Quantum Wasserstein "Metric" and Applications
Lecture 2

François Golse

École polytechnique, CMLS

VIASM, Hanoi, July 18th-19th 2024

Based on works with E. Caglioti, S. Jin, C. Mouhot, T. Paul

Outline of Lecture 2

In this lecture, we shall discuss several applications of the quantum Wasserstein pseudometric $\mathfrak{d}$ introduced in lecture 1. These applications include

•various limits of many-body problems in quantum mechanics

•proofs of the uniform in $\hbar$ convergence of some numerical schemes for quantum dynamics

•some observation inequalities for the Schrödinger and Heisenberg equations

BASICS OF QUANTUM DYNAMICS

J.-L. Basdevant, J. Dalibard: "Quantum Mechanics", Springer 2002
C. Cohen-Tannoudji, B. Diu, F. Laloë: "Quantum Mechanics I", Wiley 1977
B.C. Hall: "Quantum Theory for Mathematicians", Springer 2013

Point particle of mass m with position, momentum $q(t), p(t) \in \mathbf{R}^d$
Hamiltonian

$$H(q,p) = \underbrace{|p|^2/2m}_{\text{kinetic}} + \underbrace{V(q)}_{\text{potential}} = \text{energy}$$

•Newton's 2nd law of motion in Hamiltonian form

$$\dot{q}(t) = \partial H/\partial p = p(t)/m\,, \quad \dot{p}(t) = -\partial H/\partial q = -\nabla V(q(t))$$

•Liouville equation for $f \equiv f(t,x,\xi)$ = probability density of finding the point at x with momentum ξ at time t

$$\partial_t f(t,x,\xi) + \underbrace{\tfrac{1}{m}\xi \cdot \nabla_x f(t,x,\xi) - \nabla V(x) \cdot \nabla_\xi f(t,x,\xi)}_{=\{H,f(t,\cdot,\cdot)\} \text{ (Poisson bracket)}} = 0$$

Wave function $\psi \equiv \psi(t,x) \in L^2(\mathbf{R}^d;\mathbf{C}) =: \mathfrak{H}$ s.t. $\|\psi(t,\cdot)\|_{\mathfrak{H}} = 1$
Quantum Hamiltonian = unbounded operator on $\mathfrak{H}$

$$\mathbf{H} = -\frac{\hbar^2}{2m}\Delta_x + V(x) = \mathbf{H}^*$$

Correspondence principle

$$V(q) \to \text{multiplication by } V(x) \text{ and } p_j \to -i\hbar\partial_{q_j} = \hbar D_{q_j}$$

Schrödinger equation

$$i\hbar\partial_t\psi = \mathbf{H}\psi \implies \psi(t,\cdot) = \underbrace{e^{-it\mathbf{H}/\hbar}}_{\text{unitary}}\psi(0,\cdot)$$

von Neumann equation for $R(t)$ = projection on $\mathbf{C}\psi(t,\cdot)$

$$i\hbar\partial_t R(t) = \underbrace{\mathbf{H}R(t) - R(t)\mathbf{H}}_{=:[\mathbf{H},R(t)]} \implies R(t) = e^{-it\mathbf{H}/\hbar}R(0)e^{it\mathbf{H}/\hbar}$$

Asymptotic regime $\hbar \ll$ "typical" action of the particle

(a) **WKB ansatz** seek wave function in the form of the formal series

$$\psi(t,x) = \sum_{n\geq 0} \hbar^n a_n(t,x) e^{iS(t,x)/\hbar}, \quad S(t,x) \text{ and } a_n(t,x) \in \mathbf{R}$$

Leading order equations (usually only local in time due to caustics)

$$\partial_t S + H(\nabla_x S, x) = 0, \quad \partial_t a_0^2 + \mathrm{div}_x(a_0^2 \nabla_x S(t,x)) = 0$$

(b) **Schrödinger coherent states** wave function $|q(t), p(t)\rangle$ = plane wave with $O(\hbar)$ wavelength and a Gaussian envelope of width $O(\sqrt{\hbar})$; what is the (classical) dynamics of $q(t), p(t)$ for such states to approximately follow the quantum dynamics?

Let $R \in \mathcal{L}(\mathfrak{H})$ be the integral operator

$$R\phi(x) = \int_{\mathbf{R}^d} r(x,y)\phi(y)dy$$

Ex for $R =$ projection on $\mathbf{C}\psi$ with $\|\psi\|_{\mathfrak{H}} = 1$, denoted $R = |\psi\rangle\langle\psi|$

$$R\phi(x) = \underbrace{\left(\int_{\mathbf{R}^d} \overline{\psi(y)}\phi(y)dy\right)}_{=:\langle\psi|\phi\rangle}\psi(x) \implies r(x,y) = \psi(x)\overline{\psi(y)}$$

Wigner transform of R

$$W_\hbar[R](q,p) := \frac{1}{(2\pi)^d}\int_{\mathbf{R}^d} r(q + \tfrac{1}{2}\hbar y, q - \tfrac{1}{2}\hbar y)e^{ip\cdot y}dy$$

Observe that

$$R = R^* \implies W_\hbar[R](q,p) \in \mathbf{R} \quad \text{BUT} \quad R \geq 0 \not\Longrightarrow W_\hbar[R] \geq 0$$

(1) Prove that

$$\mathcal{H}[R](q,p) = \exp(\tfrac{1}{4}\hbar(\Delta_q + \Delta_p))W_\hbar[R](q,p)$$

(Hint: recall the formula for the Fourier transform of a Gaussian.)

