Quantum Wasserstein “Metric” and Applications
Lecture 1

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

Our general purpose is to extend optimal transport (Wasserstein) distances, defined on Borel probability measures on phase space, i.e. $\mathbf{R}^d \times \mathbf{R}^d$, to their quantum analogue, i.e. to density operators on the Hilbert space $L^2(\mathbf{R}^d)$

In this first lecture, we

- recall some fundamental results on classical optimal transport
- recall some material trace-class and Hilbert-Schmidt operators
- introduce one first noncommutative extension of optimal transport
- present our quantum extension of the quadratic Wasserstein metric
- discuss some basic estimates and examples of computations

A CRASH COURSE ON CLASSICAL OPTIMAL TRANSPORT

C. Villani: "Topics in Optimal Transportation", AMS 2003

L. Ambrosio, N. Gigli, G. Savaré: "Gradient Flows in Metric Spaces and in the Space of Probability Measures", 2nd ed., Birkhäuser 2008

C.R. Givens, R.M. Shortt: Michigan Math. J. **31** (1984) 231–240

Monge's pbm For $\mu, \nu \in \mathcal{P}_1(\mathbf{R}^n)$, find $T : \mathbf{R}^n \to \mathbf{R}^n$ measurable s.t. $T\#\mu = \nu$

$$\int_{\mathbf{R}^n} |T(x) - x|\mu(dx) = \inf_{\substack{F:\mathbf{R}^n \to \mathbf{R}^n \\ F\#\mu=\nu}} \int_{\mathbf{R}^n} |F(x) - x|\mu(dx)$$

where

$$\mathcal{P}_k(\mathbf{R}^n) := \left\{\mu \in \mathcal{P}(\mathbf{R}^n) \text{ s.t. } \int_{\mathbf{R}^n} |x|^k \mu(dx) < \infty\right\}$$

Kantorovich relaxation of Monge's pbm For $\mu, \nu \in \mathcal{P}_1(\mathbf{R}^n)$, find

$$\mathcal{W}_1(\mu, \nu) := \min_{\rho \in \mathcal{C}(\mu,\nu)} \iint_{\mathbf{R}^n \times \mathbf{R}^n} |x - y|\rho(dxdy)$$

where $\mathcal{C}(\mu, \nu) := \left\{\rho \in \mathcal{P}(\mathbf{R}^{2n}) \,\middle|\, \begin{array}{l} \rho(A \times \mathbf{R}^n) = \mu(A), \\ \rho(\mathbf{R}^n \times A) = \nu(A), \end{array} \quad A \in \mathrm{Bor}(\mathbf{R}^n)\right\}$

Remark T solves Monge's pbm $\implies$ $\rho(dxdy) = \mu(dx)\delta_{T(x)}(dy)$ solves the Kantorovich relaxed pbm

Kantorovich-Rubinstein Duality using convex duality shows that

$$\mathcal{W}_1(\mu,\nu) = \sup_{\substack{\chi\in\mathrm{Lip}(\mathbf{R}^n,\mathbf{R})\\ \mathrm{Lip}(\chi)\le 1}} \left| \int_{\mathbf{R}^n} \chi(z)\mu(dz) - \int_{\mathbf{R}^n} \chi(z)\nu(dz) \right|$$

Consequences

(1) $\mathcal{W}_1$ is a metric on $\mathcal{P}_1(\mathbf{R}^n)$

(2) Let $\mu \in \mathcal{P}_1(\mathbf{R}^n)$ and μ_j be a sequence of elements of $\mathcal{P}_1(\mathbf{R}^n)$. Then the three conditions below are equivalent

(a) $\mathcal{W}_1(\mu_n,\mu) \to 0$

(b) $\mu_j \to \mu$ weakly and

$$\lim_{R\to\infty} \sup_{j\ge 1} \int_{|x|>R} |x|\mu_j(dx) = 0$$

(c) $\mu_j \to \mu$ weakly and

$$\lim_{j\to\infty} \int_{\mathbf{R}^n} |x|\mu_j(dx) = \int_{\mathbf{R}^n} |x|\mu(dx)$$

Kantorovich pbm for $\mu, \nu \in \mathcal{P}_2(\mathbf{R}^n)$

$$\mathcal{W}_2(\mu,\nu) := \left(\min_{\rho \in \mathcal{C}(\mu,\nu)} \iint_{\mathbf{R}^n \times \mathbf{R}^n} |x-y|^2 \rho(dxdy) \right)^{1/2}$$

Kantorovich Duality for $\mathcal{W}_2$

$$\mathcal{W}_2(\mu,\nu)^2 = \sup_{\substack{a(x)+b(y) \le |x-y|^2 \\ a,b \in C_b(\mathbf{R}^n)}} \int_{\mathbf{R}^n} a(x)\mu(dx) + \int_{\mathbf{R}^n} b(x)\nu(dx)$$

