

## Colloquium du CERMICS



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## Quantum Wasserstein and Observability

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- Schrödinger's equation

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

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.  $\text{tr}_{L^2}(R(t)) = 1$

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

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

# Observing Solutions of a PDE: an Example

Let  $U \subset \mathbf{C}$  be a domain, and let  $\emptyset \neq \Omega \subset U$  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)

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

**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

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

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

## von Neumann dynamics

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

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

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

**Control problem**

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

**Observability problem**

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

**Control operator**

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

**Observation operator**

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

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

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

## Conclusion

- (1) It holds  $\mathcal{O} = \mathcal{C}^*$  so that  $\overline{\text{ran}(\mathcal{C})} = \ker(\mathcal{O})^\perp$
- (2) The existence of  $C_{OBS} > 0$  implies that  $\text{ran}(\mathcal{C}) = \ker(\mathcal{O})^\perp$

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

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

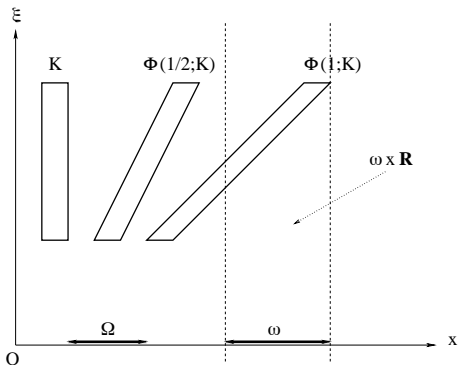
In other words,  $(X, \Xi)(t; x, \xi)$  is the solution at time  $t$  of

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

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

(GC) for each  $(x, \xi) \in K$  there exists  $t \in (0, T)$   
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  $\Omega$  satisfies the geometric condition with  $T = 1$ , at variance with  $\omega$ . Indeed, phase-space points on the bottom side of  $K$  stay out of the strip  $\omega \times \mathbf{R}$  for all  $t \in [0, 1]$ .

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

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

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

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

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

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

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

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

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

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

$$\begin{aligned} \mathfrak{D}_\lambda(f, R)^2 &:= \inf_{Q \in \mathcal{C}(f, R)} \iint_{\mathbf{R}^{2d}} \text{tr}_{\mathfrak{H}}(Q(x, \xi)^{\frac{1}{2}} c_h^\lambda(x, \xi) Q(x, \xi)^{\frac{1}{2}}) dx d\xi \\ &\geq \lambda d \hbar \end{aligned}$$

**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

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

with

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

Since

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

one has

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

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

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

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

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

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

Set

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

Then

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

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  $Q(t; x, \xi) = U(t)Q^{in}(\Phi(t, x, \xi))U(t)^*$ ;

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

Then

$$\mathfrak{D}_\lambda(f(t, \cdot), R(t))^2 \leq \iint_{\mathbf{R}^{2d}} \operatorname{tr}_{\mathfrak{H}} \left( Q(t, x, \xi)^{\frac{1}{2}} c_h^\lambda(x, \xi) Q(t, x, \xi)^{\frac{1}{2}} \right) dx d\xi$$

(2) Moreover

$$\begin{aligned} & \frac{d}{dt} \iint_{\mathbf{R}^{2d}} \operatorname{tr}_{\mathfrak{H}} \left( Q(t, x, \xi)^{\frac{1}{2}} c_h^\lambda(x, \xi) Q(t, x, \xi)^{\frac{1}{2}} \right) dx d\xi \\ & \leq \iint_{\mathbf{R}^{2d}} \operatorname{tr}_{\mathfrak{H}} \left( Q(t, x, \xi)^{\frac{1}{2}} \left\{ \frac{1}{2}|\xi|^2 + V(x); c_h^\lambda(x, \xi) \right\} Q(t, x, \xi)^{\frac{1}{2}} \right) dx d\xi \\ & + \iint_{\mathbf{R}^{2d}} \operatorname{tr}_{\mathfrak{H}} \left( Q(t, x, \xi)^{\frac{1}{2}} \frac{i}{\hbar} \left[ -\frac{\hbar^2}{2} \Delta + V; c_h^\lambda(x, \xi) \right] Q(t, x, \xi)^{\frac{1}{2}} \right) dx d\xi \end{aligned}$$

