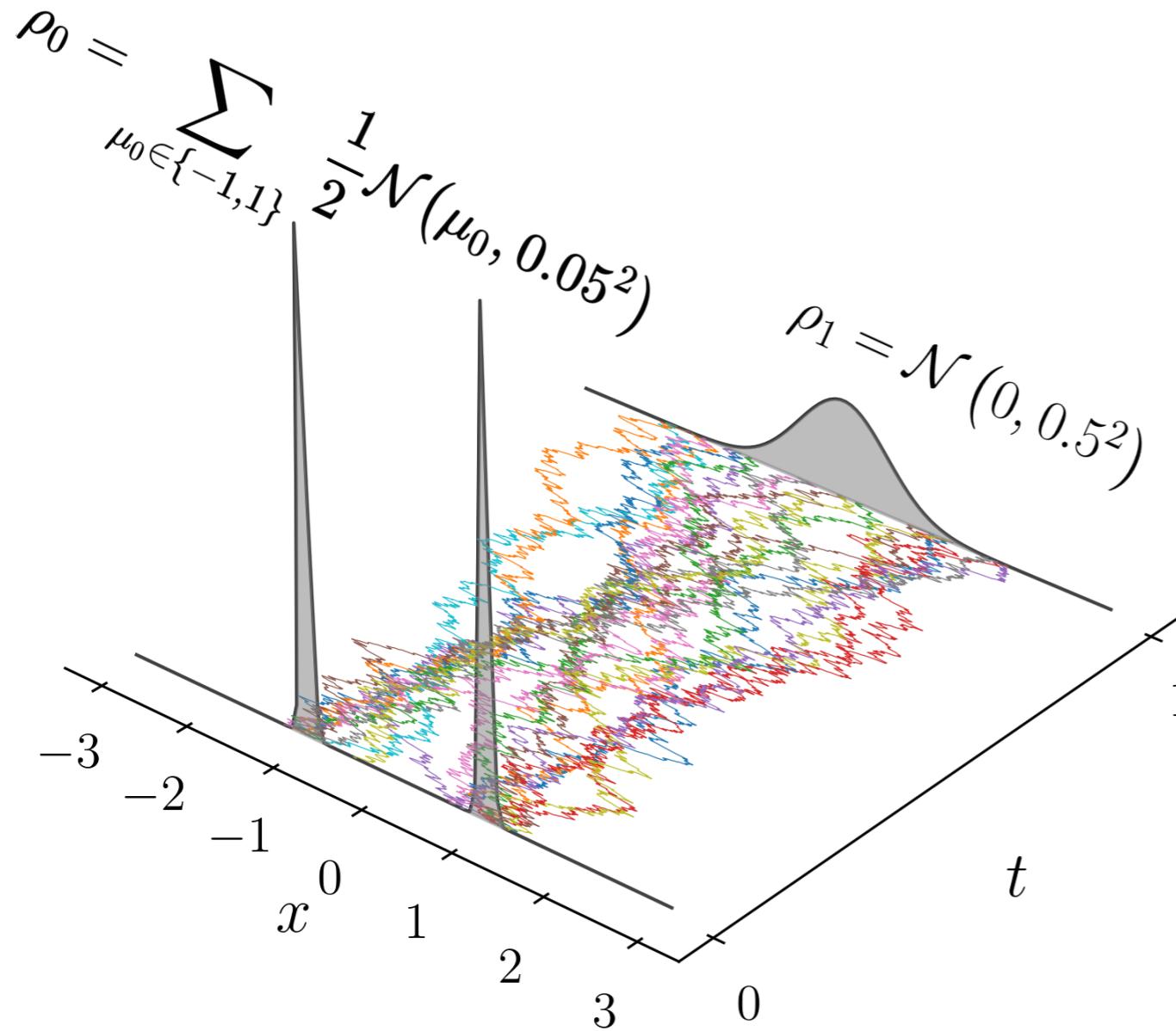
$$q(x) = x^\top Q x, Q \succeq 0$$

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



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:



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PEOPLE AND
ROBOTS