Optimal Couplings

(a) (Knott-Smith Thm) $\rho \in \mathcal{C}(\mu,\nu)$ optimal coupling for $\mathcal{W}_2$ iff there exists a proper convex l.c.s. function $\Phi : \mathbf{R}^n \to \mathbf{R} \cup \{+\infty\}$ s.t.

$$\text{supp}(\rho) \subset \text{graph}(\partial\Phi)$$

(b) (Brenier's Thm) if $\mathcal{H} - \dim(S) \le n-1 \implies \mu(S) = 0$, there is a unique optimal coupling for $\mathcal{W}_2$

$$\rho(dxdy) = \mu(dx)\delta_{\nabla\Phi(x)}(dy) \quad \text{with } \Phi : \mathbf{R}^n \to \mathbf{R} \cup \{+\infty\} \text{ convex}$$

Properties of $\mathcal{W}_2$

(1) $\mathcal{W}_2$ is a metric on $\mathcal{P}_2(\mathbf{R}^n)$ (the triangle inequality is not obvious). In particular

$$\mathcal{W}_2(\mu,\nu)=0 \iff \mu=\nu$$

Optimal coupling $\rho(dxdy)=\mu(dx)\delta_x(dy)$, transport map $\mathrm{Id}=\nabla\frac{1}{2}|x|^2$.
(2) Let $\mu\in\mathcal{P}_2(\mathbf{R}^n)$ and μ_j be a sequence of elements of $\mathcal{P}_2(\mathbf{R}^n)$. Then the two conditions below are equivalent

(a) $\mathcal{W}_2(\mu_n,\mu)\to 0$
(b) $\mu_j\to\mu$ weakly and

$$\lim_{R\to\infty}\sup_{j\ge 1}\int_{|x|>R}|x|^2\mu_j(dx)=0$$

(3) G_1, G_2 Gaussian with means m_1, m_2 & covariance matrices A_1, A_2

$$\mathcal{W}_2(G_1,G_2)^2=|m_1-m_2|^2+\operatorname{tr}\left(A_1+A_2-2\left(\sqrt{A_1}A_2\sqrt{A_1}\right)^{\frac{1}{2}}\right)$$

$$\mathcal{W}_2(\delta_{m_1},\delta_{m_2})=|m_1-m_2|$$

(QUANTUM) DENSITY OPERATORS

L. Hörmander: "The Analysis of Linear Partial Differential Operators III", Springer 1994

B. Simon: "Trace Ideals and Their Applications", AMS 2005

F.G., T. Paul: C. R. Acad. Sci. Paris, Ser. I 356 (2018) 177–197

Trace Hilbert space $\mathfrak{H} := L^2(\mathbf{R}^d)$; for $T \in \mathcal{L}(\mathfrak{H})$ s.t. $T = T^* \geq 0$

$$\mathrm{tr}(T) := \sum_{j\geq 1}(e_j|Te_j) \in [0,+\infty] \text{ for all Hilbert basis } (e_j)_{j\geq 0} \text{ of } \mathfrak{H}$$

Trace-class $\mathcal{L}^1(\mathfrak{H}) := \{T\in\mathcal{L}(\mathfrak{H}) : \|T\|_1 := \mathrm{tr}(|T|) < \infty\} \subset \mathcal{K}(\mathfrak{H})$

•the trace tr extends as a linear functional on $\mathcal{L}^1(\mathfrak{H})$ such that

$$A \in \mathcal{L}(\mathfrak{H}) \text{ and } T \in \mathcal{L}^1(\mathfrak{H}) \implies AT \text{ and } TA \in \mathcal{L}^1(\mathfrak{H})$$
$$\mathrm{tr}(AT) = \mathrm{tr}(TA) \text{ and } |\mathrm{tr}(AT)| \leq \|A\|\|T\|_1$$

•$\mathcal{L}^1(\mathfrak{H})$ is a Banach space for the trace-norm $T \mapsto \|T\|_1$, with

$$\mathcal{K}(\mathfrak{H})' = \mathcal{L}^1(\mathfrak{H})\,, \quad \mathcal{L}^1(\mathfrak{H})' = \mathcal{L}(\mathfrak{H})$$

Partial Trace

Let $T \in \mathcal{L}^1(\mathfrak{H}_1 \otimes \mathfrak{H}_2)$; then one defines $T_1 = \operatorname{tr}_2(T) \in \mathcal{L}^1(\mathfrak{H}_1)$ by the formula

$$\operatorname{tr}_{\mathfrak{H}_1}(T_1 A) = \operatorname{tr}_{\mathfrak{H}_1 \otimes \mathfrak{H}_2}(T(A \otimes I_{\mathfrak{H}_2})), \qquad A \in \mathcal{L}(\mathfrak{H})$$

Similar definition for $\operatorname{tr}_1(T) \in \mathcal{L}^1(\mathfrak{H}_2)$.

