Weyl Calculus and Exactly Solvable Schrödinger Bridges with Quadratic State Cost

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The Problem

Solve linear reaction-diffusion PDE IVP:

$$\frac{\partial}{\partial t}\widehat{\varphi} = -\mathcal{L}\widehat{\varphi}, \quad \widehat{\varphi}(t = t_0, \boldsymbol{x}) = \widehat{\varphi}_0(\boldsymbol{x}) \text{ (given)}$$

where $\mathcal{L} \equiv -\Delta_{\boldsymbol{x}} + q(\boldsymbol{x})$

given bounded continuous reaction rate

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Our contribution: closed-form Green's function for convex quadratic $q(\boldsymbol{x})$

$$\widehat{\varphi}(t, \boldsymbol{x}) = \int_{\mathcal{X}} \kappa(t_0, \boldsymbol{x}, t, \boldsymbol{y})\widehat{\varphi}_0(\boldsymbol{y})\mathrm{d}\boldsymbol{y}$$

State-of-the-art

Randomized numerical solution via Feynman-Kac path integral

Estimates $\widehat{\varphi}(t, \boldsymbol{x})$ as conditional expectation

Good: meshless/particle-based

Bad: still needs function approximation

Our Motivation

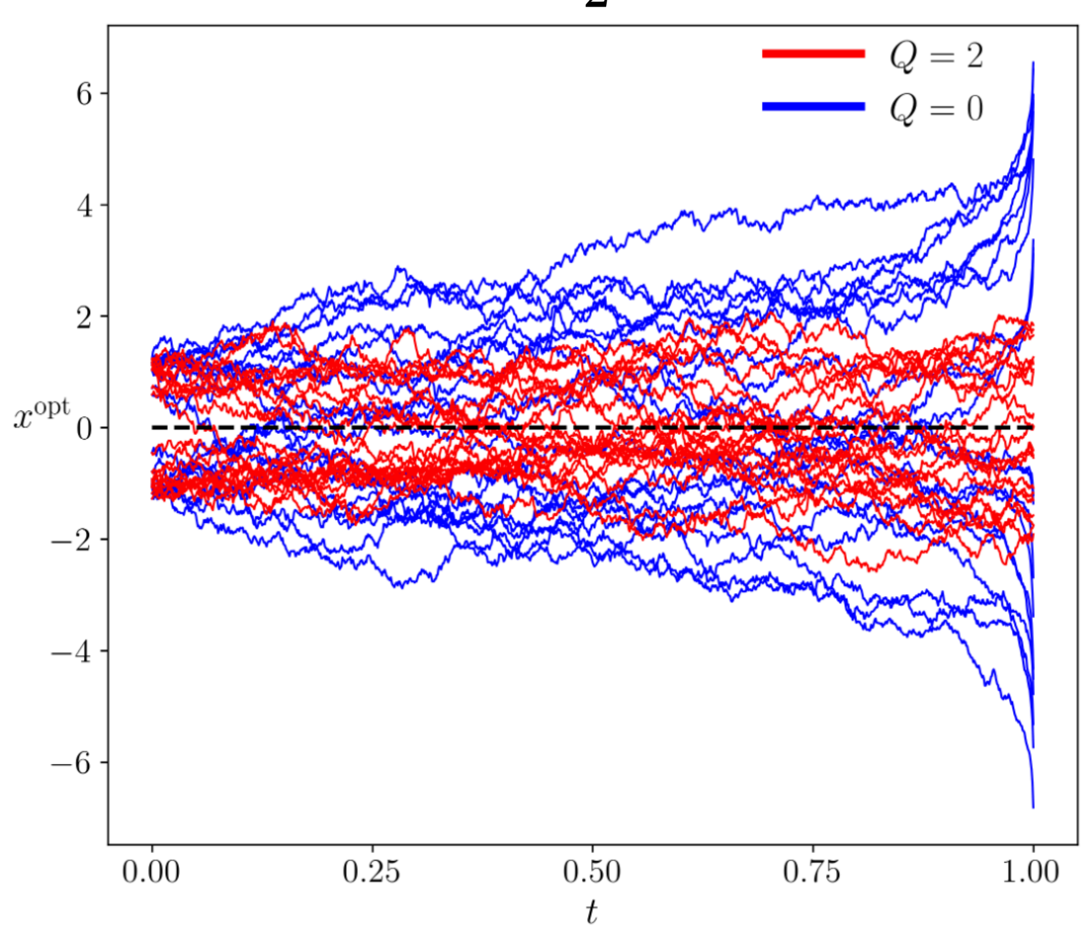
Schrödinger bridge problem with state cost

