

Contractions and Reactions in Schrödinger Bridges

Alexis M. H. Teter

Ph.D. Defense in Applied Mathematics
University of California Santa Cruz

Advisor: Abhishek Halder

Committee: Qi Gong (Chair), Abhishek Halder, Hongyun Wang, Yongxin Chen

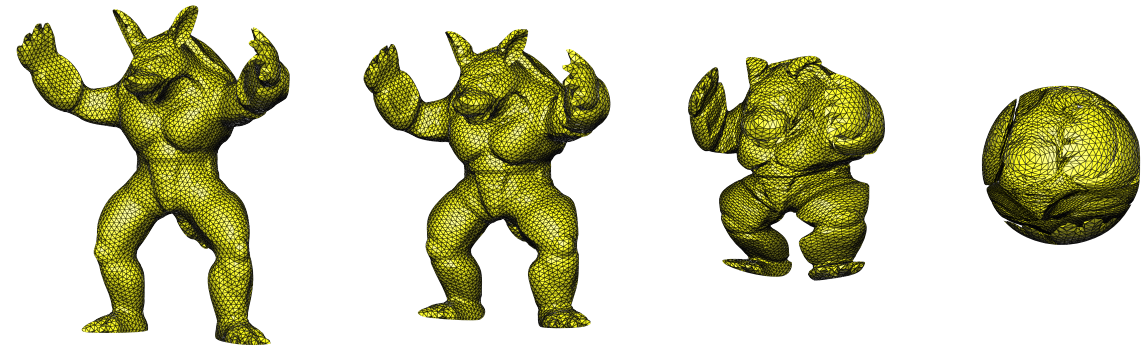
October 09, 2025

Bridge $\rightsquigarrow$ Transport from Source to Target

of goods



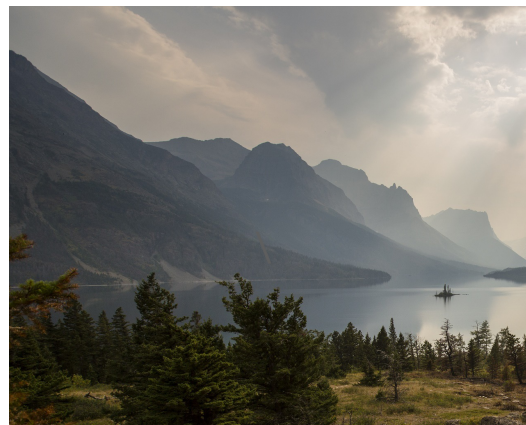
of meshes



of color



source



target



transported

of style



source



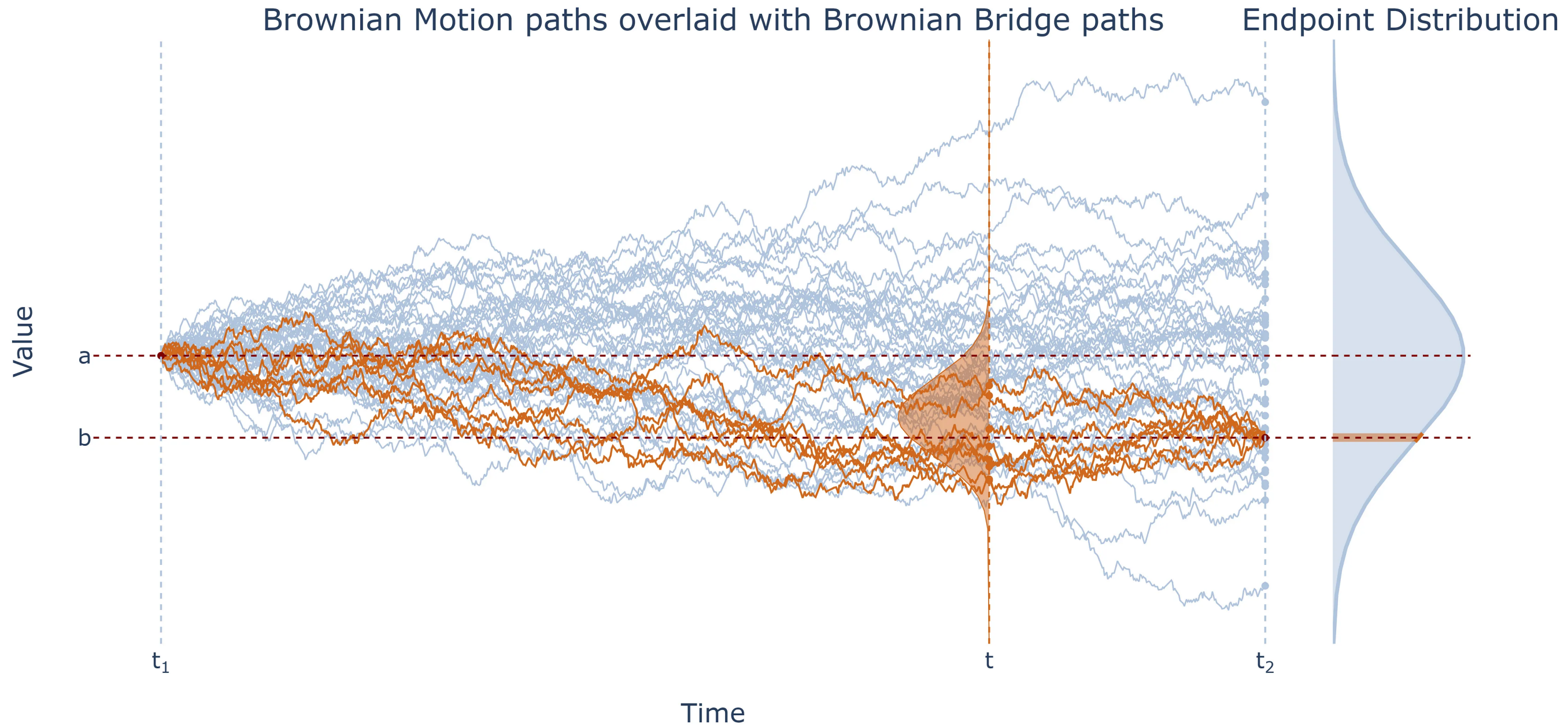
target



transported

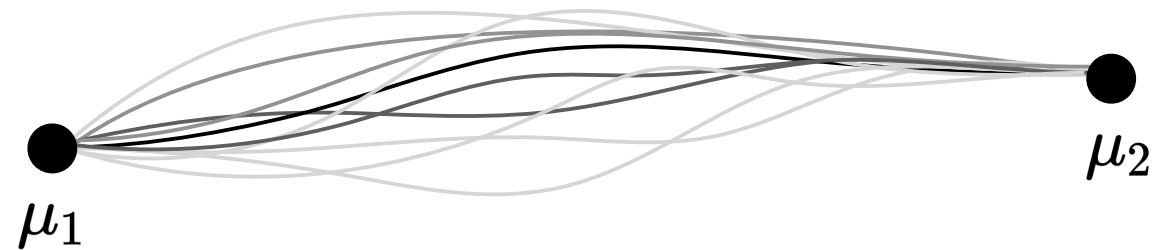
Diffusion Bridge: Transport via Diffusion

When source and target are points on the ground vector space

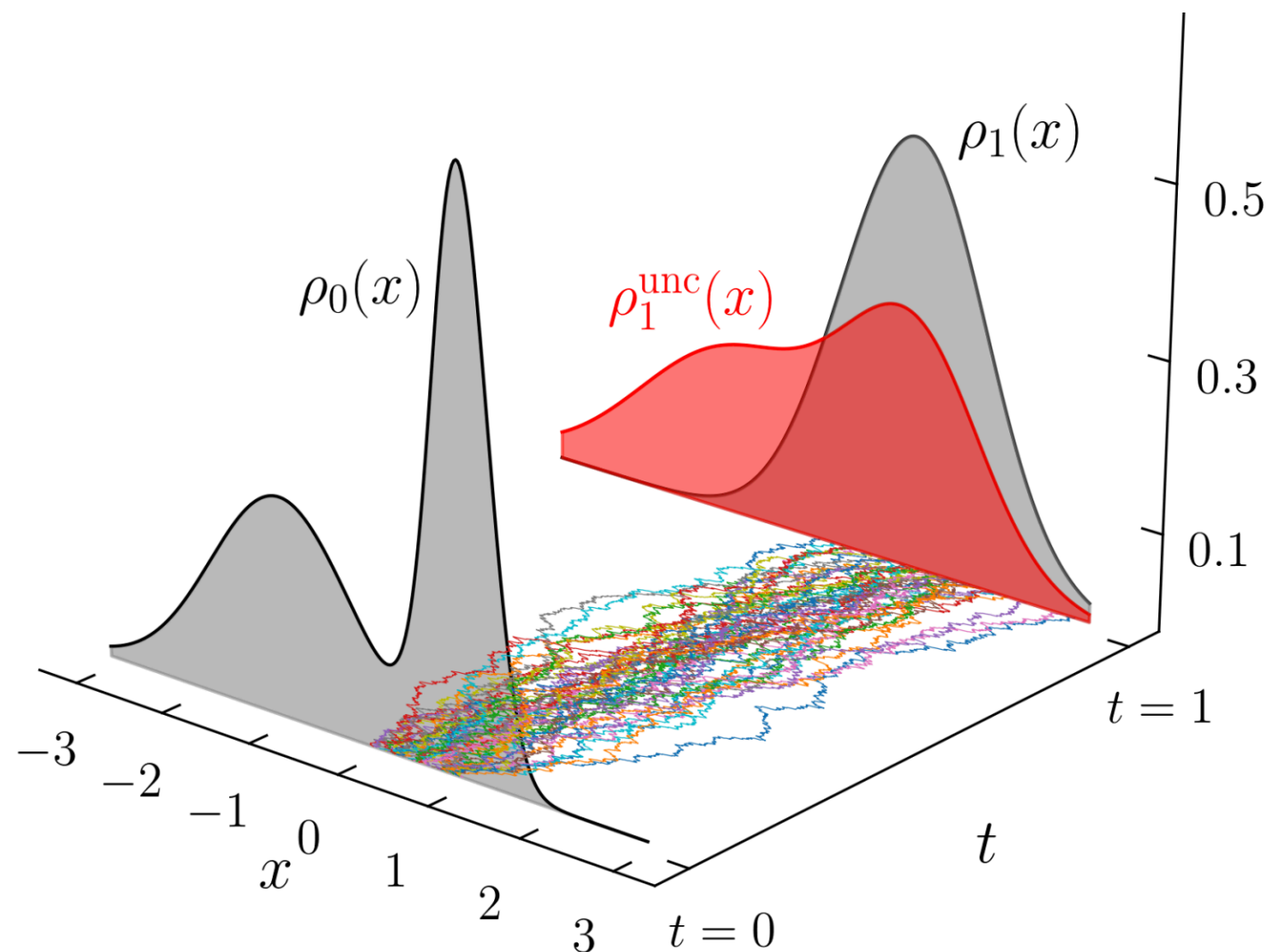


Schrödinger Bridge (SB): Transport via Diffusion

When source and target are measures or probability density functions (PDFs)



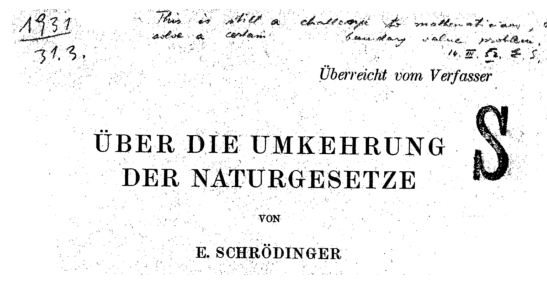
Comes with maximum likelihood guarantee on path space



Brief History of SB



formulates the problem as an attempt to give stochastic interpretation of quantum mechanics



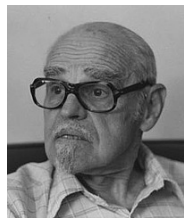
Sur la théorie relativiste de l'électron et l'interprétation de la mécanique quantique

PAR
E. SCHRÖDINGER

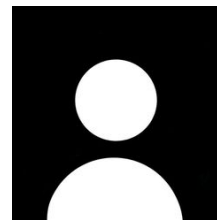
E. Schrödinger (1931-32)



R. Fortet (1940)



A. Beurling (1960)



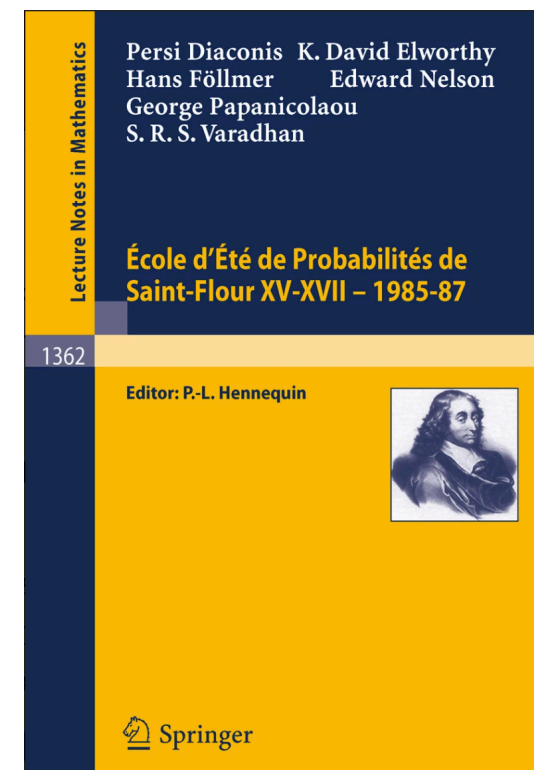
B. Jamison (1975)

establish the existence-uniqueness of the solution for classical SB



H. Föllmer (1985-87)

rigorous large deviations over path space interpretation for classical SB



T. Mikami (1990)



P. Dai Pra (1991)



M. Pavon (1991)

reformulate classical SB as minimum effort stochastic optimal control problem



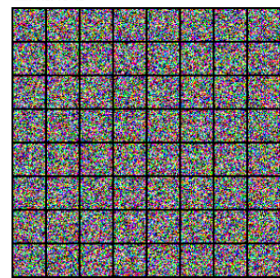
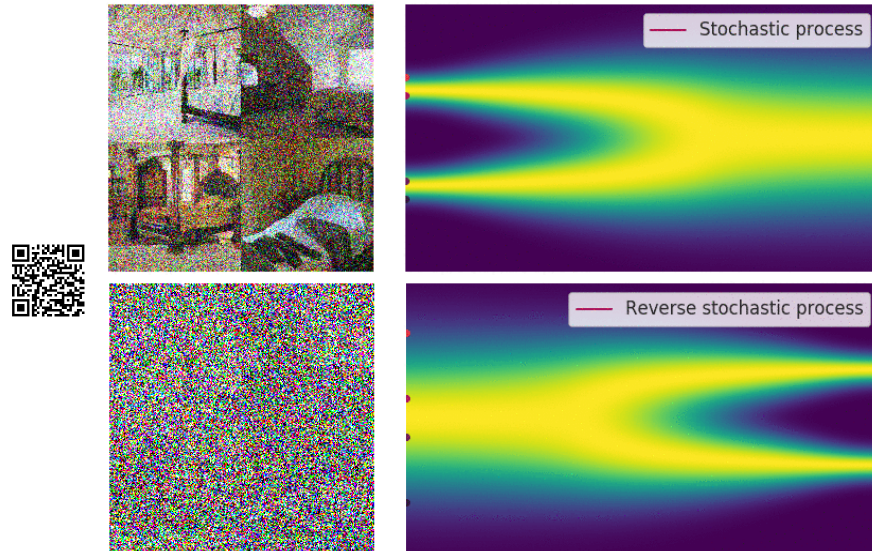
A. Wakolbinger (1991)



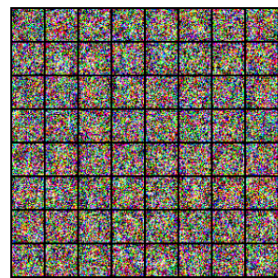
A. Blaquièr (1991)