(2) Set $\mathbf{H} := -\frac{1}{2}\hbar^2\Delta_x + \frac{1}{2}|x|^2$, and $\mathcal{U}(t) := e^{-it\mathbf{H}/\hbar}$. For each $R^{in} \in \mathcal{D}(\mathfrak{H})$, write a PDE satisfied by $W_\hbar[\mathcal{U}(t)R^{in}\mathcal{U}(-t)]$.

(3) Same question with $\mathbf{H} := -\frac{1}{2}\hbar^2\Delta_x + V(x)$. What are the assumptions needed on the potential V for the formal computation to be made rigorous?

Thm [Lions-Paul Rev. Mat. Iberoam.1993] Let $R_\hbar^{in}=(R_\hbar^{in})^*\geq 0$ be s.t.

$$W_\hbar[R_\hbar^{in}] \to f^{in} \text{ in } \mathcal{S}'(\mathbf{R}^d \times \mathbf{R}^d) \text{ as } \hbar \to 0$$

where f^{in} = probability density on $\mathbf{R}^d \times \mathbf{R}^d$. Then

$$W_\hbar[e^{-it\mathbf{H}/\hbar} R_\hbar^{in} e^{it\mathbf{H}/\hbar}] \to f(t,\cdot,\cdot) \text{ in } \mathcal{S}'(\mathbf{R}^d \times \mathbf{R}^d) \text{ as } \hbar \to 0$$

where f is the probability density solution to the Liouville equation with initial data f^{in}.

Example WKB wave function with $\|a^{in}\|_{L^2} = 1$ and $S \in \mathrm{Lip}(\mathbf{R}^d; \mathbf{R})$

$$\psi_\hbar^{in}(x) = a^{in}(x) e^{iS^{in}(x)/\hbar} \implies f^{in}(q,p) = |a^{in}(q)|^2 \delta(p - \nabla S^{in}(q))$$

Classical dynamics with $m = 1$ and denoting $L := \mathrm{Lip}(\nabla V)$, one has

$$\begin{cases} \dot{X} = \Xi \\ \dot{\Xi} = -\nabla V(X) \end{cases} \quad \text{and} \quad \begin{cases} \dot{Y} = H \\ \dot{H} = -\nabla V(Y) \end{cases}$$

$$\implies \tfrac{d}{dt}(|X - Y|^2 + |\Xi - H|^2) \leq (1 + L)(|X - Y|^2 + |\Xi - H|^2)$$

Quantum dynamics since $\mathbf{H} = -\frac{\hbar^2}{2}\Delta_x + V(x) = \mathbf{H}^*$ on $L^2(\mathbf{R}^d_x)$

$$i\hbar\partial_t\psi_1 = \mathbf{H}\psi_1 \quad \text{and} \quad i\hbar\partial_t\psi_2 = \mathbf{H}\psi_2$$

$$\implies \tfrac{d}{dt}\int_{\mathbf{R}^d} |\psi_1(t,x) - \psi_2(t,x)|^2 dx = 0$$

Uniform in $\hbar > 0$ **estimate** of $\|\psi_1(t,\cdot) - \psi_2(t,\cdot)\|_{L^2(\mathbf{R}^d)}$ without assuming regularity on the potential V (e.g. for $V \in L^\infty(\mathbf{R}^d)$) but...

MEAN-FIELD AND CLASSICAL LIMITS IN QUANTUM MECHANICS

F. G., C. Mouhot, T. Paul: Commun; Math. Phys. **343** (2016), 165–205

F. G., T. Paul: Archive Rational Mech. Anal. **223** (2017) 57–94

Mean-Field Limit vs Classical Limit

$$
\begin{array}{ccc}
\boxed{\textbf{Schrödinger}} & \stackrel{N\to\infty}{\longrightarrow} & \boxed{\textbf{Hartree}} \\
\downarrow & & \downarrow \\
\hbar \to 0 & \searrow & \hbar \to 0 \\
\downarrow & & \downarrow \\
\boxed{\textbf{Liouville}} & \stackrel{N\to\infty}{\longrightarrow} & \boxed{\textbf{Vlasov}}
\end{array}
$$

•Uniformity as $\hbar \to 0$ of the upper horizontal (mean-field) limit discussed in
[Graffi-Martinez-Pulvirenti: M3AS **13** (2003), 59–73]
[Pezzotti-Pulvirenti: Ann. Henri Poincaré **10** (2009), 145–187]
•Semiclassical limit of Hartree, no cvgce rate, including Coulomb:
[Lions-Paul Rev. Mat. Iberoam. **9** (1993), 553–618]

