Colloquium du CERMICS

Quantum Wasserstein and Observability

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20 novembre 2024

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CERMICS ENPC
November 20th 2024

In collaboration with T. Paul, M3AS **32** (2022) 941–963

•**Schrödinger's equation**

$$i\hbar\partial_t\psi(t,x) = \underbrace{\left(-\tfrac{1}{2}\hbar^2\Delta_x + V(x)\right)}_{\text{quantum Hamiltonian } \mathcal{H}}\psi(t,x)\,, \qquad x \in \mathbf{R}^d$$

for the unknown wave function $\psi \equiv \psi(t,x) \in \mathbf{C}$ s.t. $\|\psi(t,\cdot)\|_{L^2} = 1$

•**von Neumann equation**

$$i\hbar\partial_t R(t) = [\mathcal{H}, R(t)]$$

Unknown operator $R(t)=R(t)^*\geq 0$ on $L^2(\mathbf{R}^d)$ s.t. $\operatorname{tr}_{L^2}(R(t))=1$

The potential V is a real-valued function s.t. $\mathcal{H}$ has a self-adjoint extension to $\mathfrak{H} = L^2(\mathbf{R}^d)$, so that $U(t) := e^{-it\mathcal{H}/\hbar}$ is a unitary group on $\mathfrak{H}$ by Stone's theorem, and

$$\psi(t,\cdot) = U(t)\psi(0,\cdot)\,, \qquad R(t) = U(t)R(0)U(t)^*$$

Observing Solutions of a PDE: an Example

Let $U \subset \mathbf{C}$ be a domain, and let $\varnothing \neq \Omega \subset U$ be open.
Let $\bar{\partial}$ be the Cauchy-Riemann operator and let $f \in \mathcal{D}'(U)$ satisfy

$$\bar{\partial} f = 0$$

Then (by analytic continuation)

$$f\big|_{\Omega} = 0 \implies f = 0 \text{ on } U$$

Pbm Existence of a constant $C[\Omega, U] > 0$ such that

$$\bar{\partial} f = 0 \text{ on } U \implies \sup_{z \in U} |f(z)| \leq C[\Omega, U] \sup_{z \in \Omega} |f(z)|?$$

Observation Inequality

A class $\mathcal{K}$ of quantum states at $t = 0$ is "observable" in $\Omega \subset \mathbf{R}^d$ open for a time $T > 0$ if there exists $C_{OBS} > 0$ such that

Schrödinger's dynamics

$$1 = \|\psi(0,\cdot)\|_{\mathfrak{H}}^2 \leq C_{OBS} \int_0^T \int_\Omega |\psi(t,x)|^2 dxdt$$

for initial data (orthogonal projection on $\mathbf{C}\psi(0,\cdot)$) in $\mathcal{K}$

von Neumann dynamics

$$1 = \operatorname{tr}_{\mathfrak{H}}(R(0)) \leq C_{OBS} \int_0^T \operatorname{tr}_{\mathfrak{H}}(\mathbf{1}_\Omega R(t))dt$$

for all initial data $R(0)$ in $\mathcal{K}$

J.L. Lions HUM for Schrödinger

Self-adjoint Hamiltonian $H = -\frac{1}{2}\Delta_x + V(x) = H^*$

Control problem

$$\begin{cases} i\partial_t\phi = H\phi + \mathbf{1}_{(0,T)\times\omega} f \\ \phi\big|_{t=T} = 0 \end{cases}$$

Observability problem

$$\begin{cases} i\partial_t\psi = H\psi \\ \psi\big|_{t=0} = \psi^{in} \end{cases}$$

Control operator

$$\mathcal{C} : L^2((0,T)\times\omega) \ni f \mapsto -i\phi\big|_{t=0} \in L^2(\mathbf{R}^d)$$

Observation operator

$$\mathcal{O} : L^2(\mathbf{R}^d) \ni \psi^{in} \mapsto \psi\big|_{(0,T)\times\omega} \in L^2((0,T)\times\omega)$$