SB in the 21st Century

Generative AI



$t = 0$



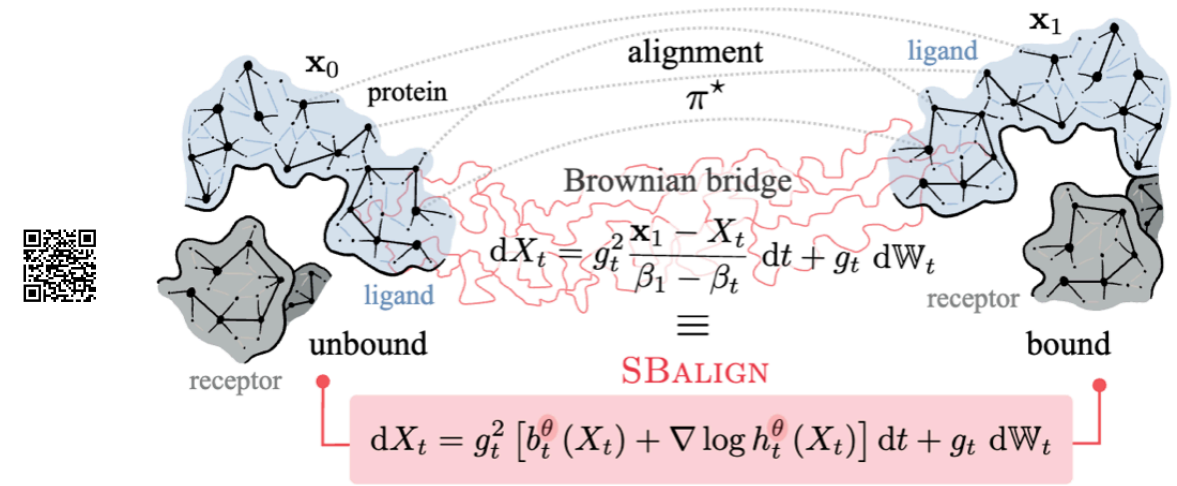
$t = 0.31$



$t = 0.60$



$t = 0.63$



Inpainting



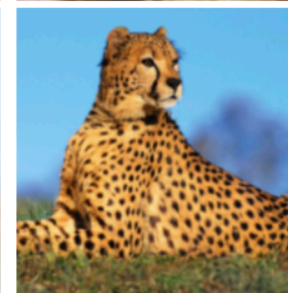
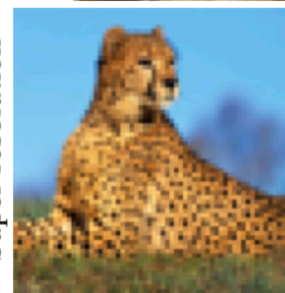
I²SB output



Deblurring



Super-resolution

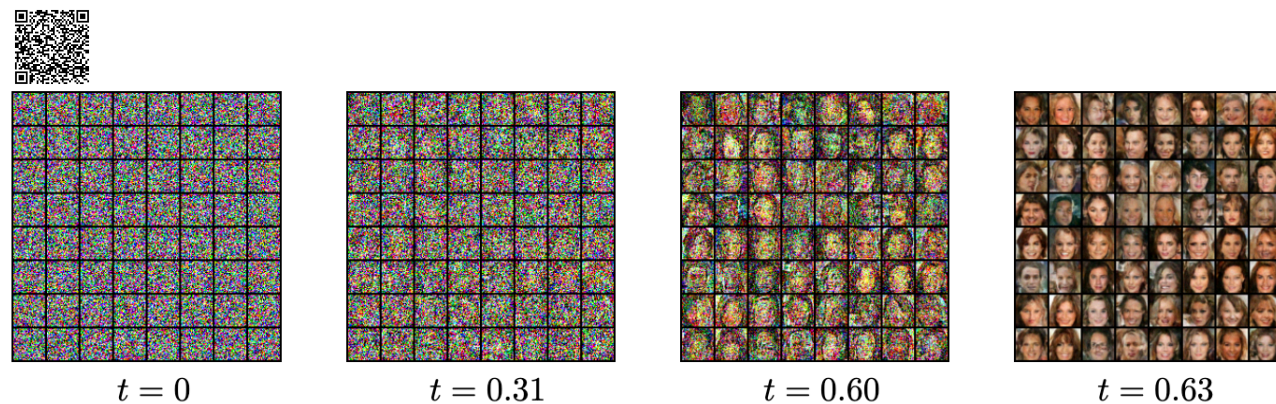
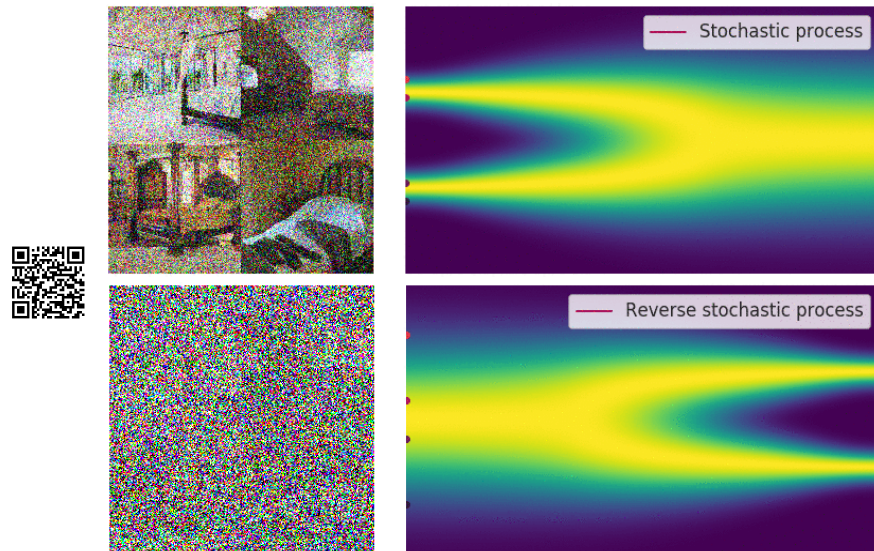


JPEG restoration



SB in the 21st Century

Generative AI



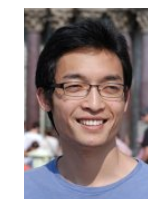
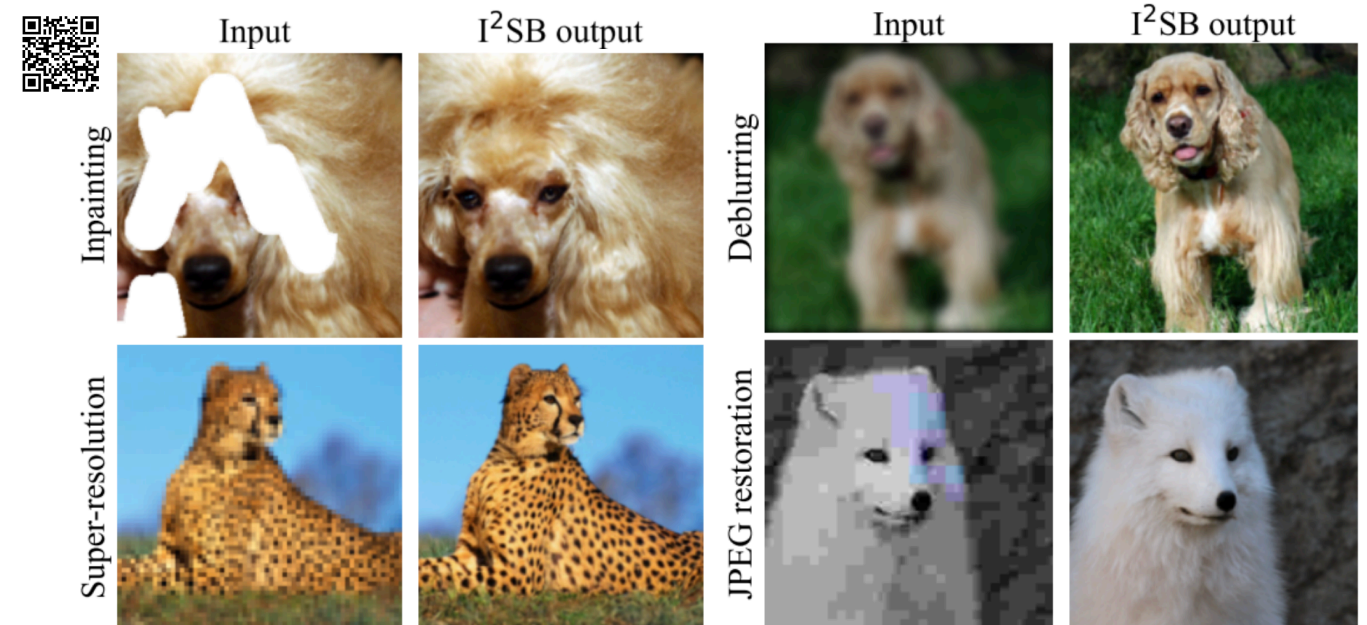
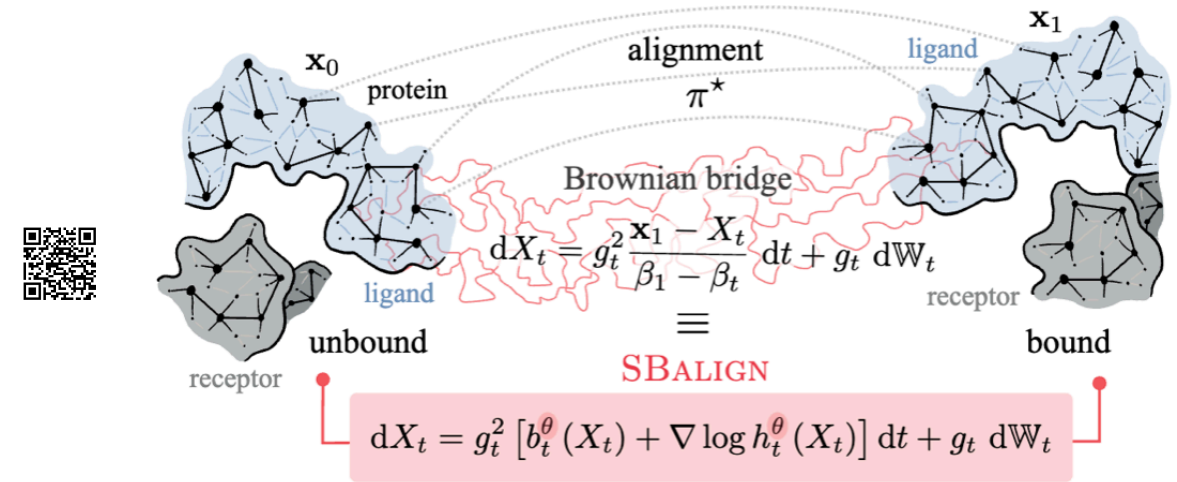
Stochastic Control

Linear Quadratic distribution control a.k.a. LQSB ~2015

generalized SB with nonlinear drift ~2020

reflected SB for deterministic path constraints ~2021

control non-affine SB: application to colloidal self-assembly ~2023



Y. Chen



T. Georgiou



M. Pavon



K. Caluya



A. Halder



I. Nodozi



C. Yan



J. O'Leary



M. Khare



A. Mesbah

Outline of This Talk

Background

Stochastic control formulation + solution structure + dynamic Sinkhorn algorithm

Brief recap of my pre-advancement results

Contraction coefficient for LQSB

Lambertian SB

Post-advancement results

Control-affine SB (CASB) and Hopf-Cole transform

Markov kernel for classical SB: Hermite + Weyl Calculus

Markov kernel for LQSB

Back to quantum: CASB and classical SB

Outro

Summary + publications + acknowledgement

Background

Generalized SB: Stochastic Control Formulation

$$\begin{aligned}
 & \arg \inf_{(\rho, \mathbf{u}) \in \mathcal{P}_{01} \times \mathcal{U}} \int_{t_0}^{t_1} \int_{\mathbb{R}^n} \overbrace{(q(\mathbf{x}) + r(\mathbf{u}))}^{\text{state cost} + \text{control cost}} \rho(t, \mathbf{x}) \, d\mathbf{x} \, dt \\
 & \quad \frac{\partial \rho}{\partial t} + \nabla_{\mathbf{x}} \cdot (\rho \mathbf{f}(t, \mathbf{x}, \mathbf{u})) = \overbrace{\Delta_{\Sigma}(t, \mathbf{x}, \mathbf{u}) \rho}^{\text{weighted Laplacian}} \sum_{i,j=1}^n \frac{\partial^2}{\partial x_i \partial x_j} ((\Sigma)_{ij} \rho) \\
 & \quad \rho(t_0, \mathbf{x}) = \rho_0(\mathbf{x}), \quad \rho(t_1, \mathbf{x}) = \rho_1(\mathbf{x}).
 \end{aligned}$$

PDF dynamics for the
controlled Itô SDE

$$d\mathbf{x} = \overbrace{\mathbf{f}(t, \mathbf{x}, \mathbf{u})}^{\text{prior drift}} dt + \overbrace{\boldsymbol{\sigma}(t, \mathbf{x}, \mathbf{u})}^{\text{prior diffusion}} d\mathbf{w}, \quad \overbrace{\Sigma}^{\text{diffusion tensor}} := \boldsymbol{\sigma} \boldsymbol{\sigma}^\top$$

Generalized SB: Stochastic Control Formulation

$$\begin{aligned}
 & \arg \inf_{(\rho, \mathbf{u}) \in \mathcal{P}_{01} \times \mathcal{U}} \int_{t_0}^{t_1} \int_{\mathbb{R}^n} \overbrace{(q(\mathbf{x}) + r(\mathbf{u}))}^{\text{state cost} + \text{control cost}} \rho(t, \mathbf{x}) \, d\mathbf{x} \, dt \\
 & \quad \frac{\partial \rho}{\partial t} + \nabla_{\mathbf{x}} \cdot (\rho \mathbf{f}(t, \mathbf{x}, \mathbf{u})) = \overbrace{\Delta_{\Sigma}(t, \mathbf{x}, \mathbf{u}) \rho}^{\text{weighted Laplacian}} \sum_{i,j=1}^n \frac{\partial^2}{\partial x_i \partial x_j} ((\Sigma)_{ij} \rho) \\
 & \quad \rho(t_0, \mathbf{x}) = \rho_0(\mathbf{x}), \quad \rho(t_1, \mathbf{x}) = \rho_1(\mathbf{x}).
 \end{aligned}$$

PDF dynamics for the
controlled Itô SDE

$$d\mathbf{x} = \overbrace{\mathbf{f}(t, \mathbf{x}, \mathbf{u})}^{\text{prior drift}} dt + \overbrace{\boldsymbol{\sigma}(t, \mathbf{x}, \mathbf{u})}^{\text{prior diffusion}} d\mathbf{w}, \quad \overbrace{\Sigma}^{\text{diffusion tensor}} := \boldsymbol{\sigma} \boldsymbol{\sigma}^\top$$

$\mathcal{P}_{01} := \{\text{PDF valued curves } \rho(t, \cdot) \text{ continuous in } t \in [t_0, t_1] \\ \text{such that } \rho(t_0, \cdot) = \rho_0(\cdot), \rho(t_1, \cdot) = \rho_1(\cdot)\}$

$\mathcal{U} := \{\text{Finite energy Markovian policies } \mathbf{u}(t, \mathbf{x})\}$

Classical SB: $q = 0, r = \frac{1}{2} \|\cdot\|_2^2, f = u, \sigma = \sqrt{2\varepsilon} I$

Controlled Itô SDE $d\mathbf{x} = \mathbf{u} dt + \sqrt{2\varepsilon} d\mathbf{w}$

First order conditions for optimality

$$\frac{\partial S}{\partial t} + \frac{1}{2} \|\nabla_{\mathbf{x}} S\|_2^2 + \varepsilon \Delta_{\mathbf{x}} S = 0$$

Dual PDE in
value function S

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

Primal PDE in ρ_{opt}

Boundary conditions

$$\rho_{\text{opt}}(t_0, \mathbf{x}) = \rho_0(\mathbf{x}), \quad \rho_{\text{opt}}(t_1, \mathbf{x}) = \rho_1(\mathbf{x})$$

Optimal control

$$\mathbf{u}_{\text{opt}}(t, \mathbf{x}) = \nabla_{\mathbf{x}} S$$

Classical SB: Solution Structure

Apply Hopf-Cole transform $\varphi_\varepsilon := \exp\left(\frac{S}{2\varepsilon}\right)$, $\hat{\varphi}_\varepsilon := \rho_{\text{opt}} \exp\left(-\frac{S}{2\varepsilon}\right)$

$\uparrow$ Schrödinger factors $\uparrow$

Decoupled linear PDEs $\frac{\partial \varphi_\varepsilon}{\partial t} = -\varepsilon \Delta_{\mathbf{x}} \varphi_\varepsilon \quad \frac{\partial \hat{\varphi}_\varepsilon}{\partial t} = \varepsilon \Delta_{\mathbf{x}} \hat{\varphi}_\varepsilon$

forward and backward heat PDEs

Coupled boundary conditions

$$\hat{\varphi}_\varepsilon(t_0, \mathbf{x}) \varphi_\varepsilon(t_0, \mathbf{x}) = \rho_0, \quad \hat{\varphi}_\varepsilon(t_1, \mathbf{x}) \varphi_\varepsilon(t_1, \mathbf{x}) = \rho_1$$