Assumptions on the interaction potential

$$V \in C^{1,1}(\mathbf{R}^d) \quad \text{with } V^- \in L^\infty(\mathbf{R}^d) \quad \text{and} \quad V(z) = V(-z) \in \mathbf{R}$$

Quantum N-particle Hamiltonian with $N \gg 1$ and $\hbar \ll 1$

$$\mathbf{H}_N := \sum_{k=1}^{N} -\tfrac{1}{2}\hbar^2 \Delta_{x_k} + \tfrac{1}{N} \sum_{1\le k<l\le N} V(x_k - x_l)\,, \quad \mathrm{Dom}(\mathbf{H}_N) = H^2(\mathbf{R}^{dN})$$

is self-adjoint on $\mathfrak{H}_N := \mathfrak{H}^{\otimes N} \simeq L^2(\mathbf{R}^{dN})$; let $\mathcal{U}_N(t) := e^{-it\mathbf{H}_N/\hbar}$.

•The operator $R_N(t) = \mathcal{U}_N(t) R_N^{in} \mathcal{U}_N(t)^*$ solves Heisenberg's eqn:

$$i\hbar\partial_t R_N(t) = [\mathbf{H}_N, R_{\hbar,N}(t)]\,, \qquad R_{\hbar,N}(0) = R_N^{in} \in \mathcal{D}(\mathfrak{H}_N)$$

•**Pure state** $R_N(t) = |\mathcal{U}_N(t)\Psi_N\rangle\langle\mathcal{U}_N(t)\Psi_N|$ with $\|\Psi_N\|_{\mathfrak{H}_N} = 1$

Time-dependent Hartree equation for pure states

$$i\hbar\partial_t\psi(t,x) = -\tfrac{1}{2}\hbar^2\Delta_x\psi(t,x) + \psi(t,x)V\star_x|\psi|^2(t,x)\,, \quad x\in\mathbf{R}^d$$

For mixed states

$$i\hbar\partial_t R(t) = [-\tfrac{1}{2}\hbar^2\Delta_x + V_{R(t)}, R(t)]\,, \qquad R(0) = R^{in}\in\mathcal{D}(\mathfrak{H})$$

with mean-field potential defined by the formula

$$V_{R(t)}(x) := \operatorname{tr}_{\mathfrak{H}}(V(\cdot - x)R(t))\,, \qquad x\in\mathbf{R}^d$$

Vlasov equation: $\frac{i}{\hbar}[\cdot,\cdot]\to\{\cdot,\cdot\}$ (Poisson bracket on $C^1(\mathbf{R}^d\times\mathbf{R}^d)$)

$$\begin{cases}\partial_t f(t,x,\xi) + \underbrace{\xi\cdot\nabla_x f(t,x,\xi) - (\nabla V\star_{x,\xi} f(t,x,\xi))\cdot\nabla_\xi f(t,x,\xi)}_{\{\frac{1}{2}|\xi|^2 + V\star_{x,\xi} f(t,x,\xi), f(t,x,\xi)\}} = 0\\ f(0,x,\xi) = f^{in}(x,\xi)\,, \qquad x,\xi\in\mathbf{R}^d\end{cases}$$

• From N-body Heisenberg to Hartree

Theorem 1 Setting $L := 2 + \max(4\text{Lip}(\nabla V)^2, 1)$, choose an initial (1-particle) distribution function f^{in} such that $f^{in} dx d\xi \in \mathcal{P}_2(\mathbf{R}^{2d})$. Set the Hartree initial data to be $R^{in} = \mathcal{T}[f^{in}]$. For each $t > 0$

$$\underbrace{\frac{\mathfrak{d}\left(R(t)^{\otimes N}, \mathcal{U}_N(t)\mathcal{T}[(f^{in})^{\otimes N}]\mathcal{U}_N(t)^*\right)^2}{N}}_{\substack{\text{Normalized OT square pseudometric}\\ \text{per degree of freedom}}} \le \underbrace{2d\hbar e^{Lt}}_{\substack{\text{classical}\\ \hbar\to 0}} + \underbrace{\frac{8\|\nabla V\|_{L^\infty}}{N-1}\frac{e^{Lt}-1}{L}}_{\substack{\text{mean field}\\ N\to\infty}}$$

In particular — see Theorem 1 (2) in Lecture 1 — one has

$$\underbrace{\frac{\mathcal{W}_2\left(\mathcal{H}[R(t)^{\otimes N}], \mathcal{H}[\mathcal{U}_N(t)\mathcal{T}[(f^{in})^{\otimes N}]\mathcal{U}_N(t)^*]\right)^2}{N}}_{\substack{\text{Normalized Wasserstein-2 distance}\\ \text{per degree of freedom}}} \le \frac{8\|\nabla V\|_{L^\infty}}{N-1}\frac{e^{Lt}-1}{L}$$

$$+ 2d\hbar\left(e^{Lt}+1\right)$$

•From N-body Heisenberg to Vlasov

Theorem 2 Under the same assumptions as above,

$$\underbrace{\frac{\mathfrak{d}\left(f(t,\cdot)^{\otimes N},\mathcal{U}_N(t)\mathcal{T}[(f^{in})^{\otimes N}]\mathcal{U}_N(t)^*\right)^2}{N}}_{\substack{\text{Normalized OT square pseudometric}\\\text{per degree of freedom}}}\le\underbrace{d\hbar e^{Lt}}_{\substack{\text{classical}\\\hbar\to 0}}+\underbrace{\frac{8\|\nabla V\|_{L^\infty}}{N-1}\frac{e^{Lt}-1}{L}}_{\substack{\text{mean field}\\N\to\infty}}$$