For each $\psi^{in} \in L^2(\Omega)$ and each $f \in L^2((0,T)\times\omega)$, one has

$$\begin{aligned}\int_0^T\int_\omega \overline{\mathcal{O}\psi^{in}}(t,x)f(t,x)dxdt &= \int_0^T\int_{\mathbf{R}^d} \overline{\psi(t,x)}(i\partial_t\phi - H\phi)(t,x)dxdt \\ &= \int_0^T\int_{\mathbf{R}^d} (\overline{\psi}i\partial_t\phi - \overline{H\psi}\phi)(t,x)dxdt \\ &= \int_0^T\int_{\mathbf{R}^d} (\overline{\psi}i\partial_t\phi + \phi i\partial_t\overline{\psi})(t,x)dxdt \\ &= \left[i\int_{\mathbf{R}^d}\overline{\psi}\phi(t,x)dx\right]_{t=0}^{t=T} \\ &= \int_{\mathbf{R}^d}\overline{\psi^{in}}\mathcal{C}f(x)dx\end{aligned}$$

Conclusion

(1) It holds $\mathcal{O} = \mathcal{C}^*$ so that $\overline{\mathrm{ran}(\mathcal{C})} = \ker(\mathcal{O})^\perp$

(2) The existence of $C_{OBS} > 0$ implies that $\mathrm{ran}(\mathcal{C}) = \ker(\mathcal{O})^\perp$

Let $(X, \Xi)(t; x, \xi) \in \mathbf{R}^{2d}$ be the flow of the classical Hamiltonian

$$H(x, \xi) := \tfrac{1}{2}|\xi|^2 + V(x)$$

In other words, $(X, \Xi)(t; x, \xi)$ is the solution at time t of

$$\begin{cases} \dot{X} = \frac{\partial H}{\partial \Xi}(X, \Xi) = \Xi \,, \\ \dot{\Xi} = -\frac{\partial H}{\partial X}(X, \Xi) = -\nabla V(X) \,, \end{cases} \qquad (X, \Xi)\big|_{t=0} = (x, \xi)$$

Geometric condition for a triple (K, Ω, T) with $K \subset \mathbf{R}^{2d}$ compact, $\Omega \subset \mathbf{R}^d$ open and $T > 0$:

$$(GC) \qquad \text{for each } (x, \xi) \in K \text{ there exists } t \in (0, T) \text{ such that } X(t; x, \xi) \in \Omega$$

Illustration for the Geometric Condition

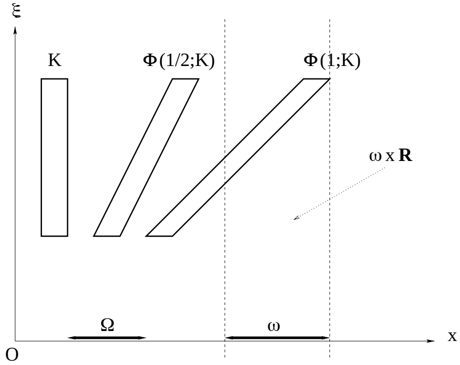

Figure: The geometric condition in space dimension $d = 1$, with $V \equiv 0$. The classical free flow is $\Phi(t; x, \xi) := (X(t; x, \xi), \Xi(t; x, \xi)) = (x + t\xi, \xi)$. The picture represents the image of the closed phase-space rectangle K by the map $(x, \xi) \mapsto \Phi(t; x, \xi)$ at time $t = \frac{1}{2}$ and $t = 1$. The interval Ω satisfies the geometric condition with $T = 1$, at variance with ω. Indeed, phase-space points on the bottom side of K stay out of the strip $\omega \times \mathbf{R}$ for all $t \in [0, 1]$.

Classical to Quantum Couplings [FG-TP ARMA 2017]

Coupling of $f \in \mathcal{P}^{ac}(\mathbf{R}^{2d})$ (probability density on $\mathbf{R}^{2d}$) with a density operator $R \in \mathcal{D}(\mathfrak{H}) := \{0 \le T = T^* \in \mathcal{L}(\mathfrak{H}) \text{ s.t. } \operatorname{tr}_{\mathfrak{H}}(T) = 1\}$

$$\mathbf{R}^{2d} \ni (x,\xi) \mapsto Q(x,\xi) = Q(x,\xi)^* \in \mathcal{L}(\mathfrak{H}) \text{ s.t. } Q(x,\xi) \ge 0 \text{ a.e.}$$

$$\text{s.t. } \operatorname{tr}_{\mathfrak{H}}(Q(x,\xi)) = f(x,\xi) \text{ a.e., and } \iint_{\mathbf{R}^{2d}} Q(x,\xi)dxd\xi = R$$