(Existence+uniqueness of T_1:

$$\mathcal{K}(\mathfrak{H}_1) \ni A \mapsto \operatorname{tr}_{\mathfrak{H}_1 \otimes \mathfrak{H}_2}(T(A \otimes I_{\mathfrak{H}_2})) \in \mathbf{C}$$

is a norm-continuous linear functional on $\mathcal{K}(\mathfrak{H})$, and is therefore represented by a unique trace-class operator T_1. That the identity holds for all $A \in \mathcal{L}(\mathfrak{H}_1)$ follows from a density argument.)

Hilbert-Schmidt Operators

Hilbert-Schmidt class $\mathcal{L}^2(\mathfrak{H}) := \{T \in \mathcal{L}(\mathfrak{H}) : \operatorname{tr}(T^*T) < \infty\}$

•The Hilbert-Schmidt class is a Hilbert space for the inner product

$$(T_1|T_2)_2 := \operatorname{tr}(T_1^* T_2)\,, \quad \text{Hilbert-Schmidt norm } \|T\|_2 := \sqrt{\operatorname{tr}(T^*T)}$$

•$\mathcal{L}^1(\mathfrak{H}) \subset \mathcal{L}^2(\mathfrak{H}) \subset \mathcal{K}(\mathfrak{H}) \subset \mathcal{L}(\mathfrak{H})$ with continuous inclusions, and

$$\|T\| \le \|T\|_2 \le \|T\|_1$$

•if $T = T^* \in \mathcal{L}^2(\mathfrak{H})$, there exists $(e_j)_{j\ge1}$ Hilbert basis of $\mathfrak{H}$ and $(\tau_j)_{j\ge1} \in \ell^2(\mathbf{N}^*;\mathbf{R})$ s.t.

$$T = \sum_{j\ge1} \tau_j P_j\,, \quad \|T\|_2^2 = \sum_{j\ge1} |\tau_j|^2 \text{ and } P_j\phi := (e_j|\phi)_{\mathfrak{H}} e_j$$

Hence

$$T\phi(x) = \int_{\mathbf{R}^d} t(x,y)\phi(y)dy \quad \text{with} \quad t(x,y) := \sum_{j\ge1} \tau_j e_j(x)\overline{e_j(y)}$$

$$\|T\|_2^2 = \iint_{\mathbf{R}^d\times\mathbf{R}^d} |t(x,y)|^2 dxdy$$

Quiz 1: Trace-class and Hilbert-Schmidt Operators

Here $\mathfrak{H} := L^2(\mathbf{R}^d)$.

(1) Prove that any $T \in L^1(\mathfrak{H})$ can be put in the form $T = T_1 T_2$ with $T_1, T_2 \in \mathcal{L}^2(\mathfrak{H})$ and $\|T\|_1 \leq \|T_1\|_2 \|T_2\|_2$.

(2) For all $T \in L^1(\mathfrak{H})$, can one find $T_1, T_2 \in \mathcal{L}^2(\mathfrak{H})$ such that $T = T_1 T_2$ and $\|T\|_1 = \|T_1\|_2 \|T_2\|_2$?

(3) Prove that for each $T \in L^1(\mathfrak{H})$, there exists $t \equiv t(x,y)$ such that $z \mapsto t(x+z,x)$ belongs to $C_b(\mathbf{R}^d_z; L^1(\mathbf{R}^d_x))$, and

$$Tr(T) = \int_{\mathbf{R}^d} t(x,x)dx$$

Consider the Volterra operator V defined on $L^2([0,1])$ by the formula

$$V\phi(x) = \int_0^x \phi(y)dy\,.$$

(1) Prove that V is the integral operator defined by the integral kernel $v(x,y) = \mathbf{1}_{0\le y\le x}$.
(2) Is V Hilbert-Schmidt?
(3) Is $x \mapsto v(x,x)$ integrable on $[0,1]$?
(4) Is V trace-class?
(5) What are the eigenvalues of V?
(6) What is the spectral radius of V?

(Quantum) Density Operators

Density operators on $\mathfrak{H} := L^2(\mathbf{R}^d)$

$$\mathcal{D}(\mathfrak{H}) := \{T \in \mathcal{L}(\mathfrak{H}) \text{ s.t. } T = T^* \geq 0 \text{ and } \operatorname{tr}(T) = 1\} \subset \mathcal{L}^1(\mathfrak{H})$$

Quantum analogue of $\mathcal{P}(\mathbf{R}^d \times \mathbf{R}^d)$
Dirac bra-ket notation for $\phi, \psi \in \mathfrak{H}$, denote by $|\psi\rangle$ the vector ψ

$$\text{and by } \langle\phi| \text{ the linear functional } \psi \mapsto \int_{\mathbf{R}^d} \overline{\phi(x)}\psi(x)dx = \langle\phi|\psi\rangle$$

If $\|\psi\|_{\mathfrak{H}} = 1$, the notation $|\psi\rangle\langle\psi|$ = orthogonal projection on $\mathbf{C}\psi$
Example: Schrödinger coherent state for $q, p \in \mathbf{R}^d$, set

$$|q,p\rangle(x) := (2\pi\hbar)^{-d/4} \exp\left(-\tfrac{1}{2\hbar}|x-q|^2\right) \exp\left(\tfrac{i}{\hbar}p \cdot \left(x - \tfrac{q}{2}\right)\right)$$