Schrödinger system

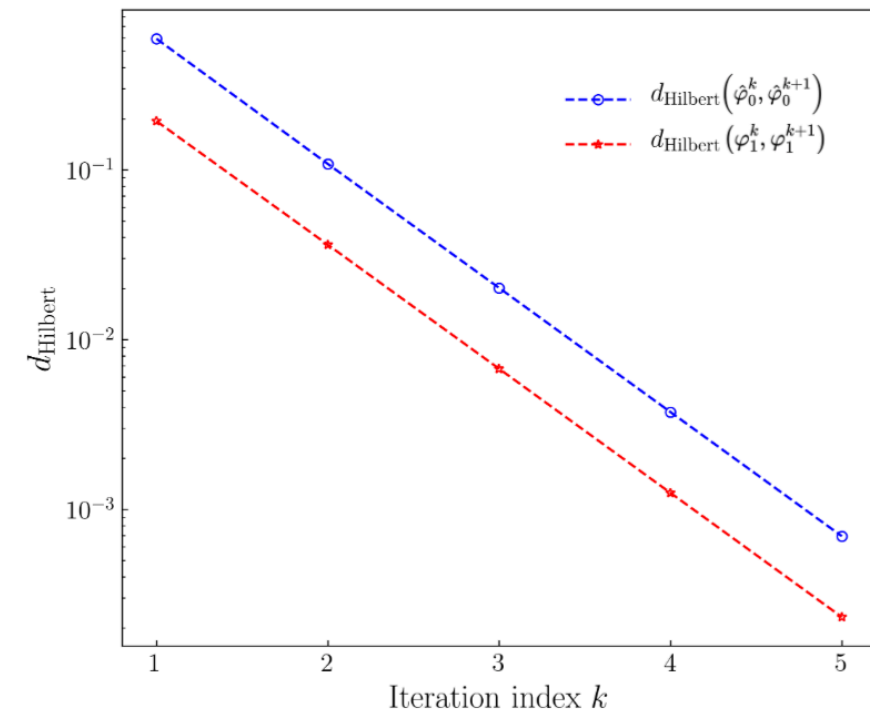
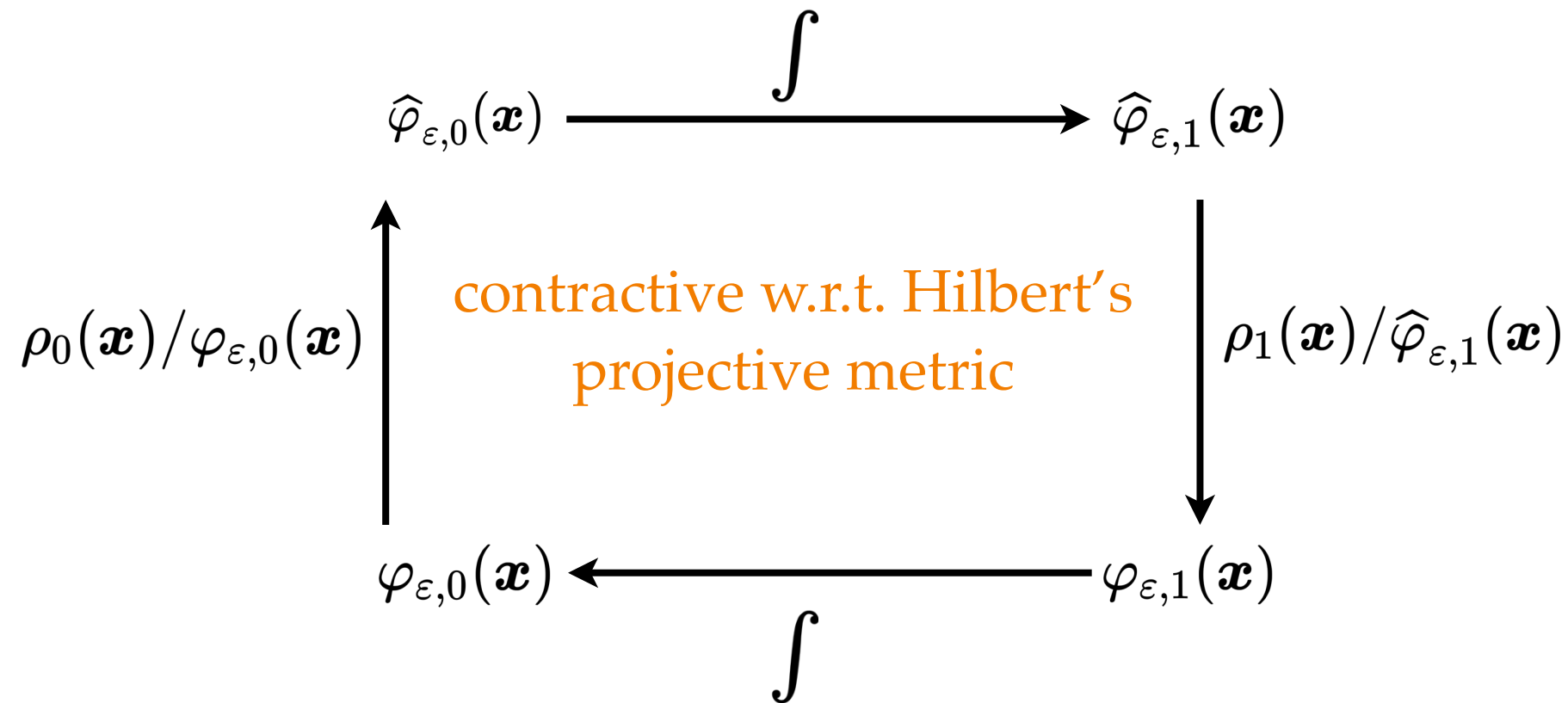
Markov kernel for the uncontrolled process

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

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

Algorithm: Dynamic Sinkhorn Recursion

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



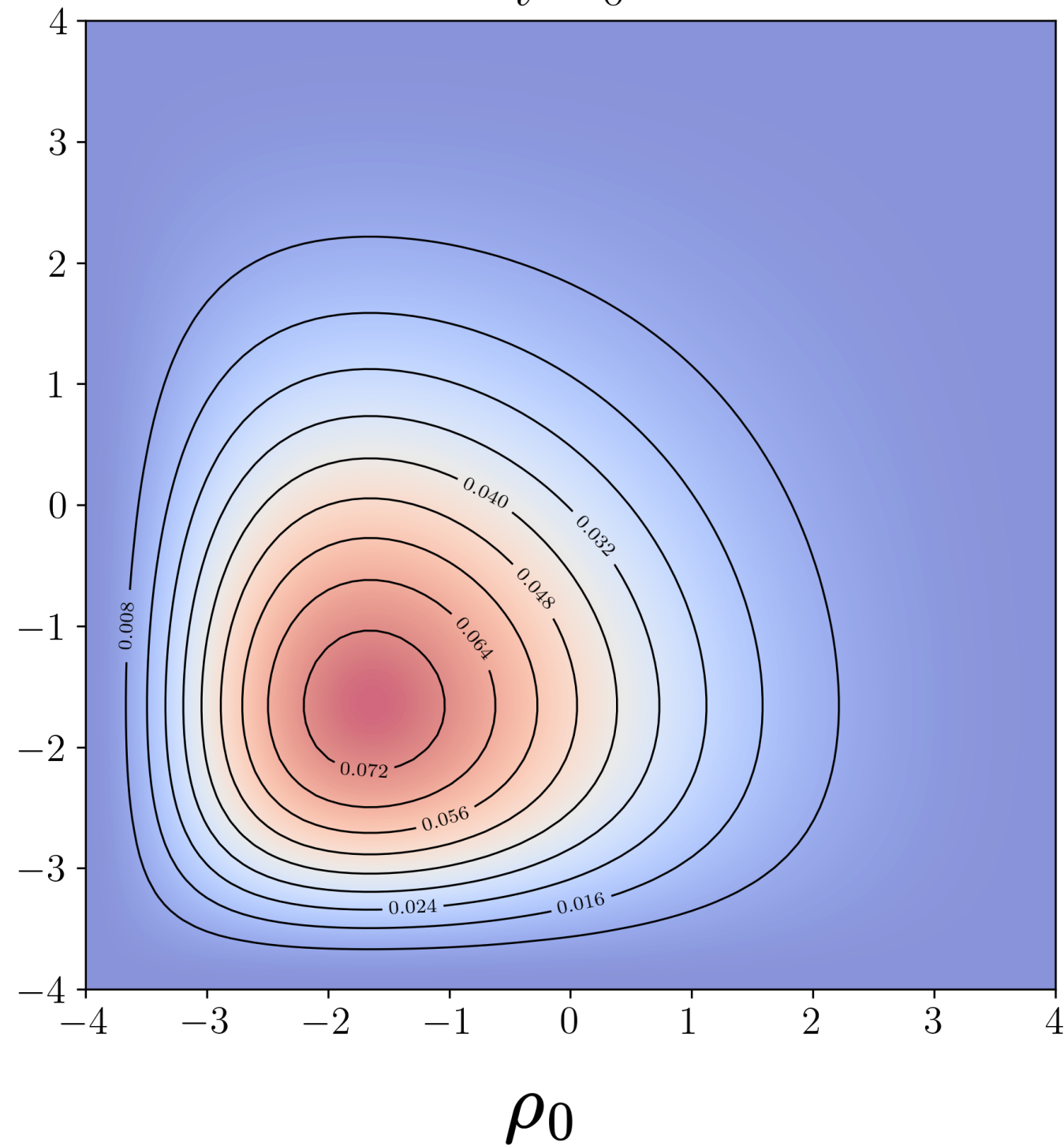
Recover original decision variables

$$\rho_{\text{opt}}(t, \mathbf{x}) = \hat{\varphi}_{\varepsilon}(t, \mathbf{x})\varphi_{\varepsilon}(t, \mathbf{x}) \quad \mathbf{u}_{\text{opt}}(t, \mathbf{x}) = 2\varepsilon \nabla_{\mathbf{x}} \log \varphi_{\varepsilon}(t, \mathbf{x})$$