In particular — see Theorem 1 (2) in Lecture 1 — one has

$$\underbrace{\frac{\mathcal{W}_2\left(f(t,\cdot)^{\otimes N},\mathcal{H}[\mathcal{U}_N(t)\mathcal{T}[(f^{in})^{\otimes N}]\mathcal{U}_N(t)^*]\right)^2}{N}}_{\substack{\text{Normalized Wasserstein-2 distance}\\\text{per degree of freedom}}}\le\frac{8\|\nabla V\|_{L^\infty}}{N-1}\frac{e^{Lt}-1}{L}$$

$$+\,d\hbar\left(e^{Lt}+1\right)$$

(1) Pick $\mathcal{Q}_N^{in} \in \mathcal{C}(R_N^{in}, (R^{in})^{\otimes N},)$ and solve for $\mathcal{Q}_N(t) \in \mathcal{D}(\mathfrak{H}_N \otimes \mathfrak{H}_N)$

$$\begin{cases} i\hbar\partial_t \mathcal{Q}_N(t) = \left[\mathbf{H}_N \otimes I_{\mathfrak{H}_N} + I_{\mathfrak{H}_N} \otimes \sum_{k=1}^N J_{k,N}(-\frac{\hbar^2}{2}\Delta + V_{R(t)}), \mathcal{Q}_N(t)\right] \\ \mathcal{Q}_N(0) = \mathcal{Q}_N^{in}, \qquad J_{k,N}A := I_{\mathfrak{H}}^{\otimes(k-1)} \otimes A \otimes I_{\mathfrak{H}}^{\otimes(N-k)} \end{cases}$$

One checks, by taking partial traces and using uniqueness for the solution of Heisenberg's equation with time-dependent potential that

$$\mathcal{Q}_N(t) \in \mathcal{C}(R_N(t), R(t)^{\otimes N}), \qquad \text{for all } t \geq 0$$

(2) Let $D_N(t) := \frac{1}{N} \operatorname{tr}_{\mathfrak{H}_N \otimes \mathfrak{H}_N}(\mathcal{Q}_N(t)^{\frac{1}{2}} C_\hbar \mathcal{Q}_N(t)^{\frac{1}{2}})$ with $C_\hbar$ given by

$$C_\hbar \Phi :\equiv \sum_{j=1}^N (|x_j - y_j|^2 \Phi - \hbar^2 (\operatorname{div}_{x_j} - \operatorname{div}_{y_j})((\nabla_{x_j} - \nabla_{y_j})\Phi))(X_N, Y_N)$$

(3) By definition of $D_N(t)$, using (1) shows that

$$D_N(t) \geq \tfrac{1}{N}\mathfrak{d}(R_N(t), R(t)^{\otimes N})^2\,, \qquad \text{for all } t \geq 0$$

(4) On the other hand

$$i\hbar\frac{dD_N}{dt} = \tfrac{1}{N}\operatorname{tr}_{\mathfrak{H}_N\otimes\mathfrak{H}_N}(\mathcal{Q}_N(t)^{\frac{1}{2}}[\mathbf{H}_N \otimes I_{\mathfrak{H}_N}, C_\hbar]\mathcal{Q}_N(t)^{\frac{1}{2}})$$
$$+\sum_{k=1}^{N}\tfrac{1}{N}\operatorname{tr}_{\mathfrak{H}_N\otimes\mathfrak{H}_N}(\mathcal{Q}_N(t)^{\frac{1}{2}}[I_{\mathfrak{H}_N}\otimes J_{k,N}(-\tfrac{1}{2}\hbar^2\Delta + V_{R(t)}), C_\hbar]\mathcal{Q}_N(t)^{\frac{1}{2}})$$

and it remains to compute

$$Z_N = -\frac{i}{\hbar}\left[\mathbf{H}_N \otimes I_{\mathfrak{H}_N} + I_{\mathfrak{H}_N}\otimes\sum_{k=1}^{N} J_{k,N}(-\tfrac{1}{2}\hbar^2\Delta + V_{R(t)}), C_\hbar\right]$$

(5) Denoting $A \vee B = AB + BA$, one finds that

$$Z_N = \sum_{j=1}^{N} (x_j - y_j) \vee (-i\hbar\nabla_{x_j} + i\hbar\nabla_{y_j})$$

$$+ \sum_{j=1}^{N} \tfrac{1}{N} \sum_{k=1}^{N} (-\nabla V(x_j - x_k) + \nabla V_{R(t)}(y_j)) \vee (-i\hbar\nabla_{x_j} + i\hbar\nabla_{y_j})$$

and one uses the elementary operator inequality

$$AB^* + BA^* \leq AA^* + BB^*$$

to prove that

$$Z_N \leq 2C_\hbar + \sum_{j=1}^{N} \left| \nabla V_{R(t)}(y_j) - \tfrac{1}{N} \sum_{k=1}^{N} \nabla V(x_j - x_k) \right|^2$$