Set of couplings of f and R denoted $\mathcal{C}(f,R)$; one has $\mathcal{C}(f,R) \neq \varnothing$ since

$$(x,\xi) \mapsto Q(x,\xi) = f(x,\xi)R \quad \text{belongs to } \mathcal{C}(f,R)$$

Classical to Quantum Transport Cost a (differential) operator parametrized by the classical phase-space variables

$$c_\hbar^\lambda(x,\xi) \equiv c_\hbar(x,\xi,y,D_y) := \lambda^2|x-y|^2+|\xi+i\hbar\nabla_y|^2$$

Shifted harmonic oscillator; in particular (by Heisenberg's uncertainty inequality)

$$c_\hbar^\lambda(x,\xi) \geq \lambda d\hbar\, I_{\mathfrak{H}}$$

Metric if $R\in\mathcal{D}_2(\mathfrak{H}):=\{T\in\mathcal{D}(\mathfrak{H})\text{ s.t. } \mathrm{tr}_{\mathfrak{H}}(T^{\frac{1}{2}}(|x|^2-\Delta)T^{\frac{1}{2}})<\infty\}$ while $f\in\mathcal{P}_2^{ac}(\mathbf{R}^{2d}):=\{\phi\in\mathcal{P}^{ac}(\mathbf{R}^{2d})\text{ s.t. } (|x|^2+|\xi|^2)\phi\in L^1(\mathbf{R}^{2d})\}$

$$\mathfrak{d}_\lambda(f,R)^2 := \inf_{Q\in\mathcal{C}(f,R)}\iint_{\mathbf{R}^{2d}}\mathrm{tr}_{\mathfrak{H}}(Q(x,\xi)^{\frac{1}{2}}c_\hbar^\lambda(x,\xi)Q(x,\xi)^{\frac{1}{2}})dxd\xi$$
$$\geq\lambda d\hbar$$

Thm [F.G.-T. Paul (ARMA2017)] Assume $V \in C^{1,1}(\mathbf{R}^d)$ such that $\mathcal{H} := -\frac{1}{2}\hbar^2\Delta_x + V(x)$ has a self-adjoint extension to $\mathfrak{H}$, and let $U(t) := e^{-it\mathcal{H}/\hbar}$, while $\Phi(t;x,\xi) = (X,\Xi)(t;x,\xi)$ is the flow of the classical Hamiltonian $H(x,\xi) := \frac{1}{2}|\xi|^2 + V(x)$. Then

$$\mathfrak{d}_\lambda(f^{in} \circ \Phi(t,\cdot,\cdot), U(t)R^{in}U(t)^*) \le \mathfrak{d}_\lambda(f^{in}, R^{in})e^{L|t|}$$

with

$$L := \frac{1}{2}\left(\lambda + \frac{\mathrm{Lip}(\nabla V)}{\lambda}\right)$$

Pair Dispersion Estimate

Since

$$\dot{X}_t - \dot{Y}_t = \Xi_t - H_t\,, \qquad \dot{\Xi}_t - \dot{H}_t = -(\nabla V(X_t) - \nabla V(Y_t))$$

one has

$$\begin{aligned}
&\tfrac{d}{dt}(\lambda^2|X_t - Y_t|^2 + |\Xi_t - H_t|^2)\\
&= 2\lambda^2(X_t - Y_t)\cdot(\Xi_t - H_t) - 2(\Xi_t - H_t)\cdot(\nabla V(X_t) - \nabla V(Y_t))\\
&\le 2\lambda^2|X_t - Y_t||\Xi_t - H_t| + 2|\Xi_t - H_t||\nabla V(X_t) - \nabla V(Y_t)|\\
&\le 2\lambda^2|X_t - Y_t||\Xi_t - H_t| + 2\tfrac{\mathrm{Lip}(\nabla V)}{\lambda}|\Xi_t - H_t|\lambda|X_t - Y_t|\\
&\le \left(\lambda + \tfrac{\mathrm{Lip}(\nabla V)}{\lambda}\right)(\lambda^2|X_t - Y_t|^2 + |\Xi_t - H_t|^2)
\end{aligned}$$

From the drei Männer Arbeit [Born-Heisenberg-Jordan Z. Phys. **35** (1926) 557–615, eq. (15)]