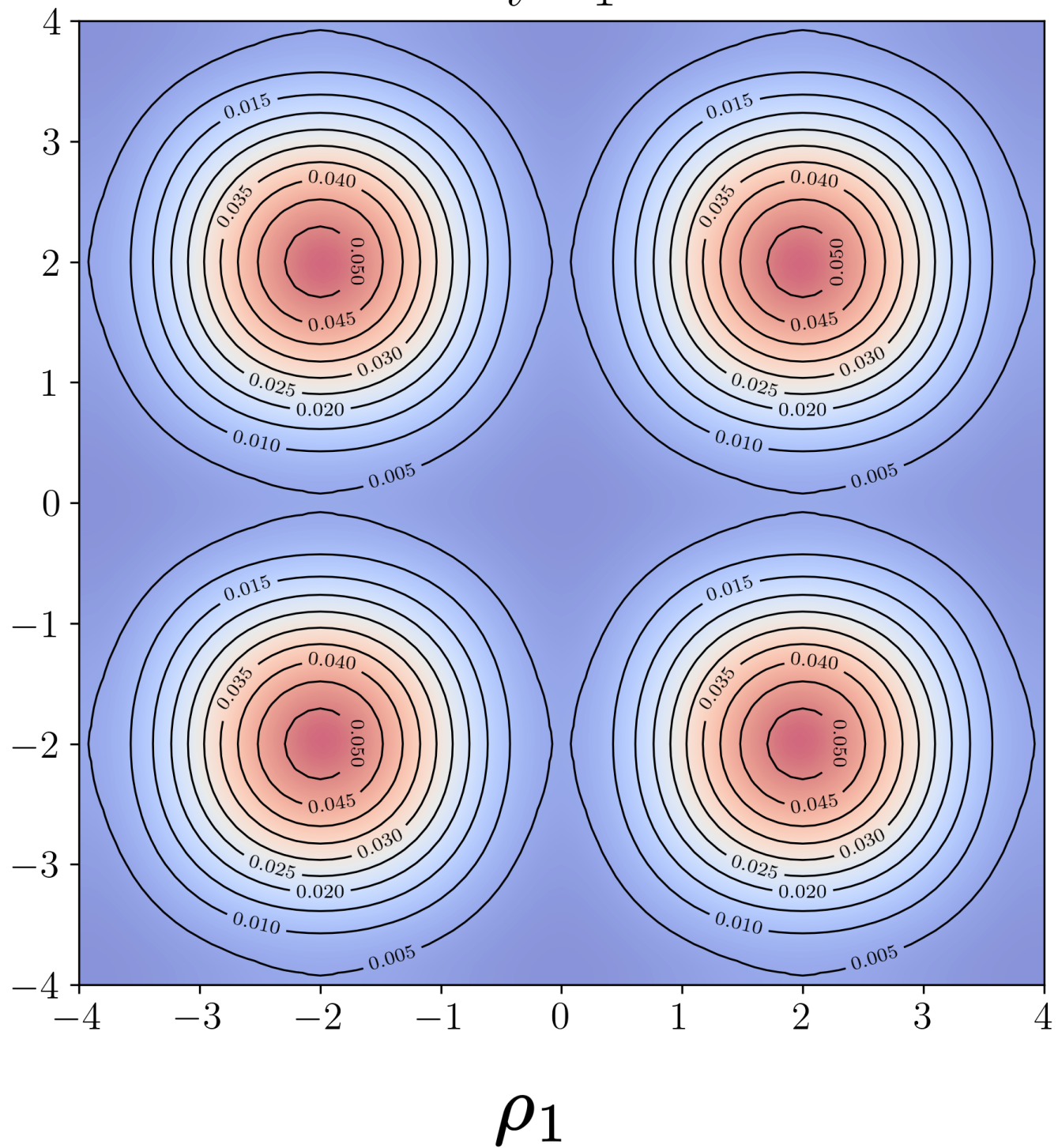
Classical SB Example: Input

$$\varepsilon = 0.3$$

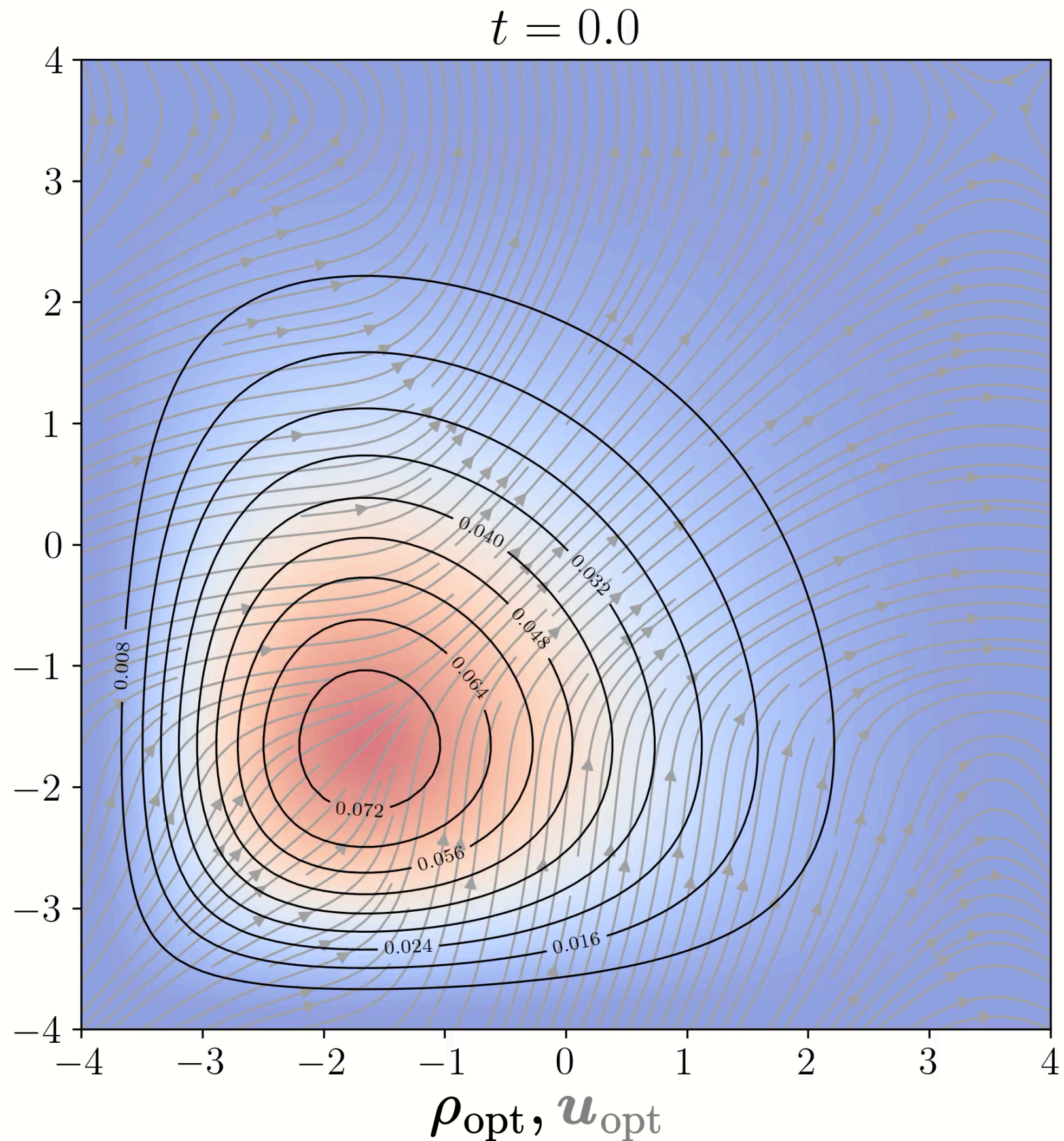
$t = 0$



$t = 1$



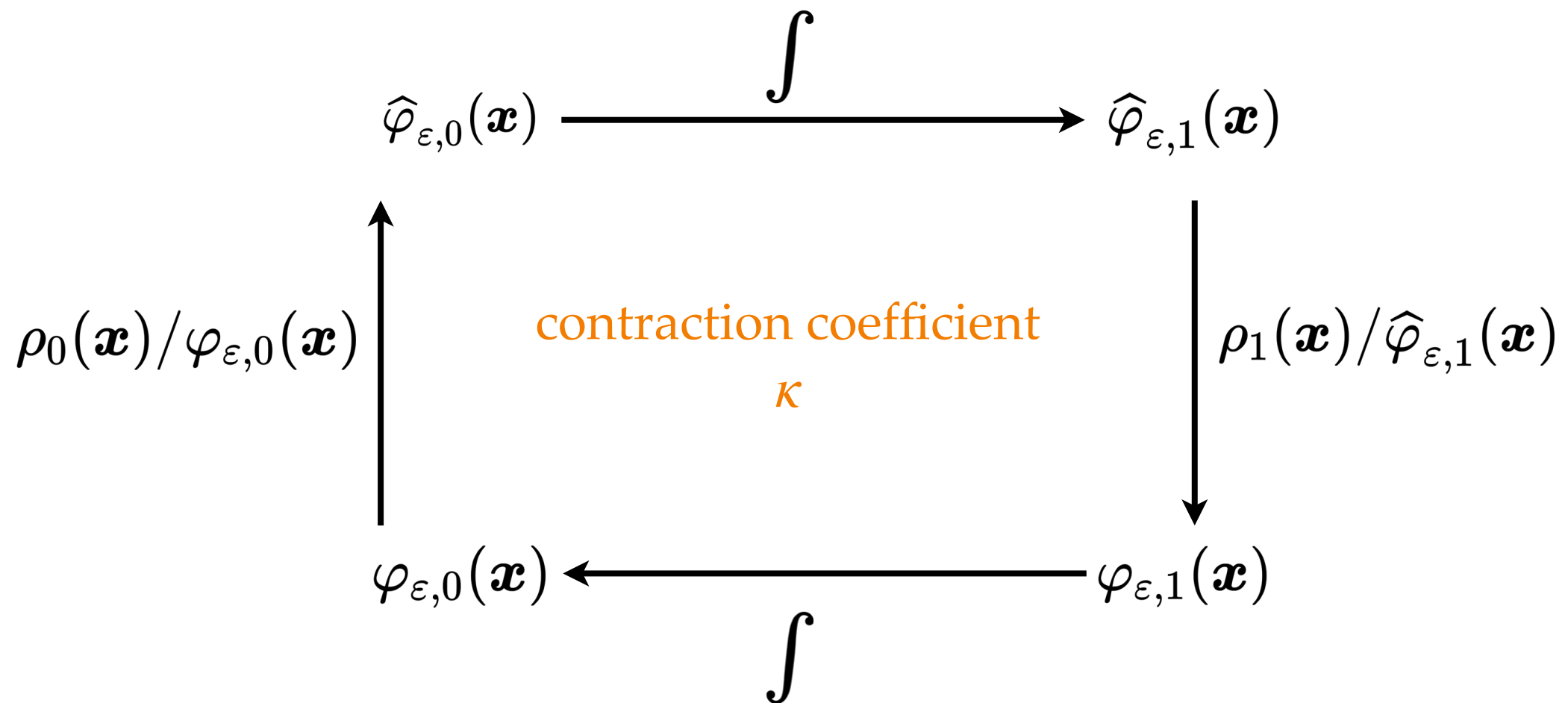
Classical SB Example: Output



Brief recap of my pre-advancement results



LQSB: $q = 0, r = \frac{1}{2} \|\cdot\|_2^2, f = A_t x + B_t u, \sigma = \sqrt{2\varepsilon} B_t$



worst-case contraction coefficient

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

$$\tilde{\alpha}_L := \max_{\mathbf{x}_0 \in \mathbf{M}_{10}^{-1/2} \Phi_{t_1 t_0} \mathcal{X}_0, \mathbf{x}_1 \in \mathbf{M}_{10}^{-1/2} \mathcal{X}_1} \|\mathbf{x}_0 - \mathbf{x}_1\|_2^2$$

$$\tilde{\beta}_L := \min_{\mathbf{x}_0 \in \mathbf{M}_{10}^{-1/2} \Phi_{t_1 t_0} \mathcal{X}_0, \mathbf{x}_1 \in \mathbf{M}_{10}^{-1/2} \mathcal{X}_1} \|\mathbf{x}_0 - \mathbf{x}_1\|_2^2$$

$$\mathbf{LQSB}: q = 0, r = \frac{1}{2} \|\cdot\|_2^2, f = A_t x + B_t u, \sigma = \sqrt{2\varepsilon} B_t$$

This result

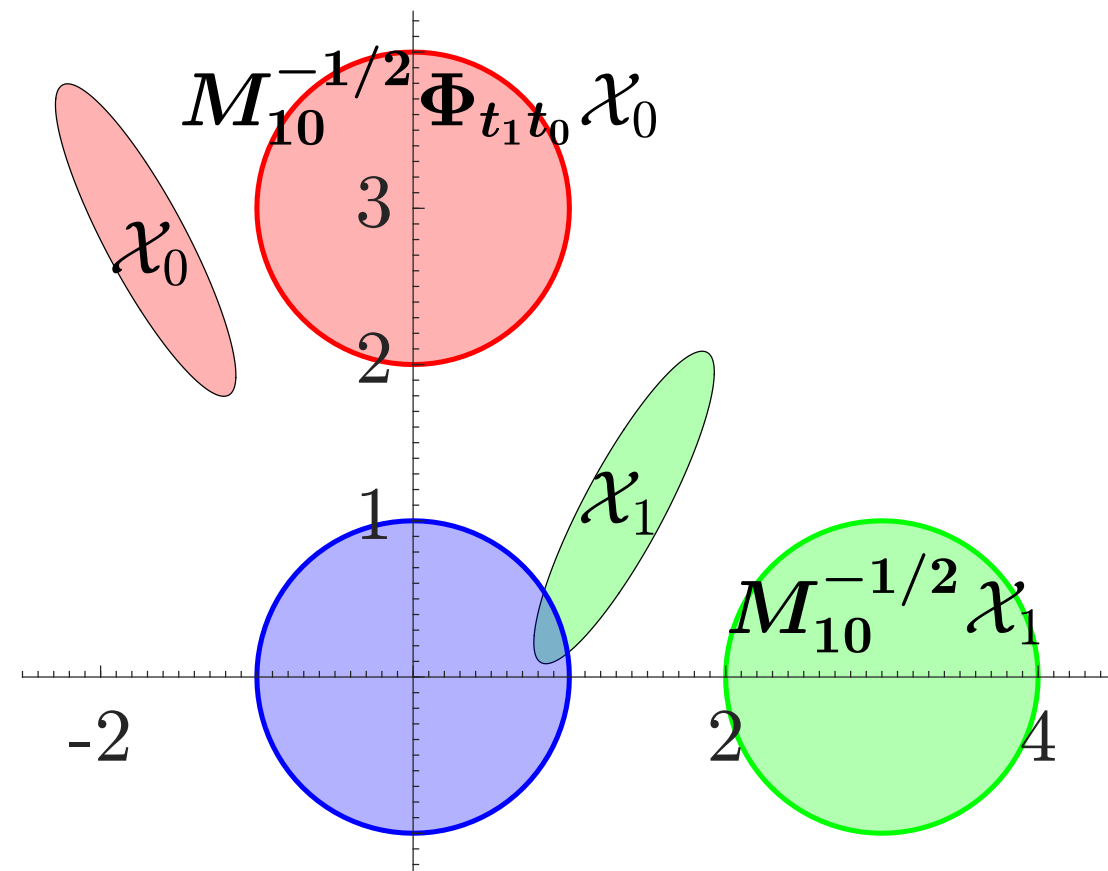
↳ yields control-theoretic + geometric interpretations:

Range of optimal state transfer cost $\tilde{\alpha}_L - \tilde{\beta}_L \uparrow \Rightarrow \gamma_L \uparrow$

Range of separation of $M_{10}^{-1/2} \Phi_{t_1 t_0} \mathcal{X}_0$ and $M_{10}^{-1/2} \mathcal{X}_1 \uparrow \Rightarrow \gamma_L \uparrow$

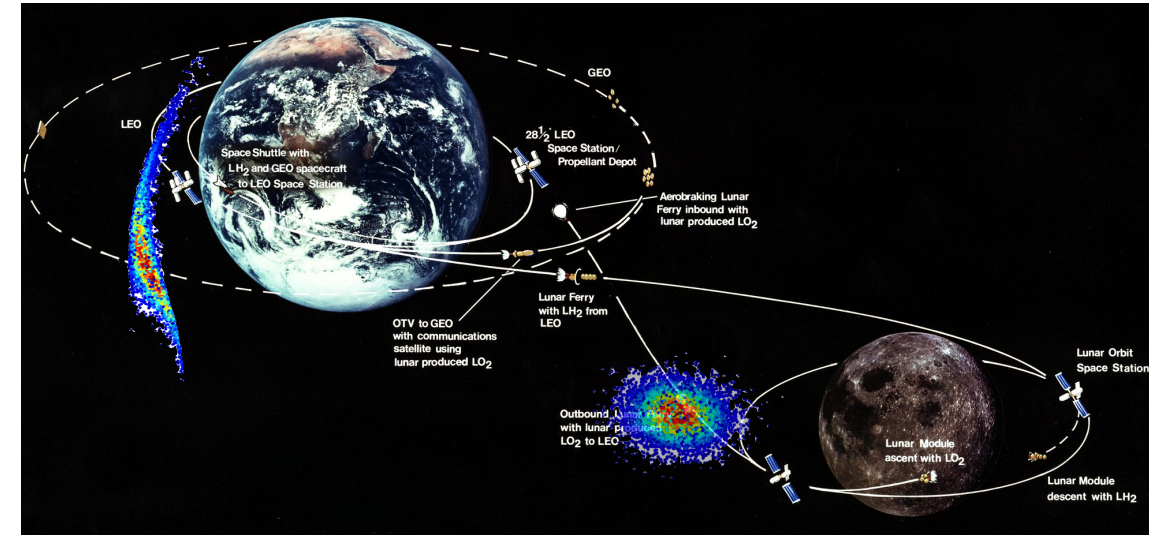
Process noise $\varepsilon \uparrow \Rightarrow \gamma_L \downarrow$

↳ suggests preconditioning



Probabilistic Lambert Problem

Position coordinate $\boldsymbol{x} = (x, y, z) \in \mathbb{R}^3$



Find velocity control policy $\dot{\mathbf{x}} := \mathbf{u}(t, \mathbf{x})$ s.t.

$$\left\{ \begin{array}{ll} \ddot{\mathbf{x}} = -\nabla_{\mathbf{x}} V(\mathbf{x}) & \text{gravitational potential } V(\mathbf{x}) = -\frac{\mu}{\|\mathbf{x}\|_2} \left(1 + \frac{J_2 R_{\text{Earth}}^2}{2\|\mathbf{x}\|_2^2} \left(1 - \frac{3z^2}{\|\mathbf{x}\|_2^2} \right) \right) \\ \mathbf{x}(t = t_0) \sim \rho_0 & \text{encodes statistical estimation errors} \\ \mathbf{x}(t = t_1) \sim \rho_1 & \text{encodes statistical performance specification} \end{array} \right.$$

Our result #1: probabilistic Lambert problem = optimal mass transport with state cost