Split the summand so as to involve the difference between the N-body and the mean-field potentials on the y_j variables only

$$
\begin{aligned}
Z_N \leq & 2C_\hbar + 2\sum_{j=1}^{N}\left|\frac{1}{N}\sum_{k=1}^{N}(\nabla V(y_j - y_k) - \nabla V(x_j - x_k))\right|^2 \\
& + 2\sum_{j=1}^{N}\left|\nabla V_{R(t)}(y_j) - \frac{1}{N}\sum_{k=1}^{N}\nabla V(y_j - y_k)\right|^2 \\
\leq & 2C_\hbar + \frac{2}{N}\operatorname{Lip}(\nabla V)^2 \underbrace{\sum_{j,k=1}^{N}|(y_j - y_k) - (x_j - x_k)|^2}_{\leq 2NC_\hbar} \\
& + 2\sum_{j=1}^{N}\left|\nabla V_{R(t)}(y_j) - \frac{1}{N}\sum_{k=1}^{N}\nabla V(y_j - y_k)\right|^2
\end{aligned}
$$

(6) It remains to bound

$$\sum_{j=1}^{N}\operatorname{tr}_{\mathfrak{H}_N\otimes\mathfrak{H}_N}\left(\mathcal{Q}_N(t)^{\frac{1}{2}}\left|\nabla V_{R(t)}(y_j)-\tfrac{1}{N}\sum_{k=1}^{N}\nabla V(y_j-y_k)\right|^2\mathcal{Q}_N(t)^{\frac{1}{2}}\right)$$

$$=\sum_{j=1}^{N}\operatorname{tr}_{\mathfrak{H}_N}\left(\left|\nabla V_{R(t)}(y_j)-\tfrac{1}{N}\sum_{k=1}^{N}\nabla V(y_j-y_k)\right|^2 R(t)^{\otimes N}\right)$$

Easy since $\mathcal{Q}_N(t)$ is replaced by the **factorized** density $R(t)^{\otimes N}$

Now, for each j, set $W_k:=\nabla V(y_k-y_j)-\nabla V_{R(t)}(y_j)$; then one has

$$\operatorname{tr}_{\mathfrak{H}}(W_kR(t))=0\implies\operatorname{tr}_{\mathfrak{H}_N}\left(\left|\tfrac{1}{N}\sum_{k=1}^{N}W_k\right|^2R(t)^{\otimes N}\right)=\frac{\operatorname{tr}_{\mathfrak{H}}(|W|^2R(t))}{N}$$

q.e.d.

Remarks (from Lecture 1)

Since density operators are characterized by their Husimi transforms, and since the Husimi transform of a density operator is a probability density, a natural idea to define optimal transport distances between density operators is to set

$$d_{ZS}(\rho_1, \rho_2) = \mathcal{W}_2(\mathcal{H}[\rho_1], \mathcal{H}[\rho_2])\,, \qquad \rho_1, \rho_2 \in \mathcal{D}_2(\mathfrak{H})$$

This definition has some advantages over the one proposed here — in the first place, one is always dealing with probability densities, i.e. functions on phase space, which are easier to manipulate than operators. This approach has been proposed by K. Zyczkowski and W. Slomczynski [J. Phys. A 31 (1998), 9095–9104].

However, there is a rather heavy price to pay with this approach, which is that the Husimi transform, and therefore d_{ZS} is not easy to propagate by usual quantum dynamics.

(1) Let $R \in \mathcal{D}_2(\mathfrak{H})$. Prove that $\mathcal{H}[R]$ is a probability density, and compute

$$\iint_{\mathbf{R}^d \times \mathbf{R}^d} (|q|^2 + |p|^2)\mathcal{H}[R](q,p)dqdp$$

(2) Let $R, S \in \mathcal{D}_2(\mathfrak{H})$, and assume that $\mathcal{H}[R] = \mathcal{H}[S]$. Prove that $R = S$. (Idea: let $r \equiv r(y,y')$ be an integral kernel of R. Set

$$J(x,\xi) = \iint_{\mathbf{R}^d \times \mathbf{R}^d} r(y,y')e^{-(|y|^2+|y'|^2)/2\hbar}e^{x\cdot(y+y')-i\xi\cdot(y-y')/\hbar}dydy'$$

Prove that J extends as a holomorphic function on $\mathbf{C}^d \times \mathbf{C}^d$, and therefore is uniquely determined by its restriction to $\mathbf{R}^d \times \mathbf{R}^d$. Conclude by (a) computing the formula relating $\mathcal{H}[R]$ to J, and (b) by computing the integral kernel r of R in terms of J.)