One easily checks that

$$\|\,|q,p\rangle\,\|_{\mathfrak{H}} = 1\,, \qquad \text{so that} \qquad \underbrace{|q,p\rangle\langle q,p| \in \mathcal{D}(\mathfrak{H})}_{\text{quantum analogue of } \delta_{q,p} \in \mathcal{P}(\mathbf{R}^d \times \mathbf{R}^d)}$$

Gaussian Wave-Packet: Envelope+Oscillations

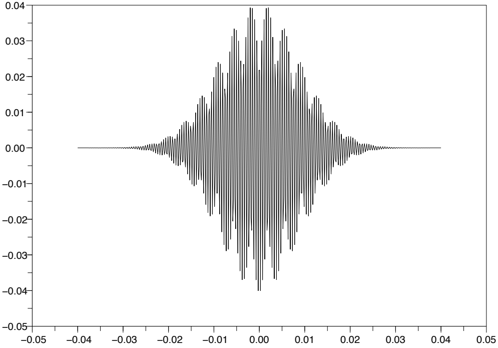

Figure: Oscillating structure of a Gaussian wave-packet

Gaussian Wave-Packet: 3d Plot

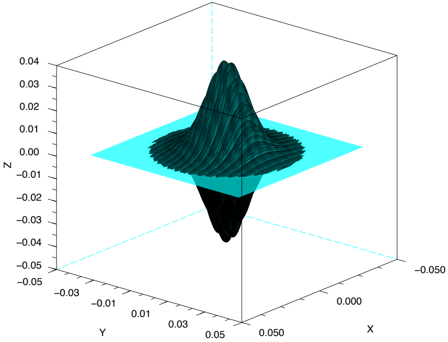

Figure: With $\hbar = 8 \cdot 10^{-5}$, plot of $Z =$ real part of the coherent state centered at $q = (0,0)$ with momentum $p = (1,0)$ with space variable $(X,Y) \in \mathbf{R}^2$

Key example for $(q_1, p_1) \neq (q_2, p_2)$, observe that

$$\underbrace{|q_1, p_1\rangle\langle q_1, p_1|}_{R_1} - \underbrace{|q_2, p_2\rangle\langle q_2, p_2|}_{R_2} = \lambda|e\rangle\langle e| - \lambda|f\rangle\langle f|$$

with $\{e, f\}$ orthonormal and $\lambda \in \mathbf{R}$, since

$$(R_1 - R_2)^* = (R_1 - R_2)\,, \quad \mathrm{tr}(R_1 - R_2) = 0\,, \quad \mathrm{rank}(R_1 - R_2) = 2$$

Therefore

$$\| \underbrace{|q_1, p_1\rangle\langle q_1, p_1|}_{R_1} - \underbrace{|q_2, p_2\rangle\langle q_2, p_2|}_{R_2} \|_1 = 2\lambda = \sqrt{2}\|R_1 - R_2\|_2$$

$$= \underbrace{2\sqrt{1 - e^{-(|q_1-q_2|^2+|p_1-p_2|^2)/2\hbar}}}_{\to\|\delta_{q_1,p_1}-\delta_{q_2,p_2}\|_{TV} \text{ as } \hbar\to 0} \to 2 \quad \text{as } \hbar \to 0$$

Conclusion $\|\cdot\|_1$ fails to capture phase space distances $\gg O(\hbar^{1/2})$

NONCOMMUTATIVE MONGE DISTANCE

A. Connes: chapter 6 of "Noncommutative Geometry", Academic Press 1994

A. Connes: Ergod. Th. Dynam. Sys **9** (1989), 207–220

Let $\mathcal{A}$ be a unital C^*-algebra (Banach *-algebra s.t. $\|a^*a\| = \|a\|^2$)
A **state** on $\mathcal{A}$ is a positive linear functional on $\mathcal{A}$ (i.e. $\omega(a^*a) \geq 0$) of norm 1 (ω positive $\iff$ $\omega(1) = 1$)

Examples of states

•$\mathcal{A} = \mathcal{L}(\mathfrak{H})$ and $\omega(A) := \langle\psi|A|\psi\rangle$ for some $\psi \in \mathfrak{H}$ with $\|\psi\|_{\mathfrak{H}} = 1$
•$\mathcal{A} = \mathcal{L}(\mathfrak{H})$ and $\omega(A) := \mathrm{tr}(RA)$ for some $R \in \mathcal{D}(\mathfrak{H})$

Let $(\mathfrak{H}, D)$ be a Fredholm module on $\mathcal{A}$ i.e.
(a) there is a *-linear representation π of $\mathcal{A}$ in $\mathfrak{H}$
(b) $D = D^*$ unbounded on $\mathfrak{H}$ s.t. $(I + D^2)^{-1} \in \mathcal{K}(\mathfrak{H})$
(c) $\{a \in \mathcal{A} \text{ s.t. } [D, \pi(a)] \in \mathcal{L}(\mathfrak{H})\}$ is norm-dense in $\mathcal{A}$