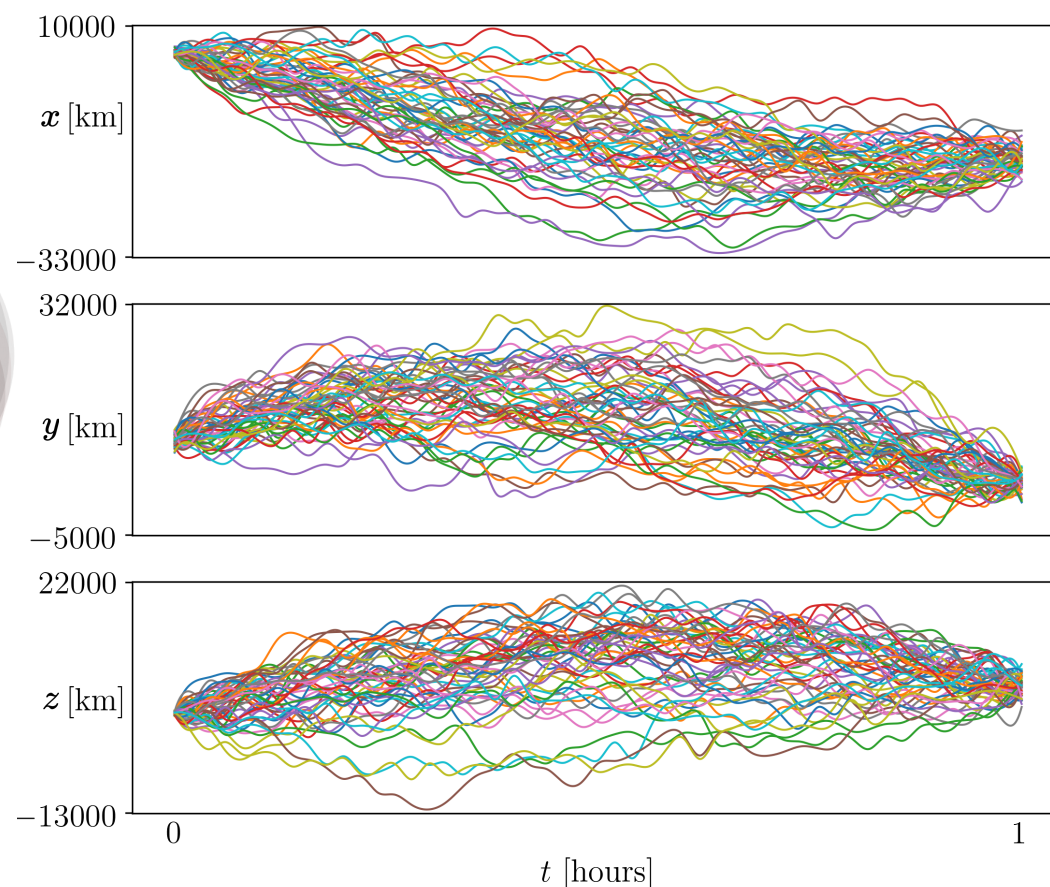
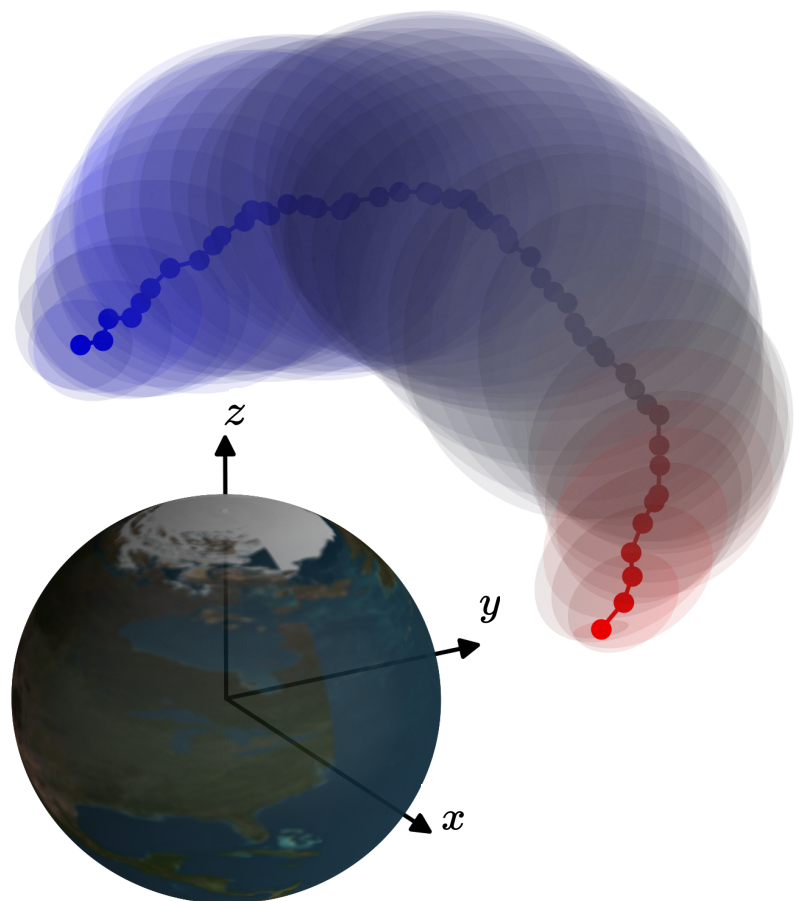
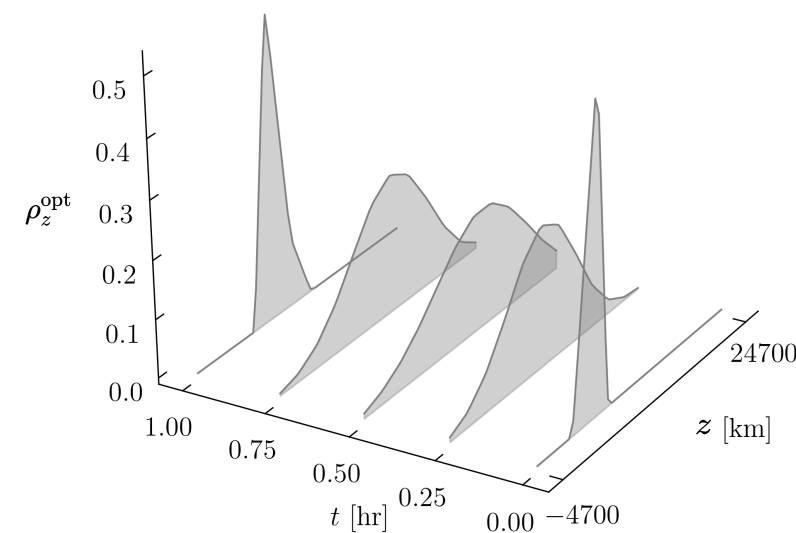
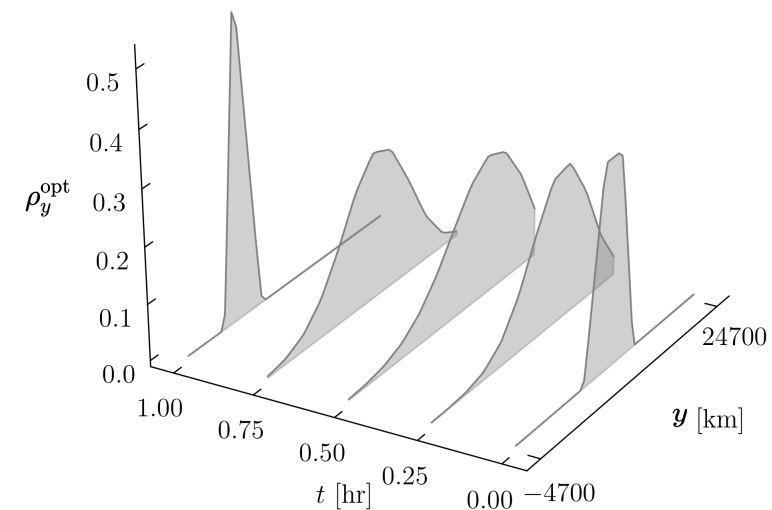
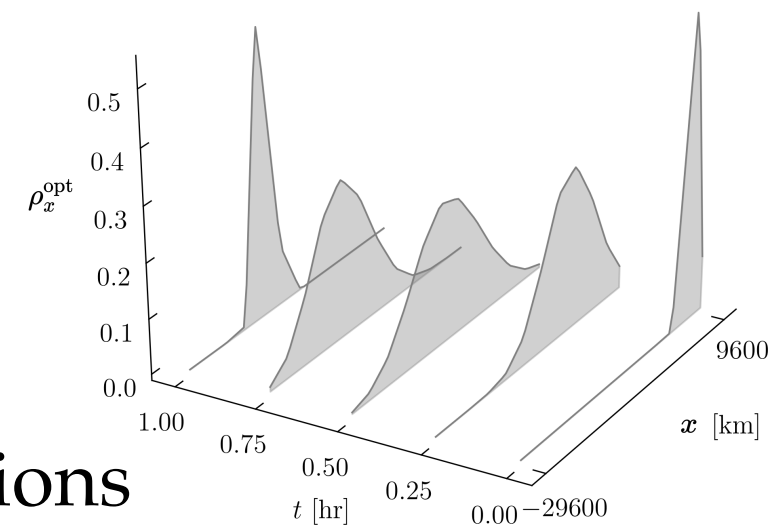
Our result #2: diffusive regularization = Lambertian SB

gravitational potential: from dynamics to state cost to reaction rate

Lambertian SB: $q = -V, r = \frac{1}{2} \|\cdot\|_2^2, f = u, \sigma = \sqrt{2\varepsilon} I$

This connection helps

- ↳ guarantee existence + uniqueness of solution
- ↳ numerical solution via dynamic Sinkhorn recursions



Post-advancement result # 1

**Control-affine SB
and Hopf-Cole transform**



Control-Affine SB: $r = \frac{1}{2} \| \cdot \|_2^2, f = A(t, \mathbf{x}) + B(t, \mathbf{x})u$

First order conditions for optimality + generalized Hopf-Cole transform

$$\varphi_\lambda := \exp\left(\frac{S}{\lambda}\right), \quad \hat{\varphi}_\lambda := \rho_{\text{opt}} \exp\left(-\frac{S}{\lambda}\right)$$

gives **coupled nonlinear reaction-advection-diffusion** PDEs!!

$$\frac{\partial \hat{\varphi}_\lambda}{\partial t} + \nabla_{\mathbf{x}} \cdot (\hat{\varphi}(\mathbf{A} + \mathbf{A}_\varphi)) - \Delta_{\Sigma} \hat{\varphi}_\lambda + \left(\frac{q}{\lambda} + q_\varphi\right) \hat{\varphi}_\lambda = 0$$

$$\frac{\partial \varphi_\lambda}{\partial t} + \langle \nabla_{\mathbf{x}} \varphi_\lambda, \mathbf{A} + \mathbf{A}_\varphi \rangle + \langle \Sigma, \text{Hess}_{\mathbf{x}} \varphi_\lambda \rangle - \left(\frac{q}{\lambda} + q_\varphi\right) \varphi_\lambda = 0$$

$$\hat{\varphi}_\lambda(t_0, \mathbf{x}) \varphi_\lambda(t_0, \mathbf{x}) = \rho_0(\mathbf{x}), \quad \hat{\varphi}_\lambda(t_1, \mathbf{x}) \varphi_\lambda(t_1, \mathbf{x}) = \rho_1(\mathbf{x})$$

where

$$\mathbf{A}_\varphi := (\lambda \mathbf{B} \mathbf{B}^\top - 2\Sigma) \nabla_{\mathbf{x}} \log \varphi_\lambda \quad \text{and} \quad q_\varphi := \frac{1}{2} (\nabla_{\mathbf{x}} \log \varphi_\lambda)^\top (\lambda \mathbf{B} \mathbf{B}^\top - 2\Sigma) \nabla_{\mathbf{x}} \log \varphi_\lambda$$

Special Case of CASB with $\mathbf{B}\mathbf{B}^\top \propto \Sigma$

Decoupled linear reaction-advection-diffusion PDEs

$$\frac{\partial \hat{\varphi}_\lambda}{\partial t} + \nabla_{\mathbf{x}} \cdot (\hat{\varphi}_\lambda \mathbf{A}) - \Delta_\Sigma \hat{\varphi}_\lambda + \frac{q \hat{\varphi}_\lambda}{\lambda} = 0$$

$$\frac{\partial \varphi_\lambda}{\partial t} + \langle \nabla_{\mathbf{x}} \varphi, \mathbf{A} \rangle + \langle \Sigma, \text{Hess}_{\mathbf{x}} \varphi_\lambda \rangle - \frac{q \varphi_\lambda}{\lambda} = 0$$

$$\hat{\varphi}_\lambda(t_0, \mathbf{x}) \varphi_\lambda(t_0, \mathbf{x}) = \rho_0(\mathbf{x}), \quad \hat{\varphi}_\lambda(t_1, \mathbf{x}) \varphi_\lambda(t_1, \mathbf{x}) = \rho_1(\mathbf{x})$$

Conclusion: Hopf-Cole leads to decoupled linear PDEs iff $\mathbf{B}\mathbf{B}^\top \propto \Sigma$

Interpretation of $\mathbf{B}\mathbf{B}^\top \propto \Sigma$

↳ Noise ↓ $\Rightarrow$ Cost of optimal control ↑

↳ Noise ↑ $\Rightarrow$ Cost of optimal control ↓



Post-advancement result # 2

**Markov kernel for classical SB with
quadratic state cost: derived 3 ways**

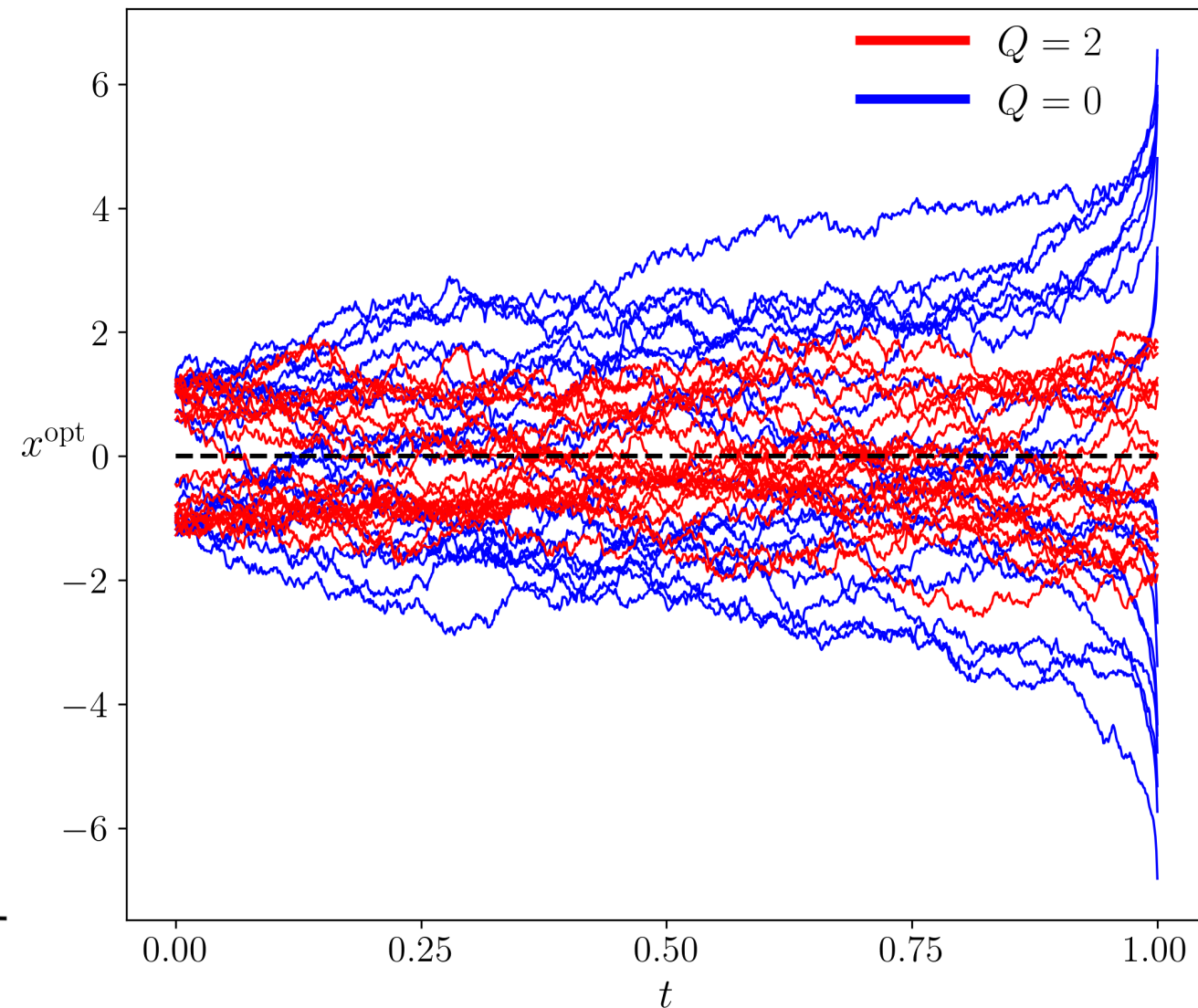


Classical SB: $q = \frac{1}{2} \mathbf{x}^\top \mathbf{Q} \mathbf{x}$, $r = \frac{1}{2} \|\cdot\|_2^2$, $f = u$, $\sigma = \sqrt{2} \mathbf{I}$

Quadratic state cost with $\mathbf{Q} \geq \mathbf{0}$

- ↳ biases sample paths toward desired level at all times
- ↳ a soft way to promote regulation/safety

After Hopf-Cole transform with $\varepsilon = 1$



$$\begin{aligned}\frac{\partial \hat{\varphi}}{\partial t} &= \left(\Delta_x - \frac{1}{2} \mathbf{x}^\top \mathbf{Q} \mathbf{x} \right) \hat{\varphi} \\ \frac{\partial \varphi}{\partial t} &= \left(-\Delta_x + \frac{1}{2} \mathbf{x}^\top \mathbf{Q} \mathbf{x} \right) \varphi\end{aligned}$$

forward-backward reaction-diffusion PDEs with quadratic reaction rate

First Way: Hermite Polynomial Gymnastics

Eigen-decomposition $\frac{1}{2}\mathbf{Q} = \mathbf{V}^\top \mathbf{\Lambda} \mathbf{V}$

Change of variable $\mathbf{y} := \mathbf{V}\mathbf{x}$ gives

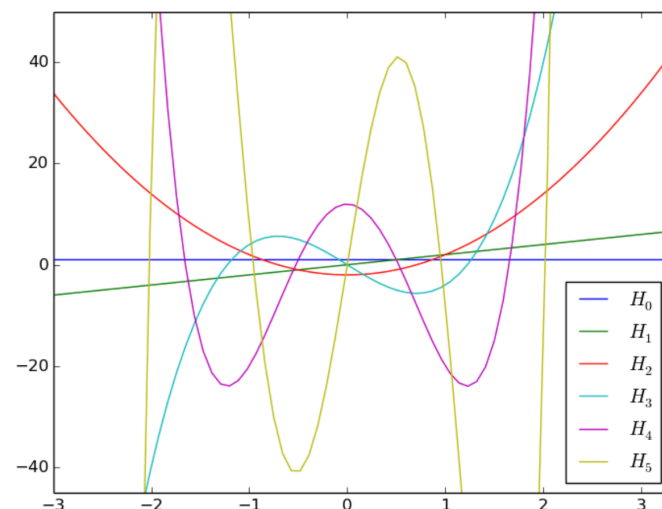
$$\frac{\partial \hat{\eta}}{\partial t} = \Delta_{\mathbf{y}} \hat{\eta} - (\mathbf{y}^\top \mathbf{\Lambda} \mathbf{y}) \hat{\eta} = \sum_{i=1}^n \left(\frac{\partial^2}{\partial y_i^2} - \lambda_i y_i^2 \right) \hat{\eta}$$

where $\hat{\eta}(0, \mathbf{y}) = \hat{\varphi}(0, \mathbf{x} = \mathbf{V}^\top \mathbf{y})$