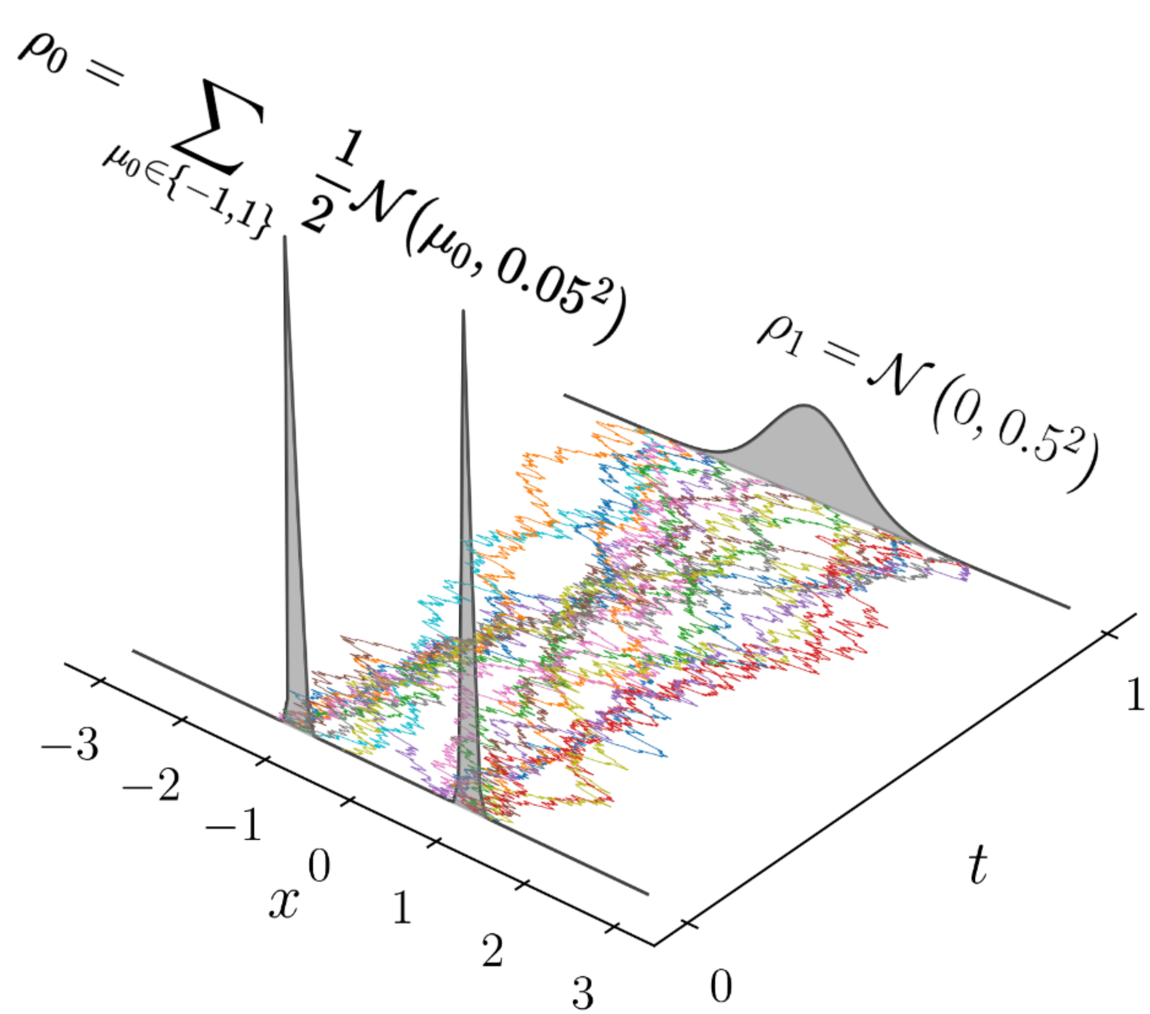
$$\inf_{(\mu^{\boldsymbol{u}},\boldsymbol{u})} \int_{\mathbb{R}^n} \int_{t_0}^{t_1} \left\{ \frac{1}{2} |\boldsymbol{u}|^2 + q(\boldsymbol{x}_t^{\boldsymbol{u}}) \right\} \mathrm{d}t \, \mathrm{d}\mu^{\boldsymbol{u}}(\boldsymbol{x}_t^{\boldsymbol{u}})$$