Let $Q, P =$ position and momentum operators (assuming $d = 1$)

$$(Q\psi)(x) := x\psi(x)\,, \qquad (P\psi)(x) := -i\hbar\psi'(x)\,, \qquad x \in \mathbf{R}$$

and let $U(t) := e^{-it\mathcal{H}/\hbar}$, where

$$\mathcal{H} := -\tfrac{1}{2}\hbar^2\partial_x^2 + V(x) = \mathcal{H}^*$$

Set

$$Q(t) := U(t)QU(t)^*\,, \qquad P(t) := U(t)PU(t)^*$$

Then

$$\tfrac{d}{dt}Q(t) = P(t)\,, \qquad \tfrac{d}{dt}P(t) = -V'(Q(t))$$

Replace (Y_t, H_t) with $(Q(t), P(t))$ in the pair dispersion inequality.

Proof of the Propagation Theorem

(1) Pick $Q^{in} \in \mathcal{C}(f^{in}, R^{in})$, set $Q(t;x,\xi) = U(t)Q^{in}(\Phi(t,x,\xi))U(t)^*$;

$$\partial_t Q + \{\tfrac{1}{2}|\xi|^2 + V(x); Q\} + \tfrac{i}{\hbar}\left[-\tfrac{1}{2}\hbar^2\Delta + V; Q\right] = 0$$

Then

$$\mathfrak{d}_\lambda(f(t,\cdot), R(t))^2 \leq \iint_{\mathbf{R}^{2d}} \mathrm{tr}_{\mathfrak{H}}(Q(t,x,\xi)^{\frac{1}{2}} c_\hbar^\lambda(x,\xi) Q(t,x,\xi)^{\frac{1}{2}}) dx d\xi$$

(2) Moreover

$$\frac{d}{dt}\iint_{\mathbf{R}^{2d}} \mathrm{tr}_{\mathfrak{H}}(Q(t,x,\xi)^{\frac{1}{2}} c_\hbar^\lambda(x,\xi) Q(t,x,\xi)^{\frac{1}{2}}) dx d\xi$$

$$\leq \iint_{\mathbf{R}^{2d}} \mathrm{tr}_{\mathfrak{H}}(Q(t,x,\xi)^{\frac{1}{2}} \{\tfrac{1}{2}|\xi|^2 + V(x); c_\hbar^\lambda(x,\xi)\} Q(t,x,\xi)^{\frac{1}{2}}) dx d\xi$$

$$+ \iint_{\mathbf{R}^{2d}} \mathrm{tr}_{\mathfrak{H}}\left(Q(t,x,\xi)^{\frac{1}{2}} \tfrac{i}{\hbar}\left[-\tfrac{\hbar^2}{2}\Delta + V; c_\hbar^\lambda(x,\xi)\right] Q(t,x,\xi)^{\frac{1}{2}}\right) dx d\xi$$

(3) With the notation $a \vee b := ab + ba$, elementary computations show that one has

$$\{\tfrac{1}{2}|\xi|^2; c_\hbar^\lambda(x,\xi)\} + \tfrac{i}{\hbar}\left[-\tfrac{\hbar^2}{2}\Delta; c_\hbar^\lambda(x,\xi)\right]$$
$$= \lambda(\xi + i\hbar\nabla_y) \vee \lambda(x-y) \leq \lambda c_\hbar^\lambda(x,\xi)$$

and

$$\{V(x); c_\hbar^\lambda(x,\xi)\} + \tfrac{i}{\hbar}\left[V; c_\hbar^\lambda(x,\xi)\right]$$
$$= \tfrac{\mathrm{Lip}(\nabla V)}{\lambda}(\xi + i\hbar\nabla_y) \vee \tfrac{\lambda}{\mathrm{Lip}(\nabla V)}(\nabla V(x) - \nabla V(y))$$
$$\leq \tfrac{\mathrm{Lip}(\nabla V)}{\lambda} c_\hbar^\lambda(x,\xi)$$

by using the elementary inequality

$$\left.\begin{array}{l} A^* = A \\ B^* = B \end{array}\right\} \implies A \vee B = AB + BA \leq A^2 + B^2$$

(4) Hence

$$\frac{d}{dt}\iint_{\mathbf{R}^{2d}} \mathrm{tr}_{\mathfrak{H}}(Q(t,x,\xi)^{\frac{1}{2}} c_\hbar^\lambda(x,\xi) Q(t,x,\xi)^{\frac{1}{2}}) dxd\xi$$
$$\leq (\lambda + \tfrac{\mathrm{Lip}(\nabla V)}{\lambda}) \iint_{\mathbf{R}^{2d}} \mathrm{tr}_{\mathfrak{H}}(Q(t,x,\xi)^{\frac{1}{2}} c_\hbar^\lambda(x,\xi) Q(t,x,\xi)^{\frac{1}{2}}) dxd\xi$$

which implies the announced inequality.