Apply separation of variables $\hat{\eta}(t, \mathbf{y}) = T(t) \prod_{i=1}^n Y_i(y_i)$

physicists' Hermite polynomial

and notice soln of $\frac{d^2 Y}{dy^2} - (\lambda y^2 + c)Y = 0$ are $Y = a \exp\left(-\frac{y^2 \sqrt{\lambda}}{2}\right) H_n(\lambda^{1/4} y)$



$$H_n(x) := (-1)^n e^{x^2} \frac{d^n}{dx^n} (e^{-x^2})$$

of degree $n = -\frac{c}{2\sqrt{\lambda}} - \frac{1}{2} \in \mathbb{N}_0$

First Way: Hermite Polynomial Gymnastics

For $\mathbf{Q} \succ \mathbf{0}$

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

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

and

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

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

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

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

First Way: Hermite Polynomial Gymnastics

For $\mathbf{Q} \succeq \mathbf{0}$

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

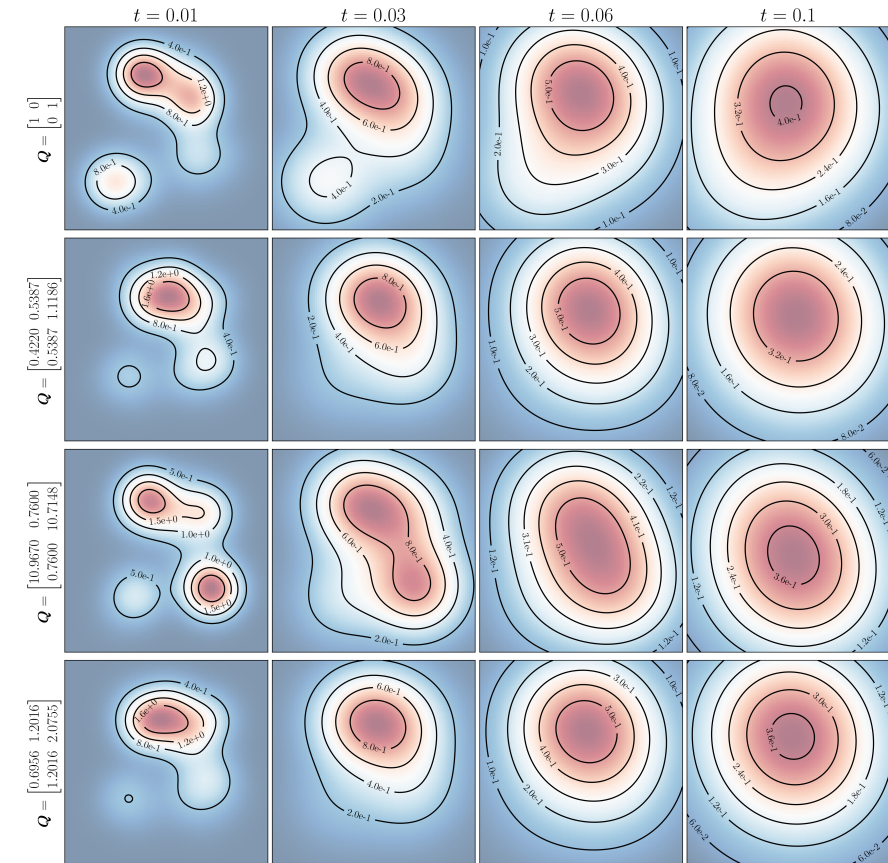
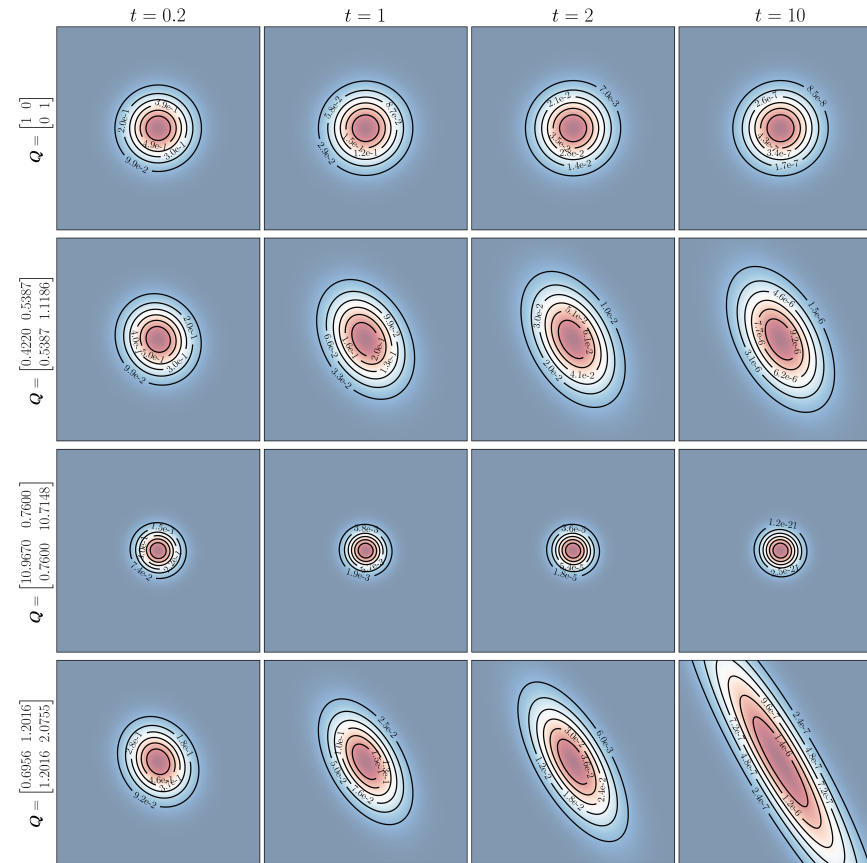
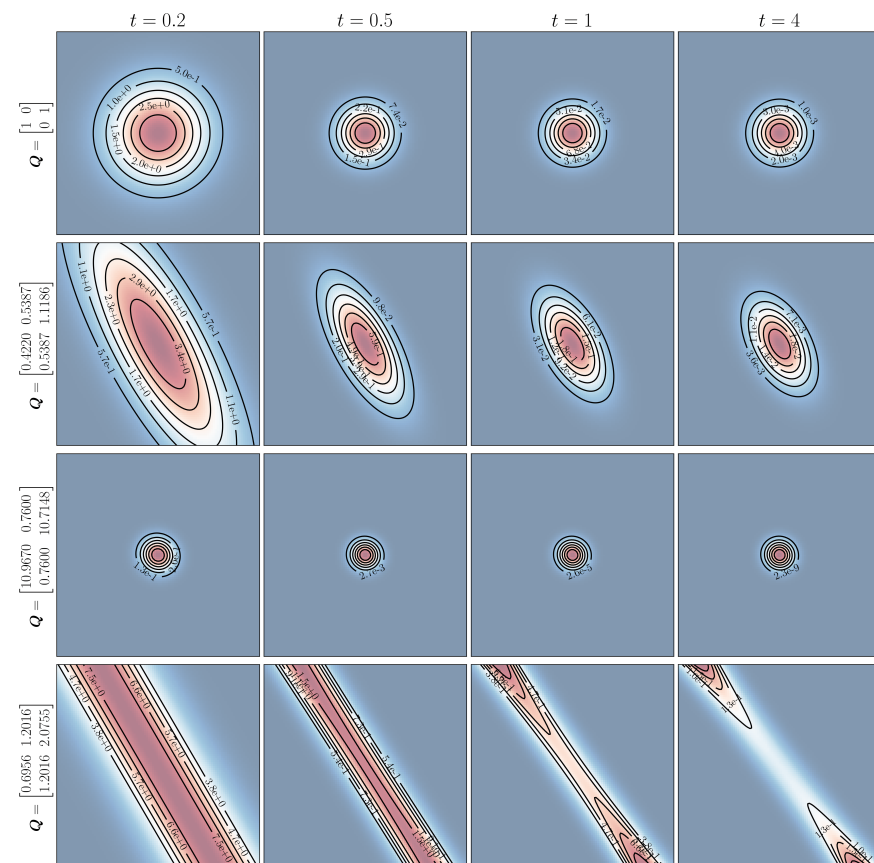
Action of kernel in $\mathbf{x}$ coordinates

$$\hat{\varphi}_0(\mathbf{x}) = \mathbf{1}$$

$$\hat{\varphi}_0(\mathbf{x}) \sim \mathcal{N}(0, \mathbf{I})$$

scaled Himmelblau function

$$\hat{\varphi}_0(\mathbf{x}) \propto \exp\left(-\frac{f(\mathbf{x}_1, \mathbf{x}_2)}{35}\right)$$



Second Way: Weyl Calculus

PDE $\longrightarrow$ Weyl operator $H(X, D) \longrightarrow$ Weyl symbol $h(x, \xi) \longrightarrow$ Kernel κ

Step 1: PDE $\longrightarrow$ Weyl operator $H(X, D)$

Let $X_k := x_k, \quad D_k := \frac{1}{i} \frac{\partial}{\partial x_k} \quad \forall k \in [n]$

$$\mathbf{X} := (X_1 \quad \dots \quad X_n)^\top, \quad \mathbf{D} := (D_1 \quad \dots \quad D_n)^\top$$

Write the semigroup $\exp(-(t - t_0)\mathcal{L})$ in terms of $\mathbf{X}, \mathbf{D}$

Weyl operator is a composition:

$$Q_\Lambda(\mathbf{X}, \mathbf{D}) := |\mathbf{D}|^2 + \sum_{k=1}^n \lambda_k X_k^2$$

$$H_\Lambda(\mathbf{X}, \mathbf{D}) = \exp(-(t - t_0)Q_\Lambda(\mathbf{X}, \mathbf{D}))$$

Second Way: Weyl Calculus

Step 2 (non-trivial): Weyl operator $H(X, D) \longrightarrow$ Weyl symbol $h(\mathbf{x}, \boldsymbol{\xi})$

Derive a PDE IVP for the Weyl symbol

$$\frac{\partial}{\partial t} h_{\Lambda}(\mathbf{x}, \boldsymbol{\xi}) = - \sum_{j=0}^2 \frac{1}{j!} \{q_{\Lambda}, h_{\Lambda}\}_j(\mathbf{x}, \boldsymbol{\xi}), \quad h_{\Lambda}|_{t=t_0} = 1$$

where $q_{\Lambda}(\mathbf{x}, \boldsymbol{\xi}) = |\boldsymbol{\xi}|^2 + \sum_{k=1}^n \lambda_k x_k^2$ and the j th order Poisson bracket

$$\{f, g\}_j(\mathbf{x}, \boldsymbol{\xi}) := \left(\frac{1}{2i}\right)^j \left(\sum_{k=1}^n \left(\frac{\partial^2}{\partial y_k \partial \xi_k} - \frac{\partial^2}{\partial x_k \partial \nu_k}\right)\right)^j f(\mathbf{x}, \boldsymbol{\xi}) g(\mathbf{y}, \boldsymbol{\eta})|_{\mathbf{y}=\mathbf{x}, \boldsymbol{\eta}=\boldsymbol{\xi}} \quad \forall j = 0, 1, 2, \dots$$

Solution of this PDE IVP:

$$h_{\Lambda}(\mathbf{x}, \boldsymbol{\xi}) = \left(\prod_{k=1}^n \frac{1}{\cosh(\sqrt{\lambda_k}(t - t_0))}\right) \exp\left(-\sum_{k=1}^n \frac{\lambda_k x_k^2 + \xi_k^2}{\sqrt{\lambda_k}} \tanh(\sqrt{\lambda_k}(t - t_0))\right)$$

Second Way: Weyl Calculus

Step 3: Weyl symbol $h(\mathbf{x}, \boldsymbol{\xi}) \longrightarrow$ Kernel κ

In general,

$$\kappa(t_0, \mathbf{x}, t, \mathbf{y}) = \frac{1}{(2\pi)^n} \int_{\mathbb{R}^n} h\left(\frac{\mathbf{x} + \mathbf{y}}{2}, \boldsymbol{\xi}\right) e^{i\langle \mathbf{x} - \mathbf{y}, \boldsymbol{\xi} \rangle} d\boldsymbol{\xi}$$

non-unitary inverse Fourier transform of $\boldsymbol{\xi} \mapsto h((\mathbf{x} + \mathbf{y})/2, \boldsymbol{\xi})$

Applying this to our Weyl symbol h_Λ gives

$$\kappa_\Lambda(t_0, \mathbf{x}, t, \mathbf{y})$$

$$= \left(\prod_{k=1}^n \frac{\lambda_k^{1/4}}{\sqrt{2\pi \sinh(2\sqrt{\lambda_k}(t - t_0))}} \right)$$

$$\times \exp \left(- \sum_{k=1}^n \frac{\sqrt{\lambda_k}}{2} (x_k^2 + y_k^2) \frac{\cosh(2\sqrt{\lambda_k}(t - t_0))}{\sinh(2\sqrt{\lambda_k}(t - t_0))} \right)$$

$$\times \exp \left(\sum_{k=1}^n \sqrt{\lambda_k} x_k y_k \left(\frac{1}{\sinh(2\sqrt{\lambda_k}(t - t_0))} \right) \right)$$

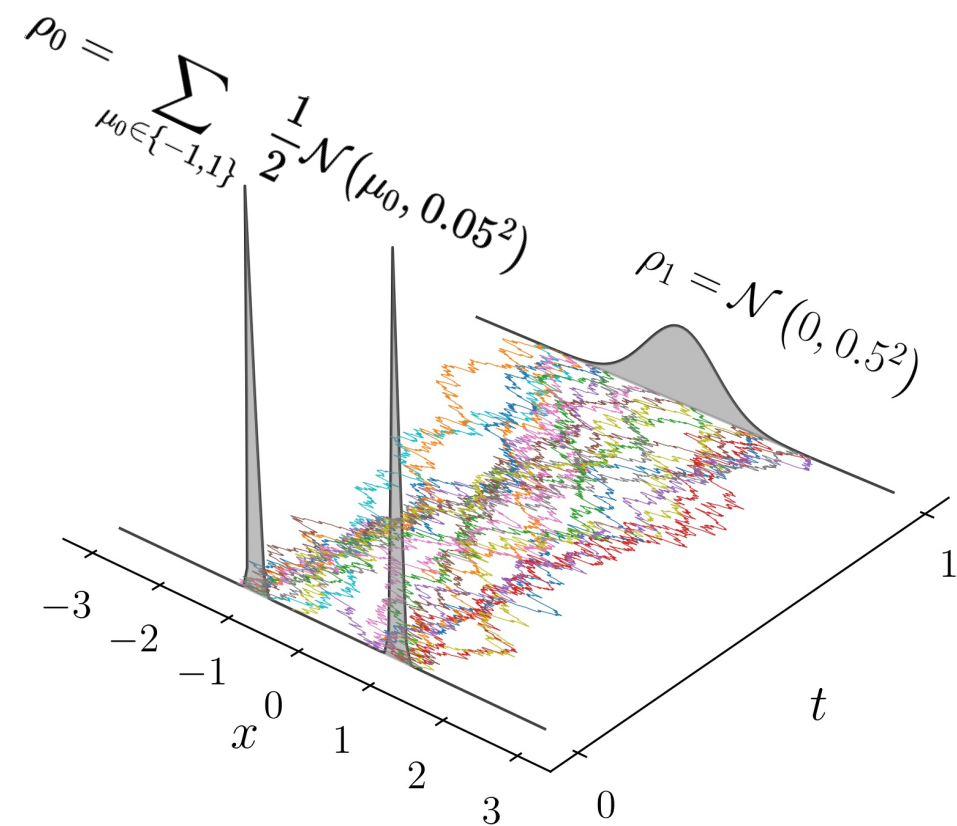
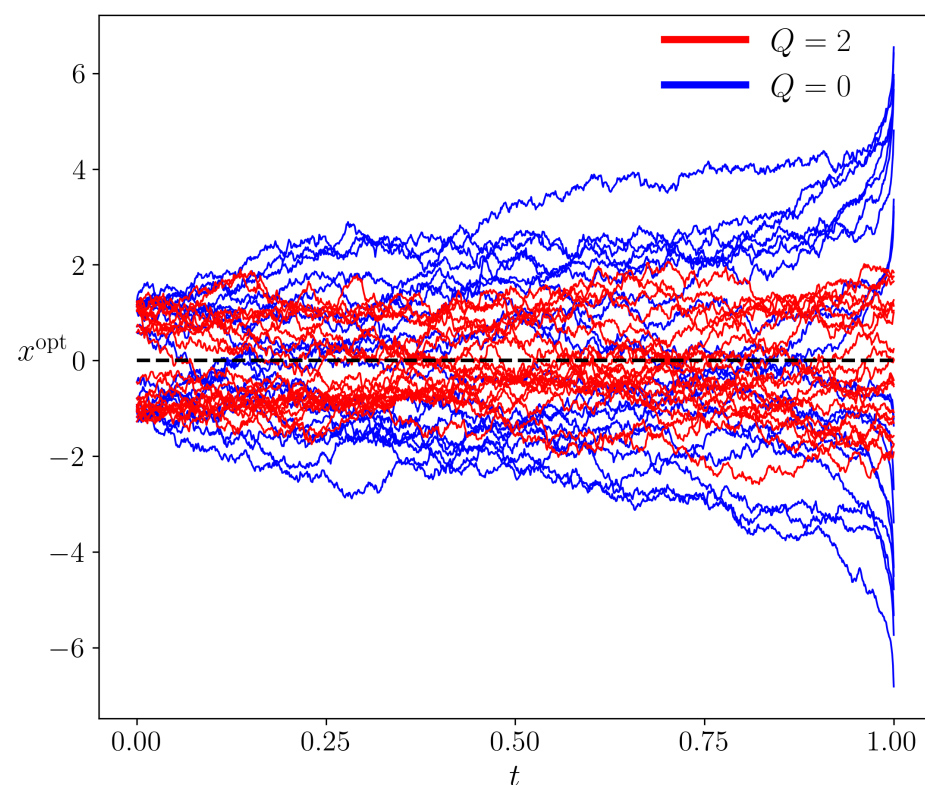
Same kernel obtained
via first way