Theorem [Connes1989] Assume that

$$\{a \in \mathcal{A} \text{ s.t. } \|[D, \pi(a)]\|_{\mathfrak{H}} \leq 1\}/\mathbf{C}1 \text{ is bounded.}$$

Then, the following formula metrizes the set of states on $\mathcal{A}$

$$\mathrm{dist}(\omega_1, \omega_2) := \sup\{|\omega_1(a) - \omega_2(a)| \text{ s.t. } \|[D, \pi(a)]\|_{\mathfrak{H}} \leq 1\}$$

Example: Dirac Operator as a Fredholm Module

Set $\mathcal{A} = C(M)$ where M =compact spin Riemannian manifold, with $\mathfrak{H} := L^2(M; S)$ where S =spinor bundle on M, and $\mathcal{A}$ acting on $\mathfrak{H}$ by scalar multiplication, while D =Dirac operator

$$\operatorname{dist}_g(x,y) = \sup\{|a(x) - a(y)| \,:\, a \in C(M) \text{ s.t. } \|[D,a]\| \le 1\}$$

Proof For $\gamma(v)\zeta$:=Clifford multiplication of $\zeta \in S_x$ by $v \in T_xM$,

$$([D,a]\xi)_x = \gamma((\operatorname{grad} a)_x)\xi_x\,, \quad \xi \in \mathfrak{H} \implies \|[D,a]\| = \|\operatorname{grad} a\|_{L^\infty(M)}$$
$$\implies \operatorname{dist}_g(x,y) \le \sup_{\operatorname{Lip}(a)\le 1} |a(x) - a(y)| \le \operatorname{dist}_g(x,y)$$

(Upper bound obvious by definition; for the lower bound, it suffices to pick $a(z) := \operatorname{dist}_g(z,y)$.)

Remarks on the Connes Distance

•Applies for instance to the case of Γ, a discrete group, with $C^*_{red}(\Gamma)$ defined as the C^* algebra generated by the left regular representation on $\mathfrak{H} := \ell^2(\Gamma)$, with $L : \Gamma \to \mathbf{R}_+$ length function (e.g. word length)

$$L(1) = 0\,, \quad L(g^{-1})L(g)\,, \quad L(gh) \leq L(g) + L(h)$$

Then $(\mathfrak{H}, D)$ is a Fredholm module on $C^*_{red}(\Gamma)$, where

$$D\xi := (L(g)\xi_g)_{g\in\Gamma} \quad \text{for all } \xi = (\xi_g)_{g\in\Gamma} \in \ell^2(\Gamma)$$

•Is there a dual formulation of the Connes distance? see [D'Andrea, Martinetti: J. Geometry Phys. (2021)]
•The Connes distance is a noncommutative analogue of the Monge distance on the space of positions, **not on a phase space**

A QUANTUM ANALOGUE TO $\mathcal{W}_2$

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

F.G. T. Paul: Arch. Ration. Mech. Anal. **223** (2017) 57–94.

Other approaches to defining a quantum analogue of $\mathcal{W}_2$:
G. De Palma, D. Trevisan: Ann. H. Poincaré **22** (2021), 3199–3234.
K. Zuckowski, W. Slominski: J. Phys. A **31** (1998), 9095–9104

Transport Cost

Phase space coordinates position $q \in \mathbf{R}^d$, momentum $p \in \mathbf{R}^d$

Quantization rule (simplest)

$$a(q) \to \text{ multiplication by } a(y) \text{ in } L^2(\mathbf{R}^d_y)\,, \quad p \mapsto -i\hbar\nabla_y$$

•**Classical-to-quantum** transport cost=operator on $L^2(\mathbf{R}^d_y)$

$$c_\hbar(x,\xi) := \underbrace{|x-y|^2 + |\xi + i\hbar\nabla_y|^2}_{\text{quantization in } (y,\eta) \text{ of } |x-q|^2+|\xi-p|^2} \geq d\hbar I_{\mathfrak{H}}$$

•**Quantum-to-quantum** transport cost=operator on $L^2(\mathbf{R}^d_x \times \mathbf{R}^d_y)$

$$C_\hbar := \underbrace{|x-y|^2 - \hbar^2(\nabla_x - \nabla_y)\cdot(\nabla_x - \nabla_y)}_{\text{quantization of } |q-q'|^2+|p-p'|^2} \geq 2d\hbar I_{\mathfrak{H}\otimes\mathfrak{H}}$$

(Lower bounds implied by **Heisenberg's uncertainty inequality**)

Finite Energy Density Operators

Example

$$\underbrace{|q|^2+|p|^2}_{\text{phase space Euclidean norm}} \to \underbrace{|x|^2-\hbar^2\Delta_x}_{\text{harmonic oscillator}}$$