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

$$\begin{aligned} & \left\{ \frac{1}{2}|\xi|^2; c_h^\lambda(x, \xi) \right\} + \frac{i}{\hbar} \left[ -\frac{\hbar^2}{2} \Delta; c_h^\lambda(x, \xi) \right] \\ &= \lambda(\xi + i\hbar \nabla_y) \vee \lambda(x - y) \leq \lambda c_h^\lambda(x, \xi) \end{aligned}$$

and

$$\begin{aligned} & \left\{ V(x); c_h^\lambda(x, \xi) \right\} + \frac{i}{\hbar} \left[ V; c_h^\lambda(x, \xi) \right] \\ &= \frac{\text{Lip}(\nabla V)}{\lambda} (\xi + i\hbar \nabla_y) \vee \frac{\lambda}{\text{Lip}(\nabla V)} (\nabla V(x) - \nabla V(y)) \\ & \leq \frac{\text{Lip}(\nabla V)}{\lambda} c_h^\lambda(x, \xi) \end{aligned}$$

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

$$\begin{aligned} & \frac{d}{dt} \iint_{\mathbf{R}^{2d}} \operatorname{tr}_{\mathfrak{H}}(Q(t, x, \xi)^{\frac{1}{2}} c_h^\lambda(x, \xi) Q(t, x, \xi)^{\frac{1}{2}}) dx d\xi \\ & \leq \left( \lambda + \frac{\operatorname{Lip}(\nabla V)}{\lambda} \right) \iint_{\mathbf{R}^{2d}} \operatorname{tr}_{\mathfrak{H}}(Q(t, x, \xi)^{\frac{1}{2}} c_h^\lambda(x, \xi) Q(t, x, \xi)^{\frac{1}{2}}) dx d\xi \end{aligned}$$

which implies the announced inequality.

## Lemma

For  $(K, \Omega, T)$  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  $\Omega$  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  $(x, \xi) \in K$

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

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  $K$ .

**Thm** Let  $V \in C^{1,1}(\mathbf{R}^d)$  and  $(K, \Omega, T)$  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

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

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

# 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)

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

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  $\psi^{in}$  leads to

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

where

$$D[T, L] := 4 \frac{e^{(1+L)T/2} - 1}{1 + L}$$

$$\begin{aligned} \Sigma[\psi^{in}]^2 := & \langle \psi^{in} | |x|^2 | \psi^{in} \rangle - |\langle \psi^{in} | x | \psi^{in} \rangle|^2 \\ & + \langle \psi^{in} | -\hbar^2 \Delta_x | \psi^{in} \rangle - |\langle \psi^{in} | -i\hbar \nabla_x | \psi^{in} \rangle|^2 \end{aligned}$$

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

$$\begin{aligned} & \left| \text{tr}_{\mathfrak{H}}(\chi R(t)) - \iint_{\mathbf{R}^{2d}} \chi(x) f(t, x, \xi) dx d\xi \right| \\ &= \left| \iint_{\mathbf{R}^{2d}} \text{tr}_{\mathfrak{H}}((\chi(x) - \chi(y)) Q(t, x, \xi)) dx d\xi \right| \\ &\leq \frac{\text{Lip}(\chi)}{\lambda} \left( \iint_{\mathbf{R}^{2d}} \text{tr}_{\mathfrak{H}}(Q_t^{\frac{1}{2}} (\lambda^2 |x-y|^2 + |\xi + i\hbar \nabla_y|^2) Q_t^{\frac{1}{2}}) dx d\xi \right)^{\frac{1}{2}} \end{aligned}$$

so that

$$\begin{aligned} \left| \text{tr}_{\mathfrak{H}}(\chi R(t)) - \iint_{\mathbf{R}^{2d}} \chi(x) f(t, x, \xi) dx d\xi \right| &\leq \frac{\text{Lip}(\chi)}{\lambda} \mathfrak{d}_{\lambda}(f(t, \cdot, \cdot), R(t)) \\ &\leq \frac{\text{Lip}(\chi)}{\lambda} \mathfrak{d}_{\lambda}(f^{in}, R^{in}) \exp \left( \frac{1}{2} t \left( \lambda + \frac{\text{Lip}(\nabla V)}{\lambda} \right) \right) \end{aligned}$$

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

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

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

□

- 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?