Second Way: Weyl Calculus

Permits generalization for affine term: $q(\mathbf{z}) = \frac{1}{2} \mathbf{z}^\top \mathbf{Q} \mathbf{z} + \mathbf{r}^\top \mathbf{z} + s, \quad \mathbf{Q} \succ \mathbf{0}$

$$\begin{aligned} & \kappa_{(\Lambda, \mathbf{r}, s)}(t_0, \mathbf{x}, t, \mathbf{y}) \\ &= \left(\prod_{k=1}^n \frac{\lambda_k^{1/4} \exp(-c_k(t - t_0))}{\sqrt{2\pi \sinh(2\sqrt{\lambda_k}(t - t_0))}} \right) \\ & \times \exp \left(\sum_{k=1}^n -\frac{\sqrt{\lambda_k}}{2} (x_k^2 + y_k^2) \frac{\cosh(2\sqrt{\lambda_k}(t - t_0))}{\sinh(2\sqrt{\lambda_k}(t - t_0))} + \frac{\sqrt{\lambda_k} x_k y_k}{\sinh(2\sqrt{\lambda_k}(t - t_0))} - \frac{\left(\frac{1}{2} \mathbf{r}^\top \mathbf{v}_k (x_k + y_k) + \frac{1}{4\lambda_k} (\mathbf{r}^\top \mathbf{v}_k)^2 \right) \tanh(\sqrt{\lambda_k}(t - t_0))}{\sqrt{\lambda_k}} \right) \end{aligned}$$

$$c_k := \frac{1}{4\lambda_k} (\mathbf{r}^\top \mathbf{v}_k)^2 - \frac{s}{n}, \quad \mathbf{v}_k \text{ is } k\text{th column of } \mathbf{V}^\top$$



Post-advancement result # 3

**Markov kernel for LQSB
(subsumes previous kernel)**



$$\text{LQSB: } q = \frac{1}{2} \mathbf{x}^\top \mathbf{Q}_t \mathbf{x}, r = \frac{1}{2} \|\cdot\|_2^2, \mathbf{f} = \mathbf{A}_t \mathbf{x} + \mathbf{B}_t \mathbf{u}, \boldsymbol{\sigma} = \sqrt{2} \mathbf{B}_t$$

Assume

↳ controllable $(\mathbf{A}_t, \mathbf{B}_t)$ and $\mathbf{Q}_t \succeq \mathbf{0}$ are continuous and bounded

↳ $\mathbf{Q}_t \succ \mathbf{0}$ for some sub-interval (measure zero is okay) of time

To solve this LQSB with **generic non-Gaussian endpoints**, determine closed-form of Markov (not transition probability) kernel k

k is Green's function for the linear reaction-advection-diffusion PDE

$$\frac{\partial k}{\partial t} = -\langle \nabla_{\mathbf{x}}, k \mathbf{A}_t \mathbf{x} \rangle + \langle \mathbf{B}_t \mathbf{B}_t^\top, \nabla_{\mathbf{x}}^2 k \rangle - \frac{1}{2} \mathbf{x}^\top \mathbf{Q}_t \mathbf{x} k$$

Previous kernel was for the special case $\mathbf{A}_t = \mathbf{0}, \mathbf{B}_t = \mathbf{I} \ \forall t \in [t_0, t_1]$

Markov Kernels and Distances

We observe that known Markov kernels (including our earlier) look like

$$k = c(t, t_0) \exp\left(-\frac{1}{2} \text{dist}_{tt_0}^2(\mathbf{x}, \mathbf{y})\right)$$

Distance function $\text{dist}_{tt_0}^2 : \mathbb{R}^n \times \mathbb{R}^n \mapsto \mathbb{R}_{\geq 0}$ induced by

$$\frac{1}{2} \text{dist}_{tt_0}^2(\mathbf{x}, \mathbf{y}) = \min_{\mathbf{u}_\tau} \int_{t_0}^t \left(\frac{1}{2} \|\mathbf{u}(\tau)\|_2^2 + q(\mathbf{z}(\tau)) \right) d\tau$$

and constrained by controlled ODE from Itô diffusion + BCs

We derive the kernel in terms of an associated Riccati matrix ODE solution

Computational Pipeline

deterministic OCP

$$\frac{1}{2} \text{dist}_{tt_0}^2(\mathbf{x}, \mathbf{y}) = \min_{\mathbf{u}_\tau} \int_{t_0}^t \left(\frac{1}{2} \|\mathbf{u}(\tau)\|_2^2 + \frac{1}{2} (\mathbf{z}(\tau))^\top \mathbf{Q}(\tau) \mathbf{z}(\tau) \right) d\tau$$
$$\dot{\mathbf{z}}(\tau) = \mathbf{A}(\tau) \mathbf{z}(\tau) + \sqrt{2} \mathbf{B}(\tau) \mathbf{u}(\tau),$$
$$\mathbf{z}(\tau = t_0) = \mathbf{x}, \quad \mathbf{z}(\tau = t) = \mathbf{y}$$

Computational Pipeline

deterministic OCP

$$\frac{1}{2} \text{dist}_{tt_0}^2(\mathbf{x}, \mathbf{y}) = \min_{\mathbf{u}_\tau} \int_{t_0}^t \left(\frac{1}{2} \|\mathbf{u}(\tau)\|_2^2 + \frac{1}{2} (\mathbf{z}(\tau))^\top \mathbf{Q}(\tau) \mathbf{z}(\tau) \right) d\tau$$

$$\begin{aligned} \dot{\mathbf{z}}(\tau) &= \mathbf{A}(\tau) \mathbf{z}(\tau) + \sqrt{2} \mathbf{B}(\tau) \mathbf{u}(\tau), \\ \mathbf{z}(\tau = t_0) &= \mathbf{x}, \quad \mathbf{z}(\tau = t) = \mathbf{y} \end{aligned}$$

.....
 : Relate to cost of min energy
 : state transfer via solution map
 : $\Pi(\tau, \mathbf{K}_1, t)$ for Riccati matrix
 : ODE IVP

$$\hat{\Phi}_{tt_0}, \hat{\Gamma}_{tt_0}$$

are the state transition matrix
and the controllability Gramian
for the closed-loop system

$$\text{dist}_{tt_0}^2(\cdot, \cdot)$$

$$\frac{1}{2} \text{dist}_{tt_0}^2(\mathbf{x}, \mathbf{y}) = \frac{1}{2} \begin{pmatrix} \mathbf{x} \\ \mathbf{y} \end{pmatrix}^\top \mathbf{M}_{tt_0} \begin{pmatrix} \mathbf{x} \\ \mathbf{y} \end{pmatrix}$$

$$\text{where } \mathbf{M}_{tt_0} := \begin{bmatrix} \hat{\Phi}_{tt_0}^\top \hat{\Gamma}_{tt_0}^{-1} \hat{\Phi}_{tt_0} + \Pi(t_0, \mathbf{0}, t) & -\hat{\Phi}_{tt_0}^\top \hat{\Gamma}_{tt_0}^{-1} \\ -\hat{\Gamma}_{tt_0}^{-1} \hat{\Phi}_{tt_0} & \hat{\Gamma}_{tt_0}^{-1} \end{bmatrix}$$

Computational Pipeline

deterministic OCP



$\text{dist}^2_{tt_0}(\cdot, \cdot)$



Markov kernel k

$$\frac{1}{2} \text{dist}^2_{tt_0}(\mathbf{x}, \mathbf{y}) = \frac{1}{2} \begin{pmatrix} \mathbf{x} \\ \mathbf{y} \end{pmatrix}^\top \mathbf{M}_{tt_0} \begin{pmatrix} \mathbf{x} \\ \mathbf{y} \end{pmatrix},$$

where $\mathbf{M}_{tt_0} := \begin{bmatrix} \hat{\Phi}_{tt_0}^\top \hat{\Gamma}_{tt_0}^{-1} \hat{\Phi}_{tt_0} + \mathbf{\Pi}(t_0, \mathbf{0}, t) & -\hat{\Phi}_{tt_0}^\top \hat{\Gamma}_{tt_0}^{-1} \\ -\hat{\Gamma}_{tt_0}^{-1} \hat{\Phi}_{tt_0} & \hat{\Gamma}_{tt_0}^{-1} \end{bmatrix}$



.....
 : Substitute k into $\frac{\partial k}{\partial t} = (L - q)k$
 : with $k_0 = \delta(\mathbf{x} - \mathbf{y})$ and solve
 : reaction-advection-diffusion PDE.
 :

$$k(t_0, \mathbf{x}, t, \mathbf{y}) = a \exp\left(-\int_{t_0}^t \theta(s) ds\right) \times \exp\left(-\frac{1}{2} \begin{pmatrix} \mathbf{x} \\ \mathbf{y} \end{pmatrix}^\top \mathbf{M}_{tt_0} \begin{pmatrix} \mathbf{x} \\ \mathbf{y} \end{pmatrix}\right)$$

where $\theta(\tau) := \text{tr}(\mathbf{A}(\tau) + \mathbf{B}(\tau)\mathbf{B}(\tau)^\top \mathbf{M}_{11}(\tau, t_0))$,

$$a := (2\pi)^{-n/2} \lim_{t \downarrow t_0} \det\left(\mathbf{M}_{11}^{1/2}(t, t_0) \times \exp \int_{t_0}^t (\mathbf{A}(\tau) + \mathbf{B}(\tau)\mathbf{B}(\tau)^\top \mathbf{M}_{11}(\tau, t_0)) d\tau\right)$$

Post-advancement result # 4

**Back to quantum: can we recast CASB
as wave steering?**



From CASB to Quantum

Recap CASB problem:

$$\begin{aligned} & \arg \inf_{(\rho, \mathbf{u}) \in \mathcal{P}_{01} \times \mathcal{U}} \int_{t_0}^{t_1} \int_{\mathbb{R}^n} \left(q(t, \mathbf{x}) + \frac{1}{2} \|\mathbf{u}\|_2^2 \right) \rho(t, \mathbf{x}) d\mathbf{x} dt \\ & \frac{\partial \rho}{\partial t} + \nabla_{\mathbf{x}} \cdot (\rho(\mathbf{A}(t, \mathbf{x}) + \mathbf{B}(t, \mathbf{x})\mathbf{u})) = \Delta_{\Sigma(t, \mathbf{x}, \mathbf{u})} \rho \\ & \rho(t = t_0, \mathbf{x}) = \rho_0, \quad \rho(t = t_1, \mathbf{x}) = \rho_1 \end{aligned}$$

Apply Madelung transform $(\rho_{\text{opt}}, S) \mapsto (\psi, \psi^\dagger)$

$$\begin{aligned} \psi &:= \exp\left(R + \frac{i}{\lambda} S\right) \quad \text{where} \quad R := \frac{1}{2} \log \rho_{\text{opt}} \\ \psi^\dagger &:= \exp\left(R - \frac{i}{\lambda} S\right) \end{aligned}$$

Born's relation

$$\rho_{\text{opt}}(t, \mathbf{x}) = \psi(t, \mathbf{x}) \psi^\dagger(t, \mathbf{x}) \quad \forall t \in [t_0, t_1]$$

Nonlinear Schrödinger PDE BVP in ψ

$$i\lambda \frac{\partial \psi}{\partial t} = -\frac{\lambda^2}{2} \Delta_{\Sigma} \psi + \overset{\text{complex-valued potential}}{V_{\text{the control-affine SB}}} \psi$$

$$\psi(t_0, \mathbf{x}) \psi^{\dagger}(t_0, \mathbf{x}) = \rho_0, \quad \psi(t_1, \mathbf{x}) \psi^{\dagger}(t_1, \mathbf{x}) = \rho_1$$

$$\begin{aligned} \Re(V_{\text{the control-affine SB}}) = & \frac{\lambda^2}{2} \langle \text{Hess}_{\mathbf{x}}, \boldsymbol{\Sigma} \rangle + \frac{\lambda^2}{2} \langle \boldsymbol{\Sigma}, \text{Hess}_{\mathbf{x}} R \rangle + \langle \nabla_{\mathbf{x}} S, \mathbf{A} \rangle \\ & + \frac{\lambda^2}{2} \|\nabla_{\mathbf{x}} R\|_{\boldsymbol{\Sigma}}^2 - \frac{1}{2} \|\nabla_{\mathbf{x}} S\|_{\boldsymbol{\Sigma}}^2 + \lambda^2 \langle \nabla_{\mathbf{x}} \cdot \boldsymbol{\Sigma}, \nabla_{\mathbf{x}} R \rangle \\ & + \frac{1}{2} \langle \nabla_{\mathbf{x}} S, \mathbf{B} \mathbf{B}^{\top} \nabla_{\mathbf{x}} S \rangle + \frac{1}{2} \langle \boldsymbol{\Sigma}, \text{Hess}_{\mathbf{x}} S \rangle - q \end{aligned}$$

$$\begin{aligned} \Im(V_{\text{the control-affine SB}}) = & \lambda \left\{ \frac{1}{2} \langle \boldsymbol{\Sigma}, \text{Hess}_{\mathbf{x}} S \rangle + (\nabla_{\mathbf{x}} R)^{\top} \boldsymbol{\Sigma} (\nabla_{\mathbf{x}} S) + \langle \nabla_{\mathbf{x}} \cdot \boldsymbol{\Sigma}, \nabla_{\mathbf{x}} S \rangle \right. \\ & - \langle \nabla_{\mathbf{x}} R, \mathbf{A} + \mathbf{B} \mathbf{B}^{\top} \nabla_{\mathbf{x}} S \rangle - \frac{1}{2} \nabla_{\mathbf{x}} \cdot (\mathbf{A} + \mathbf{B} \mathbf{B}^{\top} \nabla_{\mathbf{x}} S) \\ & \left. + \frac{1}{2} \Delta_{\Sigma} R + (\nabla_{\mathbf{x}} R)^{\top} \boldsymbol{\Sigma} \nabla_{\mathbf{x}} R + \left(\frac{1}{4} - \frac{1}{2} R \right) \langle \text{Hess}_{\mathbf{x}}, \boldsymbol{\Sigma} \rangle \right\} \end{aligned}$$

The Wave BVP Specialized for Classical SB

$$i\frac{\partial\psi}{\partial t} = -\frac{1}{2}\Delta_x\psi + \overset{\text{complex-valued potential}}{V_{\text{the classical SB}}}\psi$$

where

$$\Re(V_{\text{the classical SB}}) = \frac{1}{2}\Delta_x R + \frac{1}{2}\|\nabla_x R\|_2^2 + \frac{1}{2}\Delta_x S$$

$$\Im(V_{\text{the classical SB}}) = \frac{1}{2}\Delta_x R + \|\nabla_x R\|_2^2$$



$$\frac{\partial R}{\partial t} = -\langle \nabla_x R, \nabla_x S \rangle - \frac{1}{2}\Delta_x S + \Im(V_{\text{the classical SB}})$$

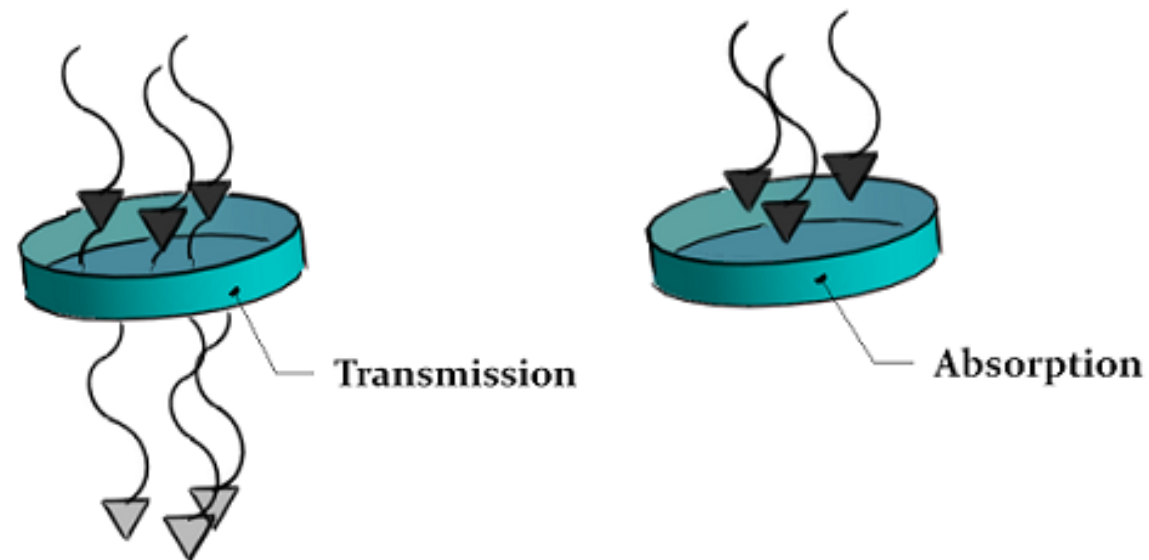
$$\frac{\partial S}{\partial t} = -\frac{1}{2}\|\nabla_x S\|_2^2 - \frac{1}{2}\Delta_x S$$