Quantum analogue of $\mathcal{P}_2(\mathbf{R}^d\times\mathbf{R}^d)$

$$\mathcal{D}_2(\mathfrak{H}):=\{R\in\mathcal{D}(\mathfrak{H})\text{ s.t. } \operatorname{tr}(R^{\frac12}(|x|^2-\hbar^2\Delta_x)R^{\frac12})<\infty\}$$

For some $\{\psi_n\in L^2(\mathbf{R}^d,|x|^2dx)\cap H^1(\mathbf{R}^d)\}$ orthonormal in $\mathfrak{H}=L^2(\mathbf{R}^d)$

$$R=\sum_{n\ge1}\rho_n|\psi_n\rangle\langle\psi_n|\in\mathcal{D}_2(\mathfrak{H}) \iff \begin{cases}\rho_n\ge0\text{ and }\sum_{n\ge1}\rho_n=1\\ \sum_{n\ge1}\rho_n(\|x\psi_n\|^2_{\mathfrak{H}}+\hbar^2\|\nabla\psi_n\|^2_{\mathfrak{H}})<\infty\end{cases}$$

Couplings

•Denote $\mathcal{C}(\mu,\nu)$ the set of (classical) couplings of $\mu,\nu\in\mathcal{P}(\mathbf{R}^{2d})$

•Set of **couplings of** 2 **quantum density** operators R,S:

$$\mathcal{C}(R,S):=\{T\in\mathcal{D}(\mathfrak{H}\otimes\mathfrak{H})\text{ s.t. }\operatorname{tr}(T(A\otimes I+I\otimes B))=\operatorname{tr}(RA+SB)\}$$

•**Coupling** Q of a probability density $f(x,\xi)$ on $\mathbf{R}^{2d}$ with $R\in\mathcal{D}(\mathfrak{H})$

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

$$\operatorname{tr}(Q(x,\xi))=f(x,\xi)\text{ a.e.,}\qquad\text{and }\int_{\mathbf{R}^{2d}}Q(x,\xi)dxd\xi=R$$

The set of couplings of f with R will be denoted $\mathcal{C}(f,R)$

Examples for all $R,S\in\mathcal{D}(\mathfrak{H})$ and each f probability density on $\mathbf{R}^{2d}$

$$R\otimes S\in\mathcal{C}(R,S)\,,\qquad\{fR=f\otimes_{\mathbf{C}}R:\,(x,\xi)\mapsto f(x,\xi)R\}\subset\mathcal{C}(f,R)$$

•For $\mu, \nu \in \mathcal{P}_2(\mathbf{R}^{2d})$, set $\mathfrak{d}(\mu, \nu) := \mathcal{W}_2(\mu, \nu)$

•For $f(x, \xi)dxd\xi \in \mathcal{P}_2(\mathbf{R}^{2d})$ and $R \in \mathcal{D}_2(\mathfrak{H})$, set

$$\mathfrak{d}(f, R) := \inf_{Q \in \mathcal{C}(f,R)} \left(\int_{\mathbf{R}^{2d}} \operatorname{tr}_{\mathfrak{H}}(Q(x,\xi)^{\frac{1}{2}} c_\hbar(x,\xi) Q(x,\xi)^{\frac{1}{2}}) dxd\xi \right)^{\frac{1}{2}}$$

•For $R, S \in \mathcal{D}_2(\mathfrak{H})$, set

$$\mathfrak{d}(R, S) := \inf_{T \in \mathcal{C}(R,S)} \left(\operatorname{tr}_{\mathfrak{H} \otimes \mathfrak{H}}(T^{\frac{1}{2}} C_\hbar T^{\frac{1}{2}}) \right)^{\frac{1}{2}}$$

Remark for $f(x, \xi)dxd\xi \in \mathcal{P}_2(\mathbf{R}^{2d})$ and $R, S \in \mathcal{D}_2(\mathfrak{H})$

$$\mathfrak{d}(f, R) \geq \sqrt{d\hbar} \qquad \text{and} \qquad \mathfrak{d}(R, S) \geq \sqrt{2d\hbar}$$

In particular $\mathfrak{d}(R, R) > 0$ (hence $\mathfrak{d}$ is not a bona fide metric)

Quiz 3: Finite Energy+2nd Moment Implies Finite $\mathfrak{d}$

Prove that $\mathfrak{d}(f, R) + \mathfrak{d}(R, S) < \infty$ for all $R, S \in \mathcal{D}_2(\mathfrak{H})$ and all probability density f with finite second order moments.