TIME-SPLITTING SCHEMES FOR QUANTUM DYNAMICS

F.G., S. Jin, T. Paul: Found. Comput. Math. **21** (2021), 613–647

Time-Splitting for Quantum Dynamics

Heisenberg equation with unkown $R(t) = R(t)^* \geq 0$

$$i\hbar\partial_t R = [\underbrace{-\tfrac{1}{2}\hbar^2\Delta_x + V(x)}_{\mathbf{H}_\hbar}, R]\,, \qquad R\big|_{t=0} = R^{in}$$

Time-split Heisenberg equation starting from $R^0 = R^{in}$

$$R^{n+\frac{1}{2}} = \exp(\tfrac{i\hbar\Delta t}{2}\Delta_x)R^n \exp(-\tfrac{i\hbar\Delta t}{2}\Delta_x)$$
$$R^{n+1} = \exp(\tfrac{\Delta t}{i\hbar}V(x))R^{n+\frac{1}{2}} \exp(-\tfrac{\Delta t}{i\hbar}V(x))$$

Error bound [S. Descombes-M. Thalhammer 2010]

$$\|\langle\hbar D_x\rangle R^{in}\langle\hbar D_x\rangle\|_1 =: M < \infty \qquad \text{with } \langle\hbar D_x\rangle := (1-\hbar^2\Delta_x)^{\frac{1}{2}}$$
$$\Longrightarrow \|R(n\Delta t) - R^n\|_1 \leq C(M, \|V\|_{W^{2,\infty}})\frac{\Delta t}{\hbar}$$

Not uniform as $\hbar \to 0$, convergence requires $\Delta t \ll \hbar$

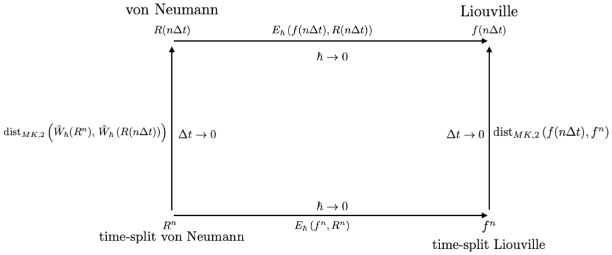

Figure: The horizontal arrows represent the semiclassical limit $\hbar \ll 1$ and the vertical arrows the convergence of the numerical scheme $\Delta t \ll 1$.

•Uniform cvgce without rate [Bao-Jin-Markowich, J. Comp. Phys. 2003]

Liouville equation with unknown $f \equiv f(t,x,\xi) \geq 0$

$$\partial_t f(t,x,\xi) + \{\underbrace{\tfrac{1}{2}|\xi|^2 + V(x)}_{=H(x,\xi)}, f(t,x,\xi)\} = 0\,, \quad f\big|_{t=0} = f^{in}$$

Method of characteristics denoting Φ_t the Hamiltonian flow of H

$$f(t,x,\xi) = f^{in}(\Phi_{-t}(x,\xi))$$

Lie-Trotter time-splitting

$$f^n(y,\eta) = f^{in}\left((K_{-\Delta t} \circ P_{-\Delta t})^n(y,\eta)\right) \qquad \begin{cases} K_t(y,\eta) := (y+t\eta,\eta) \\ P_t(y,\eta) := (y, \eta - t\nabla V(y)) \end{cases}$$

Setting $(X_t, \Xi_t) := \Phi_t(x,\xi)$ and $(Y_t, H_t) := P_t \circ K_t(y,\eta)$, one finds

$$|X_t - Y_t|^2 + |\Xi_t - H_t|^2 \leq (|x-y|^2 + |\xi-\eta|^2)e^{(2+\Lambda)|t|} + \tfrac{e^{(2+\Lambda)|t|}-1}{2+\Lambda}\tfrac{9}{4}\Lambda^2(\tfrac{1}{2}+\Lambda)^2 t^2(1+|y|^2+|\eta|^2)$$

with

$$\Lambda := \max(1, E, \|\nabla^2 V\|_{L^\infty}), \quad E := |\nabla V(0)|$$

Lemma 3 Assume that f^{in} is a probability density on $\mathbf{R}^{2d}$ such that

$$\int (|x|^2 + |\xi|^2) f^{in}(x,\xi)\,dx d\xi < \infty\,.$$

Then, for each $\Delta t \in (0,1)$ and each $n = 0, \ldots, [T/\Delta t]$, one has

$$\mathcal{W}_2(f^n, f(n\Delta t)) \leq C_T[\Lambda, E, f^{in}]\Delta t$$

Lemma 4 Let $R^{in} \in \mathcal{D}_2(\mathfrak{H})$ and $f^{in} \in \mathcal{P}_2(\mathbf{R}^{2d})$, and assume that $V \in C^{1,1}(\mathbf{R}^d)$. For each $\lambda > 0$ consider

$$\begin{cases} \partial_t f + \{\tfrac{1}{2}\lambda|\xi|^2 + V(x), f\} = 0\,, & f\big|_{t=0} = f^{in} \\ i\hbar\partial_t R = [-\tfrac{1}{2}\hbar^2\lambda\Delta + V, R]\,, & R\big|_{t=0} = R^{in} \end{cases}$$

Then $\mathfrak{d}(f(t,\cdot), R(t)) \le \mathfrak{d}(f^{in}, R^{in}) \exp(\tfrac{1}{2}t(\lambda + \max(1, \mathrm{Lip}(\nabla V)^2))$

