Gradient flows and entropy inequalities for dissipative quantum systems

Jan Maas (IST Austria)

joint work with Eric Carlen

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Starting point:
Diffusion equations via optimal transport

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Jordan–Kinderlehrer–Otto '98: Beautiful connection between

- the 2-Kantorovich metric on the space of probability measures

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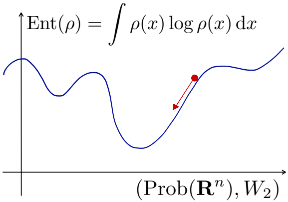
Theorem (J-K-O '98)

The heat flow is the gradient flow of the entropy w.r.t W_2.



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Gradient flows in $\mathbf{R}^n$

Let $\varphi : \mathbf{R}^n \to \mathbf{R}$ smooth and convex. For $u : \mathbf{R}_+ \to \mathbf{R}^n$ TFAE:

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$$\frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}t}|u(t) - y|^2 \leq \varphi(y) - \varphi(u(t)) \qquad \forall y \, .$$

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- applies to non-smooth problems
- leads to the synthetic notion of Ricci curvature: (Lott–Sturm–Villani theory in metric measure spaces)

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Question: Is there a discrete JKO-Theorem?

Discrete setting

Setting

- $\mathcal{X}$: finite set
- $Q(x, y)$: transition rate from x to y
- π: reversible measure, $\forall x, y \; : \; Q(x, y)\pi(x) = Q(y, x)\pi(y)$

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- Markov generator: $\mathcal{L}\psi(x) := \sum_y Q(x,y)(\psi(y) - \psi(x))$
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Relative Entropy

- $\mathcal{P}(\mathcal{X}) := \left\{ \rho : \mathcal{X} \to \mathbf{R}_+ \ \middle| \ \sum_{x\in\mathcal{X}} \rho(x)\pi(x) = 1 \right\}$
- $\mathrm{Ent}(\rho) := \sum_{x\in\mathcal{X}} \rho(x) \log \rho(x) \, \pi(x) , \qquad \rho \in \mathcal{P}(\mathcal{X}) .$

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No! (reason: $W_2(\mu_\alpha, \mu_\beta) = \sqrt{|\alpha - \beta|}$)

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What about the general discrete case?

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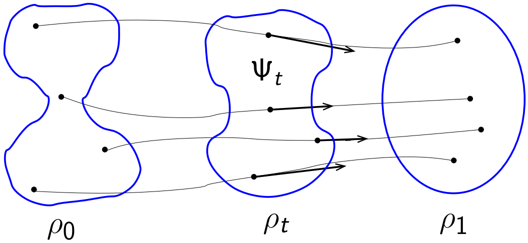

Back to $\mathbf{R}^n$: dynamical characterisation of W_2

Benamou-Brenier formula in $\mathbf{R}^n$

$$W_2(\rho_0,\rho_1)^2 = \inf_{\rho_\cdot,\Psi_\cdot} \left\{ \int_0^1 \int_{\mathbf{R}^n} |\Psi_t(x)|^2 \rho_t(x)\,\mathrm{d}x\,\mathrm{d}t \ : \right.$$

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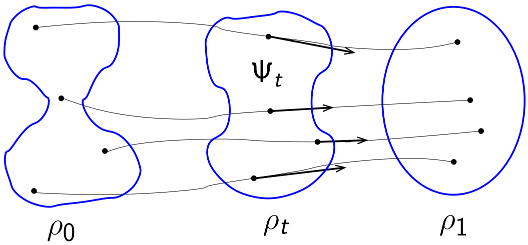

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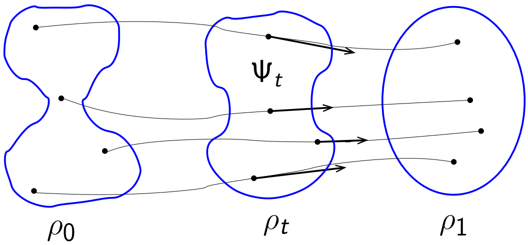

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Problem: ρ is defined on vertices, $\nabla\psi$ is defined on edges

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- Log-mean compensates for the lack of discrete chain rule:

$$\hat{\rho}(x,y) = \int_0^1 \rho(x)^{1-\alpha} \rho(y)^{\alpha} \, \mathrm{d}\alpha = \frac{\rho(x) - \rho(y)}{\log \rho(x) - \log \rho(y)}$$

Starting point for a notion of discrete Ricci curvature (with Erbar)

Is there a JKO theorem for dissipative quantum systems?

Dissipative Quantum mechanics

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- Then, $\mathcal{L}^\dagger$ can be written in Lindblad form

$$\mathcal{L}^\dagger \rho = -i[H, \rho] + \textstyle\sum_j \ [V_j, \rho V_j^*] + [V_j \rho, V_j^*] \ ,$$

where the Hamiltonian H is self-adjoint, and $V_j \in B(\mathfrak{H})$.