Wave packet For all $q, p \in \mathbf{R}^d$, set

$$|q,p\rangle(x) := (\pi\hbar)^{-d/4} \exp(-\tfrac{1}{2\hbar}|x-q|^2) \exp(\tfrac{i}{\hbar} p \cdot (x - \tfrac{q}{2}))$$

Toeplitz map To m, Radon measure on $\mathbf{R}^d$, associate the operator

$$\mathcal{T}[m] := \int_{\mathbf{R}^d} |q,p\rangle\langle q,p| m(dqdp)$$

The form-domain of $\mathcal{T}[m]$ is the set of $\phi \in \mathfrak{H}$ such that the function $(q,p) \mapsto \langle q,p|\psi\rangle$ belongs to $L^2(\mathbf{R}^{2d}; m)$

Basic properties

(1) $\mathcal{T}[1] = (2\pi\hbar)^d I_{\mathfrak{H}}$, while $m \in \mathcal{P}(\mathbf{R}^d \times \mathbf{R}^d) \implies \mathcal{T}[m] \in \mathcal{D}(\mathfrak{H})$

(2) one has $\mathcal{T}[q] = (2\pi\hbar)^d x$, while $\mathcal{T}[p] = (2\pi\hbar)^d(-i\hbar\nabla_x)$

(3) if f is a quadratic form on $\mathbf{R}^d$, then

$$\begin{cases} \mathcal{T}[f(q)] = (2\pi\hbar)^d \left(f(x) + \tfrac{1}{4}\hbar(\Delta f) I_{\mathfrak{H}}\right) \text{ and} \\ \mathcal{T}[f(p)] = (2\pi\hbar)^d \left(f(-i\hbar\nabla_x) + \tfrac{1}{4}\hbar(\Delta f) I_{\mathfrak{H}}\right) \end{cases}$$

To $T \in \mathcal{L}(\mathfrak{H})$, one associates its Husimi transform

$$\mathcal{H}[T](q,p) := \frac{1}{(2\pi\hbar)^d} \langle q,p|T|q,p\rangle$$

Properties

(1) $T = T^* \implies \mathcal{H}[T](q,p) \in \mathbf{R}$ and $T \geq 0 \implies \mathcal{H}[T] \geq 0$

(2) One has $\mathcal{H}[\mathcal{T}[m]] = e^{\frac{\hbar}{2}\Delta_{q,p}} m$ since

$$\langle q,p|q',p'\rangle = e^{-\frac{1}{4\hbar}(|q-q'|^2+|p-p'|^2)} e^{-\frac{i}{\hbar}(p\cdot q'-q\cdot p')}$$

(3) One has $\mathcal{H}[I] = (2\pi\hbar)^{-d}$, while

$$\begin{cases} \mathcal{H}[f(x)](q,p) = (2\pi\hbar)^{-d}(I + \frac{1}{4}\hbar\Delta)f(q) \text{ and} \\ \mathcal{H}[f(-i\hbar\nabla_x)](q,p) = (2\pi\hbar)^{-d}(I + \frac{1}{4}\hbar\Delta)f(p) \end{cases}$$

(4) One has

$$\operatorname{tr}(R^*\mathcal{T}[f]) = (2\pi\hbar)^d \iint_{\mathbf{R}^d\times\mathbf{R}^d} \overline{\mathcal{H}[R](q,p)} f(q,p)\,dqdp$$

Theorem 1

(1) For f, g probability densities on $\mathbf{R}^{2d}$ with finite 2nd moments

$$\mathfrak{d}(\mathcal{T}[f], \mathcal{T}[g])^2 \leq \mathcal{W}_2(f,g)^2 + 2d\hbar, \qquad \mathfrak{d}(\mathcal{T}[f], \mathcal{T}[f]) = \sqrt{2d\hbar}$$

$$\mathfrak{d}(f, \mathcal{T}[g])^2 \leq \mathcal{W}_2(f,g)^2 + d\hbar, \qquad \mathfrak{d}(f, \mathcal{T}[f]) = \sqrt{d\hbar}$$

(2) For $R, S \in \mathcal{D}_2(\mathfrak{H})$

$$\mathcal{W}_2(\mathcal{H}[R], \mathcal{H}[S])^2 \leq \mathfrak{d}(R,S)^2 + 2d\hbar$$

$$\mathcal{W}_2(f, \mathcal{H}[R])^2 \leq \mathfrak{d}(f,R)^2 + d\hbar$$

(3) Moreover, if $\operatorname{rank}(R) = 1$, then

$$\mathfrak{d}(R,S) = \operatorname{tr}_{\mathfrak{H}\otimes\mathfrak{H}}((R\otimes S)^{\frac{1}{2}} C_\hbar (R\otimes S)^{\frac{1}{2}})^{\frac{1}{2}}$$

$$\mathfrak{d}(f,R) = \left(\int_{\mathbf{R}^{2d}} f(x,\xi) \operatorname{tr}_{\mathfrak{H}}(R^{\frac{1}{2}} c_\hbar(x,\xi) R^{\frac{1}{2}}) dx d\xi\right)^{\frac{1}{2}}$$

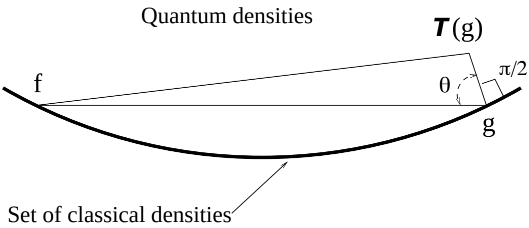

Figure: The second inequality in (1) can be recast as

$$\mathfrak{d}(f,\mathcal{T}[g])^2 \le \mathfrak{d}(f,g)^2 + \mathfrak{d}(g,\mathcal{T}[g])^2$$

$$\text{since } \mathfrak{d}(g,\mathcal{T}[g]) = \sqrt{d\hbar} = \min \mathfrak{d}$$

This suggests that

(1) "the segment $[g,\mathcal{T}[g]]$ is orthogonal to the set of classical densities",

(2) the "angle" θ is acute.