•Using Lemma 4 first with $\lambda = 1$ and $V = 0$, and then with $\lambda = 0$

$$\mathfrak{d}(f^n \circ K_{-\Delta t}, R^{n+\frac{1}{2}}) \le \mathfrak{d}(f^n, R^n) e^{\frac{\Delta t}{2}}$$

$$\mathfrak{d}(f^n \circ K_{-\Delta t} \circ P_{-\Delta t}, R^{n+1}) \le \mathfrak{d}(f^n \circ K_{-\Delta t}, R^{n+\frac{1}{2}}) e^{\frac{\Delta t}{2}\max(1, \mathrm{Lip}(\nabla V)^2)}$$

so that $\mathfrak{d}(f^n, R^n) \le \mathfrak{d}(f^{in}, R^{in}) \exp\left(\tfrac{1}{2}n\Delta t(1 + \max(1, \mathrm{Lip}(\nabla V)^2))\right)$

Error Bound

Theorem 5 Let $f^{in} \in \mathcal{P}_2(\mathbf{R}^{2d})$, and set $R^{in} = \mathcal{T}[f^{in}]$. Assume that $V \in C^{1,1}(\mathbf{R}^d)$ and set $\Lambda := \max(1, \mathrm{Lip}(\nabla V))$.
The Lie-Trotter splitting scheme for the Heisenberg equation satisfies

$$\mathfrak{d}(R^n, R(n\Delta t)) \leq C_T[\Lambda, \|V\|_{W^{2,\infty}}, f^{in}]\Delta t + 2\sqrt{d\hbar}e^{\frac{T}{2}(1+\Lambda^2)}$$

and the uniform in $\hbar$ convergence rate

$$\sup_{\max(2\|\phi\|_{L^\infty}, \mathrm{Lip}(\phi))\leq 1} \left| \int_{\mathbf{R}^{2d}} \phi(x,\xi)(\mathcal{H}[R^n] - \mathcal{H}[R(n\Delta t)])dxd\xi \right| \leq C'_T[\Lambda, \|V\|_{W^{2,\infty}}, f^{in}]\Delta t^{1/3}$$

The uniform in $\hbar$ convergence rate follows from optimizing between the uniform as $\hbar \to 0$ bound and the Descombes-Thalhammer bound.

There is a similar result with higher order splitting formulas, such as Strang splitting, leading to a uniform $O\left(\Delta t^{2/3}\right)$ estimate

OBSERVATION INEQUALITIES FOR QUANTUM DYNAMICS

FG-T. Paul: Math. Models Meth. Appl. Sci. **32** (2022) 941–963

Heisenberg equation with unkown $R(t) = R(t)^* \geq 0$

$$i\hbar\partial_t R = [\underbrace{-\tfrac{1}{2}\hbar^2\Delta_x + V(x)}_{\mathbf{H}_\hbar}, R]\,, \qquad R\Big|_{t=0} = R^{in}$$

Observing the solution R on a domain $\Omega \subset \mathbf{R}^d$ during time T

$$1(= \|R(t)\|_1) \leq C_{OBS} \int_0^T \mathrm{tr}_{\mathfrak{H}}(\mathbf{1}_\Omega R(t))dt$$

Specialists of control usually consider $R(t) = |\psi(t,\cdot)\rangle\langle\psi(t,\cdot)|$ with

$$i\hbar\partial_t\psi(t,x) = -\tfrac{1}{2}\hbar^2\Delta_x\psi(t,x) + V(x)\psi(t,x)$$

Observing the wave function ψ on the domain Ω during time T means that

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

Classical Hamiltonian $\frac{1}{2}|\xi|^2 + V(x)$, generating a flow on $\mathbf{R}^d \times \mathbf{R}^d$

$$\dot{X} = \Xi\,, \quad \dot{\Xi} = -\nabla V(X)\,, \qquad (X,\Xi)(0;x,\xi) = (x,\xi)$$

Let $K \subset \mathbf{R}^{2d}$ compact, consider a domain $\Omega \subset \mathbf{R}^d$ and let $T > 0$

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

Lemma 6 Assume that $V \in C^{1,1}(\mathbf{R}^d)$ and that K, Ω, T satisfy (GC). Then

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

Proof Since Ω is open $\mathbf{1}_\Omega$ is l.s.c., and by (GC)+Fatou's lemma

$$K \ni (x,\xi) \mapsto \int_0^T \mathbf{1}_\Omega(X(t;x,\xi))dt \in (0,+\infty) \text{ is l.s.c.}$$

Illustration for the Geometric Condition

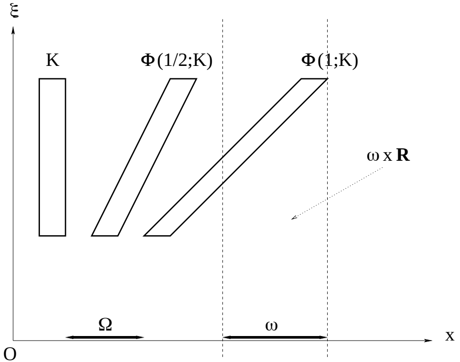

Figure: The geometric condition in space dimension $d = 1$, with $V \equiv 0$. The classical free flow is $\Phi(t; x, \xi) := (X(t; x, \xi), \Xi(t; x, \xi)) = (x + t\xi, \xi)$. The picture represents the image of the closed phase-space rectangle K by the map $(x, \xi) \mapsto \Phi(t; x, \xi)$ at time $t = \frac{1}{2}$ 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 $t \in [0, 1]$.