[Gorini/Kossakowski/Sudarshan, Lindblad 1976]

Monotonicity of the quantum relative entropy

- General form of completely positive trace preserving Markovian dynamics:

$$\partial_t \rho = \mathcal{L}^\dagger \rho \quad \text{(Lindblad equation)}$$

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Question

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- $\exists!$ stationary state: $\sigma_\beta = Z^{-1} e^{-\beta H}$,
  where $H = a^* a = \partial_x^2 - x\partial_x$ is the classical OU-operator

Conjecture: [Huber/König/Vershynina '16]

$$\mathrm{Ent}(P_t^\dagger \rho | \sigma_\beta) \le e^{-2\lambda_\beta t} \, \mathrm{Ent}(\rho | \sigma_\beta) \quad \text{where} \quad \lambda_\beta = \sinh(\beta/2) \ .$$

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Structure of Lindblad operators with detailed balance [Alicki '76]

If σ satisfies detailed balance for $(\mathcal{P}_t)$, then

$$\mathcal{L}^\dagger = \sum_j e^{\omega_j/2}\mathcal{L}_j^\dagger \ , \qquad \mathcal{L}_j^\dagger\rho = [V_j, \rho V_j^*] + [V_j\rho, V_j^*] \ ,$$

where $\{V_j\}_j = \{V_j^*\}_j$ and $[V_j, \log\sigma] = -\omega_j V_j$ for some $\omega_j \in \mathbf{R}$.

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- How to define the product $\bullet$?
  Need: non-commutative version of the classical chain rule

$$\nabla \rho = \rho \nabla \log \rho \ ?$$

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Quantum JKO

Quantum JKO-Theorem I (Carlen-M. , Mielke 2014)

Let the TPCP semigroup $\mathcal{P}_t^\dagger = e^{t\mathcal{L}^\dagger}$ satisfy det. balance w.r.t. I. Then, the Lindblad equation $\partial_t \rho = \mathcal{L}^\dagger \rho$ is the gradient flow equation for the von Neumann entropy $\text{Ent}(\rho) = \text{Tr}[\rho \log \rho]$ w.r.t $\mathcal{W}$.

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- Set $\rho_s^t = \mathcal{P}_{st}\rho_s$. Then: $\rho_0^t = \nu, \rho_1^t = \mathcal{P}_t\rho, \quad \partial_s \rho_s^t + \nabla \cdot V_s^t = 0,$ where

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$$V_s^t = P_{st} V_s - t\nabla \rho_s^t \ .$$

We obtain

$$\begin{aligned}
W_2^2(\nu, \mathcal{P}_t\rho) &\leq \int_0^1 \int_{\mathbf{R}^n} \frac{|V_s^t|^2}{\rho_s^t}\,\mathrm{d}x\,\mathrm{d}s \\
&= \int_0^1 \int_{\mathbf{R}^n} \left[\frac{|\mathcal{P}_{st} V_s|^2}{\mathcal{P}_{st}\rho_s} - 2t\frac{V_s^t \cdot \nabla \rho_s^t}{\rho_s^t} - t^2 \frac{|\nabla \rho_s^t|^2}{\rho_s^t} \right] \mathrm{d}x\,\mathrm{d}s \\
&\leq \int_0^1 \int_{\mathbf{R}^n} \frac{|V_s|^2}{\rho_s}\,\mathrm{d}x\,\mathrm{d}s - 2t\int_0^1 \partial_s \,\mathrm{Ent}(\rho_s^t)\,\mathrm{d}s \\
&= W_2^2(\nu,\rho) - 2t\Big(\mathrm{Ent}(\mathcal{P}_t\rho) - \mathrm{Ent}(\nu) \Big)
\end{aligned}$$

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- The relative entropy $\mathrm{Ent}(\cdot|\sigma_\beta)$ is geodesically λ_β-convex.

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Non-commutative analogues for quantum OU:

- $\partial_j \circ \mathcal{P}_t = e^{-\lambda_\beta t} \mathcal{P}_t \circ \partial_j$ where $\lambda_\beta = \sinh(\beta/2)$
- $(R, A) \mapsto \mathrm{Tr}\left[\int_0^\infty (tI + e^{-\omega/2} R)^{-1} A^* (tI + e^{\omega/2} R)^{-1} A \, \mathrm{d}t \right]$ is jointly convex on $\mathcal{M}_n^+ \times \mathcal{M}_n$ for all $\omega \in \mathbf{R}$

Theorem [Carlen-M. 2016]

Let $\beta > 0$ and let $\mathcal{P}_t$ be the quantum OU semigroup. Then:

- The relative entropy $\mathrm{Ent}(\cdot|\sigma_\beta)$ is geodesically λ_β-convex.
- Consequently, $\mathrm{Ent}(\mathcal{P}_t^\dagger \rho|\sigma) \leq e^{-2\lambda_\beta t} \, \mathrm{Ent}(\rho|\sigma)$

Thank you!