Lemma
For (K, Ω, T) with $K \subset \mathbf{R}^{2d}$ compact, $\Omega \subset \mathbf{R}^d$ open and $T > 0$

$$(GC) \implies C[K, \Omega, T] := \inf_{(x,\xi)\in K} \int_0^T \mathbf{1}_\Omega(X(t; x, \xi))dt > 0$$

Proof Since Ω is open, $\mathbf{1}_\Omega$ is l.s.c. By the (GC), for each $x, \xi \in \mathbf{R}^d$, there exists $t_{x,\xi} \in (0, T)$ and $\eta_{x,\xi} > 0$ such that, for all $(x, \xi) \in K$

$$|t - t_{x,\xi}| < \eta_{x,\xi} \implies \mathbf{1}_\Omega(X(t; x, \xi)) = 1$$
$$\implies \int_0^T \mathbf{1}_\Omega(X(t; x, \xi))dt \geq 2\eta_{x,\xi} > 0$$

By Fatou's lemma, the positive function $(x, \xi) \mapsto \int_0^T \mathbf{1}_\Omega(X(t; x, \xi))dt$ is l.s.c. on K compact, and therefore attains its minimum on K.

Application to Observability

Thm Let $V \in C^{1,1}(\mathbf{R}^d)$ and (K, Ω, T) satisfying (GC). Then, for all $R^{in} \in \mathcal{D}_2(\mathfrak{H})$ and all $\delta > 0$, denoting $\Omega_\delta = \Omega + B(0, \delta)$, one has

$$\int_0^T \operatorname{tr}_{\mathfrak{H}}(\mathbf{1}_{\Omega_\delta} U(t) R^{in} U(t)^*) dt \geq \underbrace{C[K, \Omega, T]}_{\text{geometric}}$$

$$\underbrace{- \frac{1}{\delta} \inf_{\lambda > 0} \frac{1}{\lambda} \frac{\exp\left(\frac{1}{2} T \left(\lambda + \frac{\operatorname{Lip}(\nabla V)}{\lambda}\right)\right) - 1}{\frac{1}{2}\left(\lambda + \frac{\operatorname{Lip}(\nabla V)}{\lambda}\right)} \inf_{\operatorname{supp}(f^{in}) \subset K} \mathfrak{d}_\lambda(f^{in}, R^{in})}_{\text{semiclassical correction}}$$

Example 1: Toeplitz Initial Data

Assume that R^{in} is of the form

$$R^{in} := \int_{\mathbf{R}^{2d}} |q,p\rangle\langle q,p|\mu(dqdp), \quad \mu \in \mathcal{P}_2(\mathbf{R}^{2d})$$

$$\text{where } |q,p\rangle(x) := (\pi\hbar)^{-d/4} e^{-|x-q|^2/2\hbar} e^{ip\cdot x/\hbar}$$

In that case (see [FG-T. Paul, ARMA2017] Thm. 2.4)

$$\lambda d\hbar \le \mathfrak{d}_\lambda(f^{in}, R^{in})^2 \le \max(1,\lambda^2) W_2(f^{in}, \mu^{in})^2 + \lambda d\hbar$$

so that

$$\text{supp}(\mu) \subset K \implies \inf_{\text{supp}(f^{in})\subset K} \mathfrak{d}_\lambda(f^{in}, R^{in}) = \sqrt{\lambda d\hbar}$$

Example 2: Pure State

Assume that $R(t) = |U(t)\psi^{in}\rangle\langle U(t)\psi^{in}|$, where $U(t) = e^{-it\mathcal{H}/\hbar}$ is the Schrödinger group.