Metric if $R \in \mathcal{D}_2(\mathfrak{H})$ while f is a probability density on $\mathbf{R}^d \times \mathbf{R}^d$ with finite 2nd order moment

$$\inf_{Q\in\mathcal{C}(f,R)} \iint_{\mathbf{R}^{2d}} \operatorname{tr}_{\mathfrak{H}}(Q(x,\xi)^{\frac{1}{2}}(\lambda^2|x-y|^2+|\xi+i\hbar\nabla_y|^2)Q(x,\xi)^{\frac{1}{2}})dxd\xi$$

$$=: \mathfrak{d}_\lambda(f,R)^2 \geq \lambda d\hbar$$

Theorem 7 [F.G.-T. Paul (ARMA2017)] Assume $V \in C^{1,1}(\mathbf{R}^d)$ such that $\mathbf{H} := -\frac{1}{2}\hbar^2\Delta_x + V(x)$ has a self-adjoint extension to $\mathfrak{H}$, and let $U(t) := e^{-it\mathbf{H}/\hbar}$, 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

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

Theorem 8
Let $V \in C^{1,1}(\mathbf{R}^d)$ and (K, Ω, T) satisfying (GC). Then, for all initial density operator $R^{in} \in \mathcal{D}_2(\mathfrak{H})$, all probability density f^{in} with finite second order moment and all $\delta > 0$, with $\Omega_\delta := \Omega + B(0,\delta)$, one has

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

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

Rmk No need that $\hbar \to 0$; observation constant **completely explicit** in terms of the Bardos-Lebeau-Rauch **geometric data**

Example 1: Töplitz 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)

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

so that

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

Example 2: Pure State

Assume that $R(t)=|U(t)\psi^{in}\rangle\langle U(t)\psi^{in}|$, where $U(t)=e^{-it\mathbf{H}/\hbar}$ 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

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

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

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

so that

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

Since

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

one has

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

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

q.e.d.

(1) Let $\mu, \nu \in \mathcal{P}_2(\mathbf{R}^n)$. Prove that

$$\mathcal{W}_2(e^{t\Delta}\mu, e^{t\Delta}\nu) \leq \mathcal{W}_2(\mu, \nu)\,.$$

(Hint: represent $e^{t\Delta}\mu(x)$ by means of the Brownian motion, and consider the process $(x + B_t, y + B_t) \in \mathbf{R}^n \times \mathbf{R}^n$, with the SAME Brownian motion B_t.)

(2) Find another proof of (1) without appealing to the representation of the solution by means of the Brownian motion. (Hint: pick $\rho_{in} \in \mathcal{C}(\mu, \nu)$ and propagate ρ_{in} by a degenerate diffusion operator A^*A, i.e. set

$$\partial_t \rho_t + A^* A \rho_t = 0\,, \qquad \rho_0 = \rho_{in}$$

where A is a 1st order differential operator such that $A|x - y|^2 = 0$.)

(3) Set $\mathfrak{H} := L^2(\mathbf{R})$ and $q\psi(y) := y\psi(y)$ while $p\psi(y) := -i\hbar\frac{d\psi}{dy}(y)$. Consider the Quantum Heat Equation

$$\partial_t R = -\tfrac{1}{\hbar^2}[p,[p,R]] - \tfrac{1}{\hbar^2}[q,[q,R]]\,, \qquad R(0) = R^{in} \in \mathcal{D}_2(\mathfrak{H})$$

Prove that the Cauchy problem above is solved by a contraction semigroup on $\mathcal{L}^2(\mathfrak{H})$, and that $R(t) \in \mathcal{D}_2(\mathfrak{H})$.

(4) Let R_1, R_2 be the solutions of

$$\partial_t R_1 = -\tfrac{1}{\hbar^2}[p,[p,R_1]] - \tfrac{1}{\hbar^2}[q,[q,R_1]]\,, \qquad R_1(0) = R_1^{in} \in \mathcal{D}_2(\mathfrak{H})$$
$$\partial_t R_2 = -\tfrac{1}{\hbar^2}[p,[p,R_2]] - \tfrac{1}{\hbar^2}[q,[q,R_2]]\,, \qquad R_2(0) = R_2^{in} \in \mathcal{D}_2(\mathfrak{H})$$

Prove that

$$\mathfrak{d}(R_1(t), R_2(t)) \le \mathfrak{d}(R_1^{in}, R_2^{in})\,, \qquad t \ge 0$$

(Hint: consider the operators $[p\otimes I + I\otimes p, q\otimes I - I\otimes q]$ and $[q\otimes I + I\otimes q, p\otimes I - I\otimes p]$.)