Interpretation of the Derived Complex Potentials

Real part = elastic scattering (transmission of wave function)

Imaginary part = inelastic scattering (absorption of wave function)

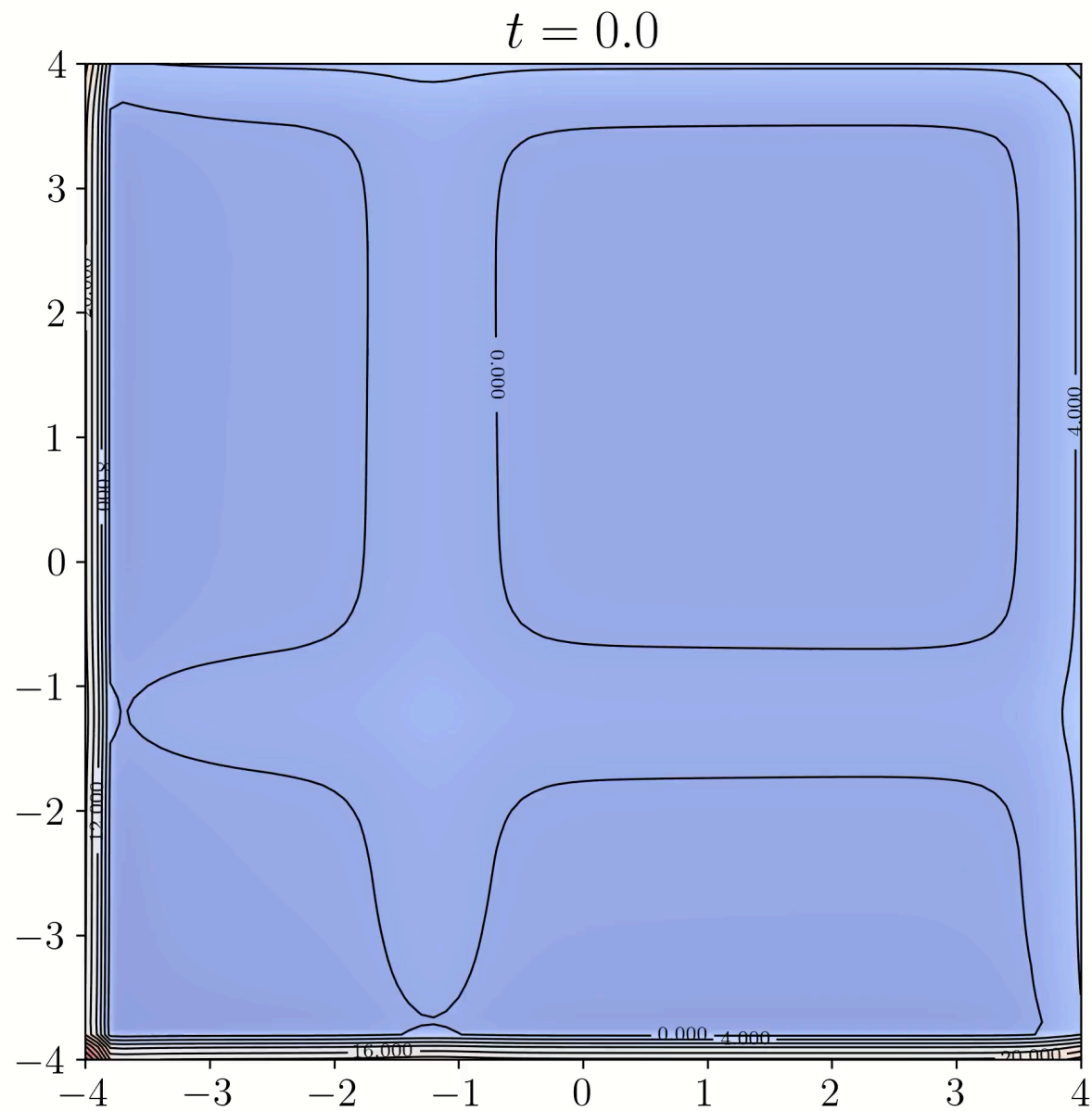
SB as a diffusion process induces a “medium”



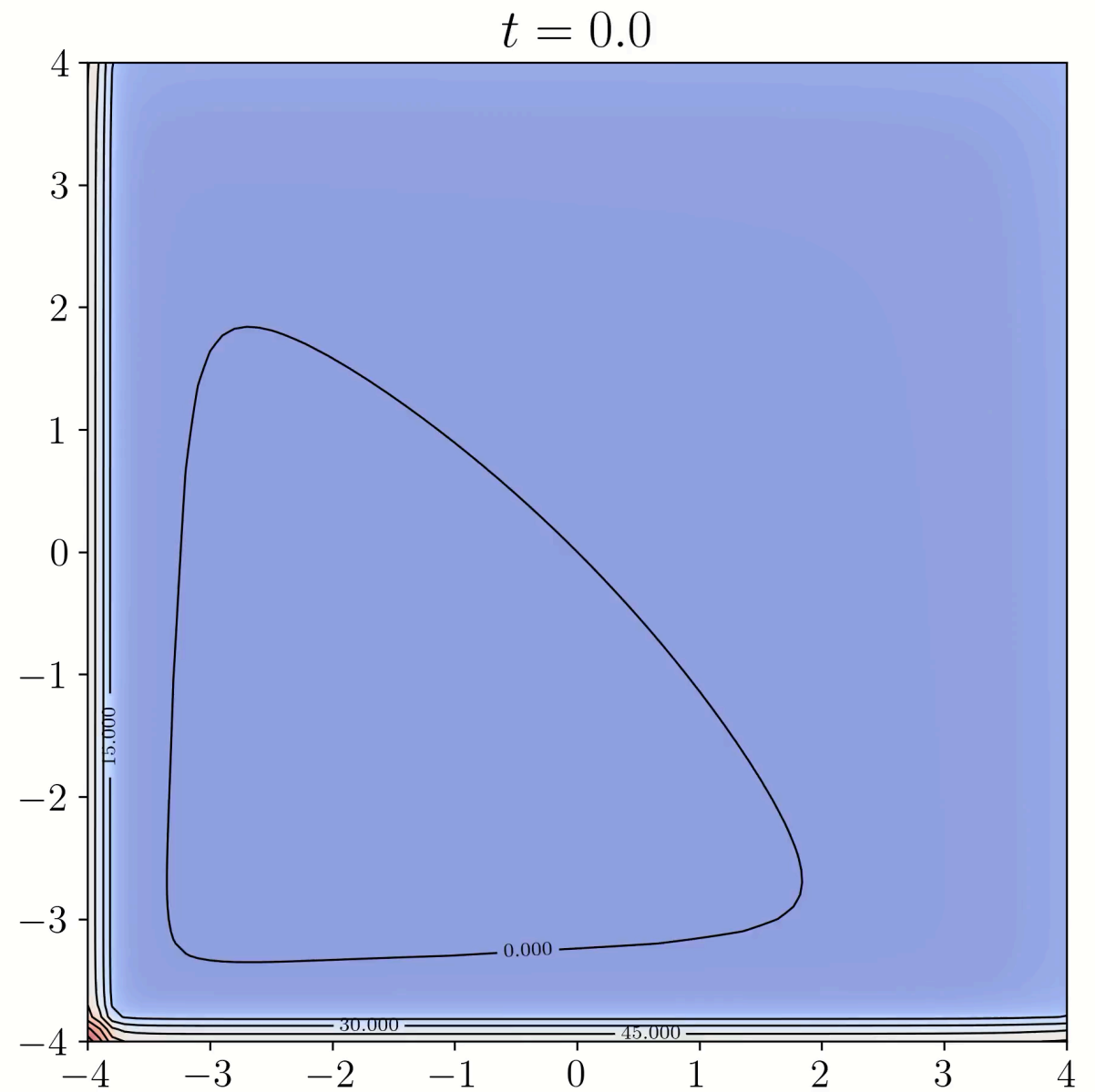
Similar to optical potential in nuclear physics

Example: Complex Potential for Classical SB

$$\Re(V_{\text{the classical SB}})$$



$$\Im(V_{\text{the classical SB}})$$



Generalization of Bohm Potential



D. Bohm (1951-54)

PHYSICAL REVIEW

VOLUME 96, NUMBER 1

OCTOBER 1, 1954

Model of the Causal Interpretation of Quantum Theory in Terms of a Fluid
with Irregular Fluctuations



PHYSICAL REVIEW

VOLUME 85, NUMBER 2

JANUARY 15, 1952

A Suggested Interpretation of the Quantum Theory in Terms of "Hidden" Variables. I



Bohm's 1952 paper:

$$\frac{\partial R}{\partial t} = -\langle \nabla_x R, \nabla_x S \rangle - \frac{1}{2} \Delta_x S$$

$$\frac{\partial S}{\partial t} = -\frac{1}{2} \|\nabla_x S\|_2^2 - \frac{1}{2} \Delta_x S - \frac{1}{2} \|\nabla_x R\|_2^2 - i\mathfrak{I}(V_{\text{the classical SB}})$$

Our result for Classical SB:

If $\mathfrak{I}(V_{\text{the classical SB}}) = 0$, SB
is a near match for Bohm

$$\frac{\partial R}{\partial t} = -\langle \nabla_x R, \nabla_x S \rangle - \frac{1}{2} \Delta_x S + \mathfrak{I}(V_{\text{the classical SB}})$$

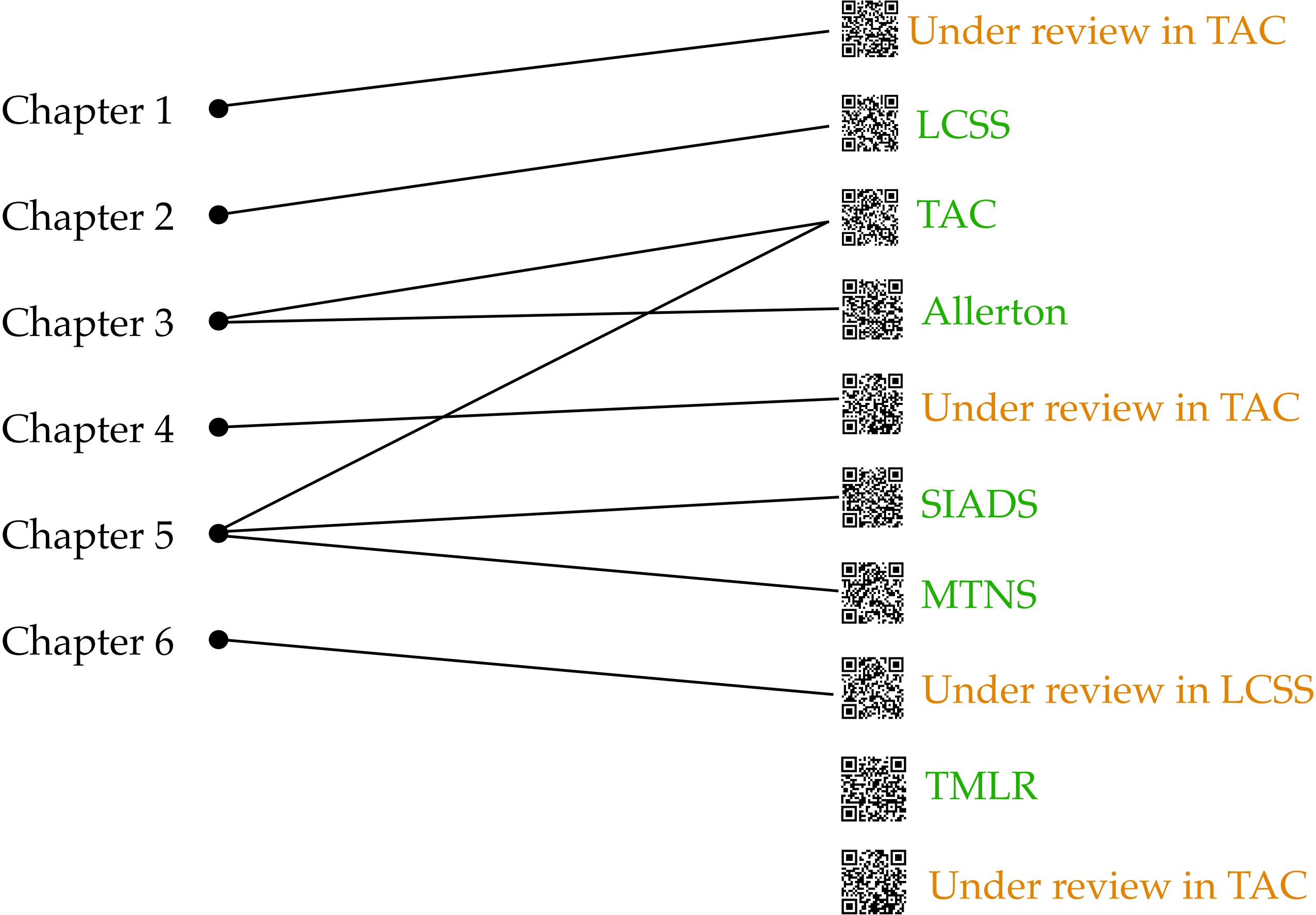
$$\frac{\partial S}{\partial t} = -\frac{1}{2} \|\nabla_x S\|_2^2 - \frac{1}{2} \Delta_x S$$

Summary

$$\text{SB} \subset \text{LQSB} \subset \text{CASB}$$

SB variant	Contributions made by this dissertation
LQSB	Derived worst-case contraction coefficient Derived Markov kernel for dynamic Sinkhorn
Lambertian SB (linear non-quadratic)	Proved probabilistic Lambert problem is generalized optimal mass transport Proved existence-uniqueness of solution for both with and without noise Dynamic Sinkhorn for numerical solution
CASB	Showed Hopf-Cole does not remove nonlinearity in general: possibility to generalize dynamic Sinkhorn Derived equiv. wave BVP: possibility for new algorithm

Publications by Dissertation Chapters



Acknowledgements

My heartfelt thanks to

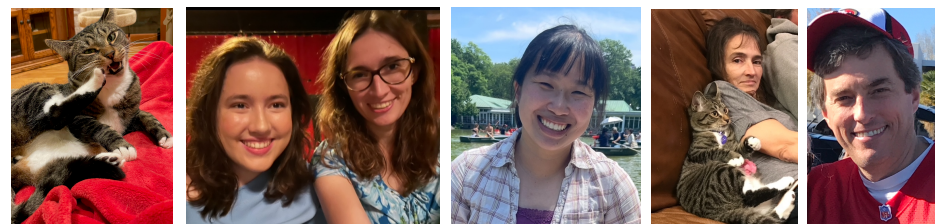
↳ my advisor



↳ my coauthors



↳ my friends and family



Generous funding supports from



2112755, 2111688



LDRD GS 25-ERD-044

Thank You

Backup Slides

Hilbert's Projective Metric d_{Hilbert}

A cone $\mathcal{K}$ is called pointed if $\mathcal{K} \cap -\mathcal{K} = \{0\}$

For any pointed convex cone $\mathcal{K}$ in a real vector space,

$$d_{\text{Hilbert}}(u, v) := \log \left(\frac{\inf\{\theta \geq 0 \mid \theta v \geq u\}}{\sup\{\theta \geq 0 \mid u \geq \theta v\}} \right) \quad \forall u, v \in \text{interior}(\mathcal{K})$$

Example. For $\mathcal{K} = \mathbb{R}_{\geq 0}^n$,

$$d_{\text{Hilbert}}(u, v) = \log \left(\frac{\max_{i=1, \dots, n} u_i / v_i}{\min_{i=1, \dots, n} u_i / v_i} \right)$$

Example. For $\mathcal{K} = \mathbb{S}_+^n$,

$$d_{\text{Hilbert}}(u, v) = \log \max\{\lambda_{\max}(u^{-1}v), \lambda_{\max}(v^{-1}u)\}$$

Hilbert's Projective Metric d_{Hilbert}

Nonnegativity. $d_{\text{Hilbert}}(u, v) \geq 0 \quad \forall (u, v) \in \text{interior}(\mathcal{K})$

Indiscernability. $d_{\text{Hilbert}}(u, v) = 0$ iff $u = \beta v$ for some $\beta > 0$

Symmetry. $d_{\text{Hilbert}}(u, v) = d_{\text{Hilbert}}(v, u)$

Triangle inequality. $d_{\text{Hilbert}}(u, w) \leq d_{\text{Hilbert}}(u, v) + d_{\text{Hilbert}}(v, w)$

Scale invariance. $d_{\text{Hilbert}}(\alpha u, \beta v) = d_{\text{Hilbert}}(u, v) \quad \forall \alpha, \beta > 0$