$$\text{subject to} \quad \mathrm{d}\boldsymbol{x}_t^{\boldsymbol{u}} = \boldsymbol{u}_t(t, \boldsymbol{x}_t^{\boldsymbol{u}}) \, \mathrm{d}t + \sqrt{2} \, \mathrm{d}\boldsymbol{w}_t,$$

$$\boldsymbol{x}_t^{\boldsymbol{u}}(t = t_0) \sim \mu_0, \quad \boldsymbol{x}_t^{\boldsymbol{u}}(t = t_1) \sim \mu_1,$$

$$q(x) = \frac{1}{2} Q x^2$$





Can be reduced to solving

Nonlinearly boundary coupled system of linear PDEs

$$\frac{\partial \widehat{\varphi}}{\partial t} = (\Delta_{\boldsymbol{x}} - q(\boldsymbol{x}))\widehat{\varphi},$$
$$\frac{\partial \varphi}{\partial t} = (-\Delta_{\boldsymbol{x}} + q(\boldsymbol{x}))\varphi,$$
$$\widehat{\varphi}(t=t_0,\cdot)\varphi(t=t_0,\cdot) = \mu_0, \quad \widehat{\varphi}(t=t_0,\cdot)\varphi(t=t_1,\cdot) = \mu_1$$

Equivalently, nonlinear integral equations (Schrödinger system)

$$\mu_0(\boldsymbol{x}) = \widehat{\varphi}_0(\boldsymbol{x}) \int \kappa(t_0,\boldsymbol{x},t_1,\boldsymbol{y})\varphi_1(\boldsymbol{y})\mathrm{d}\boldsymbol{y}$$
$$\mu_1(\boldsymbol{x}) = \widehat{\varphi}_1(\boldsymbol{x}) \int \kappa(t_0,\boldsymbol{y},t_1,\boldsymbol{x})\widehat{\varphi}_0(\boldsymbol{y})\mathrm{d}\boldsymbol{y}$$

Optimal solution: $\mu^{\boldsymbol{u}}_{\mathrm{opt}}(t,\cdot) = \widehat{\varphi}(t,\cdot)\varphi(t,\cdot), \quad \boldsymbol{u}_{\mathrm{opt}}(t,\cdot) = \nabla_{(\cdot)} \log \varphi(t,\cdot)$

The Case $q(x) = \frac{1}{2}x^\top Q x, \quad Q \geq 0$

Gaussian endpoints $\mu_0 = \mathcal{N}(\mathbf{0}, \mathbf{\Sigma}_0), \quad \mu_1 = \mathcal{N}(\mathbf{0}, \mathbf{\Sigma}_1)$

$\rightsquigarrow$ coupled Riccati ODEs studied in Chen, Georgiu, Pavon, *ACC 2015*

Non-Gaussian endpoints

$\rightsquigarrow$ need κ

Closed-form derivation of κ using Hermite polynomials
(elementary + painful + difficult to generalize)

arXiv:2406.00503

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ALEXIS M.H. TETER†, WENQING WANG‡, AND ABHISHEK HALDER§

More disciplined alternative: Weyl calculus

New Idea: Weyl Calculus to Compute κ

Originally developed for quantum mechanics

Appears less known to solve problems outside quantum mechanics

Many names: Weyl quantization, Wigner-Weyl transform

Proposed computational steps:

PDE $\longrightarrow$ Weyl operator $H(\boldsymbol{X}, D)$ $\longrightarrow$ Weyl symbol $h\left(\boldsymbol{x}, \boldsymbol{\xi}\right)$ $\longrightarrow$ Kernel κ

Step 1: PDE $\longrightarrow$ Weyl Operator $H(\boldsymbol{X}, \boldsymbol{D})$

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

$$\boldsymbol{X} := \begin{pmatrix} X_1 & \dots & X_n \end{pmatrix}^\top, \quad \boldsymbol{D} := \begin{pmatrix} D_1 & \dots & D_n \end{pmatrix}^\top$$