Choosing $f^{in}(q,p) := \frac{|\langle q,p|\psi^{in}\rangle|^2}{(2\pi\hbar)^d}$ = Husimi transform of ψ^{in} leads to

$$\frac{1}{C_{OBS}} = C[K,\Omega,T]\iint_K |\langle q,p|\psi^{in}\rangle|^2 \frac{dqdp}{(2\pi\hbar)^d} - D[T,\mathrm{Lip}(\nabla V)]\frac{\Sigma[\psi^{in}]}{\delta}$$

where

$$\begin{aligned} D[T,L] &:= 4\frac{e^{(1+L)T/2}-1}{1+L} \\ \Sigma[\psi^{in}]^2 &:= \langle\psi^{in}|\,|x|^2|\psi^{in}\rangle - |\langle\psi^{in}|x|\psi^{in}\rangle|^2 \\ &\quad + \langle\psi^{in}| - \hbar^2\Delta_x|\psi^{in}\rangle - |\langle\psi^{in}| - i\hbar\nabla_x|\psi^{in}\rangle|^2 \end{aligned}$$

Proof

Call $f(t,\cdot,\cdot) := f^{in}\circ\Phi(t;\cdot,\cdot)$ and $R(t) := U(t)R^{in}U(t)^*$. For all $Q(t)\in\mathcal{C}(f(t,\cdot,\cdot),R(t))$, one has

$$\left|\mathrm{tr}_{\mathfrak{H}}(\chi R(t)) - \iint_{\mathbf{R}^{2d}}\chi(x)f(t,x,\xi)dxd\xi\right|$$
$$= \left|\iint_{\mathbf{R}^{2d}}\mathrm{tr}_{\mathfrak{H}}((\chi(x)-\chi(y))Q(t,x,\xi)dxd\xi\right|$$
$$\le \frac{\mathrm{Lip}(\chi)}{\lambda}\left(\iint_{\mathbf{R}^{2d}}\mathrm{tr}_{\mathfrak{H}}(Q_t^{\frac{1}{2}}(\lambda^2|x-y|^2+|\xi+i\hbar\nabla_y|^2)Q_t^{\frac{1}{2}})dxd\xi\right)^{\frac{1}{2}}$$

so that

$$\left|\mathrm{tr}_{\mathfrak{H}}(\chi R(t)) - \iint_{\mathbf{R}^{2d}}\chi(x)f(t,x,\xi)dxd\xi\right| \le \frac{\mathrm{Lip}(\chi)}{\lambda}\mathfrak{d}_\lambda(f(t,\cdot,\cdot),R(t))$$
$$\le \frac{\mathrm{Lip}(\chi)}{\lambda}\mathfrak{d}_\lambda(f^{in},R^{in})\exp\left(\tfrac{1}{2}t\left(\lambda+\frac{\mathrm{Lip}(\nabla V)}{\lambda}\right)\right)$$

Since

$$\iint_{\mathbf{R}^{2d}} \chi(x) f(t,x,\xi)\,dx\,d\xi = \iint_{\mathbf{R}^{2d}} \chi(X(t;x,\xi)) f^{in}(x,\xi)\,dx\,d\xi$$

one has

$$\int_0^T \operatorname{tr}_{\mathfrak{H}}(\chi R(t))dt \geq \inf_{(x,\xi)\in K} \int_0^T \chi(X(t;x,\xi))dt \iint_K f^{in}(x,\xi)dxd\xi$$
$$- \frac{\operatorname{Lip}(\chi)}{\lambda} \frac{\exp\left(\frac{1}{2}T\left(\lambda + \frac{\operatorname{Lip}(\nabla V)}{\lambda}\right)\right) - 1}{\frac{1}{2}\left(\lambda + \frac{\operatorname{Lip}(\nabla V)}{\lambda}\right)} \mathfrak{d}_\lambda(f^{in}, R^{in})$$

Conclude by choosing $\chi(x) := \left(1 - \frac{\operatorname{dist}(x,\Omega)}{\delta}\right)_+$, so that $\operatorname{Lip}(\chi) = \frac{1}{\delta}$

$\square$

Conclusions/Perspectives

•We have proved an observation inequality for the quantum dynamics under the only assumption that V is regular enough for the existence and uniqueness of the classical dynamics ($C^{1,1}$ potential)
•The observation constant is explicit in terms of the geometric data of the Bardos-Lebeau-Rauch controllability condition
•Approach based on a quantum analogue of the Wasserstein distance to measure the difference between a classical and a quantum density

Possible extensions
•Obtaining a controllability statement (by duality as in HUM)
•Including magnetic fields (I. Ben Porath's PhD thesis)
•Other dispersive dynamics? Klein-Gordon?