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

Example (Heat PDE).

$$\mathcal{L} \equiv -\Delta_{\boldsymbol{x}}, \quad |\boldsymbol{D}|^2 := \langle \boldsymbol{D}, \boldsymbol{D} \rangle = (-\mathrm{i})^2 \langle \nabla_{\boldsymbol{x}}, \nabla_{\boldsymbol{x}} \rangle = -\Delta_{\boldsymbol{x}}$$

Therefore, $\quad H_{\mathrm{heat}}(\boldsymbol{X}, \boldsymbol{D}) = \exp\Big(-(t - t_0)|\boldsymbol{D}|^2\Big)$

Step 1: PDE $\longrightarrow$ Weyl Operator $H(\boldsymbol{X}, \boldsymbol{D})$

Reaction-diffusion PDE:

$$\frac{\partial \widehat{\varphi}}{\partial t} = \left(\Delta_{\boldsymbol{z}} - \frac{1}{2}\boldsymbol{z}^\top \boldsymbol{Q}\boldsymbol{z}\right)\widehat{\varphi}, \quad \widehat{\varphi}(t_0, \cdot) = \widehat{\varphi}_0, \quad \text{w. l. o. g. } \boldsymbol{Q} \succ \boldsymbol{0}$$

$$\frac{1}{2}\boldsymbol{Q} = \boldsymbol{V}^\top \boldsymbol{\Lambda} \boldsymbol{V}$$

$$\boldsymbol{z} \mapsto \boldsymbol{x} := \boldsymbol{V}\boldsymbol{z}, \quad \hat{\nu}(t, \boldsymbol{x}) := \widehat{\varphi}\left(t, \boldsymbol{z} = \boldsymbol{V}^\top \boldsymbol{x}\right)$$

$$\frac{\partial \hat{\nu}}{\partial t} = \Delta_{\boldsymbol{x}}\hat{\nu} - \left(\boldsymbol{x}^\top \boldsymbol{\Lambda}\boldsymbol{x}\right)\hat{\nu} = \sum_{k=1}^{n}\left(\frac{\partial^2}{\partial x_k^2} - \lambda_k x_k^2\right)\hat{\nu}$$

Weyl operator is a composition:

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

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

Step 2: Weyl Operator $H(X, D) \longrightarrow$ Weyl Symbol $h(\boldsymbol{x}, \boldsymbol{\xi})$

Derive a PDE IVP for the Weyl symbol

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

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

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

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Solution of this PDE IVP:

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

Step 3: Weyl Symbol $h\left(\boldsymbol{x},\boldsymbol{\xi}\right) \longrightarrow$ Kernel κ

In general,

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

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

Applying this to our Weyl symbol $h_{\boldsymbol{\Lambda}}$ gives

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

Summary for the Derived κ_{Λ}

Recovers the formula in

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Limit $\frac{1}{2}\boldsymbol{Q} = \boldsymbol{\Lambda} \downarrow \boldsymbol{0}$ recovers the heat kernel

Special case $\frac{1}{2}\boldsymbol{Q} = \boldsymbol{\Lambda} = \boldsymbol{I}_n$ recovers the Mehler kernel in quantum mechanics

Summary for the Derived κ_{Λ} (contd.)

Permits generalization: $q(z) = \dfrac{1}{2} z^\top \boldsymbol{Q} z + \boldsymbol{r}^\top z + s, \quad \boldsymbol{Q} \succ \boldsymbol{0}$

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

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

Helps in solving the Schrödinger bridge problem with quadratic state cost:

$$\widehat{\varphi}(t,\boldsymbol{z}) = \hat{\nu}(t,\boldsymbol{x})\big|_{\boldsymbol{x}=\boldsymbol{V}\boldsymbol{z}} = \int_{\mathbb{R}^n} \kappa_{(\boldsymbol{\Lambda},\boldsymbol{r},s)}(t_0,\boldsymbol{V}\boldsymbol{z},t,\boldsymbol{y})\varphi_0\big(\boldsymbol{V}^\top\boldsymbol{y}\big)\mathrm{d}\boldsymbol{y}$$

Thank You

Details:

Support: 2112755, 2111688