Hence the set of quantum densities lies on the "concave" side of the set of classical densities

Let $\nabla\Phi$ (with Φ convex) be the Brenier map pushing f to g. The optimal coupling of f and g for $\mathcal{W}_2$ is

$$\Lambda := f(x,\xi)\delta_{\nabla\Phi(x,\xi)}(dyd\eta)dxd\xi$$

Hence

$$\mathcal{T}[\Lambda]\in\mathcal{C}(\mathcal{T}[f],\mathcal{T}[g]) \quad \text{and} \quad (x,\xi)\mapsto f(x,\xi)\mathcal{T}[\delta_{\nabla\Phi(x,\xi)}]\in\mathcal{C}(f,\mathcal{T}[g])$$

On the other hand

$$\mathcal{H}[C_\hbar](q,p,q',p') = (2\pi\hbar)^{-2d}(|q-q'|^2+|p-p'|^2+2d\hbar)$$
$$\mathcal{H}[c_\hbar(x,\xi)](q,p) = (2\pi\hbar)^{-d}(|x-q|^2+|\xi-p|^2+d\hbar)$$

Therefore

$$\mathfrak{d}(\mathcal{T}[f],\mathcal{T}[g])^2 \le \operatorname{tr}_{\mathfrak{H}\otimes\mathfrak{H}}(\mathcal{T}[\Lambda]^{\frac{1}{2}} C_\hbar \mathcal{T}[\Lambda]^{\frac{1}{2}})$$

$$= \int_{\mathbf{R}^{4d}} \underbrace{(|q-q'|^2+|p-p'|^2+2d\hbar)}_{=(2\pi\hbar)^{2d}\overline{\mathcal{H}[C_\hbar](q,p)}} \Lambda(dqdpdq'dp')$$

$$= \mathcal{W}_2(f,g)^2 + 2d\hbar$$

and

$$\mathfrak{d}(f,\mathcal{T}[g])^2 \le \int_{\mathbf{R}^{2d}} \operatorname{tr}_{\mathfrak{H}}(\mathcal{T}[\delta_{\nabla\Phi(x,\xi)}]^{\frac{1}{2}} c_\hbar(x,\xi)\mathcal{T}[\delta_{\nabla\Phi(x,\xi)}]^{\frac{1}{2}}) f(x,\xi)dxd\xi$$

$$= \int_{\mathbf{R}^{2d}} \underbrace{(|(x,\xi)-\nabla\Phi(x,\xi)|^2+d\hbar)}_{=(2\pi\hbar)^{d}\overline{\mathcal{H}[c_\hbar(x,\xi)](\nabla\Phi(x,\xi))}} f(x,\xi)dxd\xi = \mathcal{W}_2(f,g)^2 + d\hbar$$

q.e.d.

Proof of Theorem 1 (2)

Pick $a_n, b_n \in C_b(\mathbf{R}^{2d};\mathbf{R})$ such that

$$a_n(q,p)+b_n(q',p')\le|q-q'|^2+|p-p'|^2\,,\qquad\text{and}$$

$$\underbrace{\int_{\mathbf{R}^{2d}}a_n(q,p)\mathcal{H}[R](q,p)dqdp}_{=(2\pi\hbar)^{-d}\operatorname{tr}_{\mathfrak{H}}(\mathcal{T}[a_n]R)}+\underbrace{\int_{\mathbf{R}^{2d}}b_n(q',p')\mathcal{H}[S](q',p')dq'dp'}_{=(2\pi\hbar)^{-d}\operatorname{tr}_{\mathfrak{H}}(\mathcal{T}[b_n]S)}$$

$$\to\mathcal{W}_2(\mathcal{H}[R],\mathcal{H}[S])^2$$

On the other hand, for each $T\in\mathcal{C}(R,S)$, one has

$$\begin{aligned}&(2\pi\hbar)^{-d}\operatorname{tr}_{\mathfrak{H}}(\mathcal{T}[a_n]R)+(2\pi\hbar)^{-d}\operatorname{tr}_{\mathfrak{H}}(\mathcal{T}[b_n]S)\\&=(2\pi\hbar)^{-d}\operatorname{tr}_{\mathfrak{H}\otimes\mathfrak{H}}(T^{\frac12}(\mathcal{T}[a_n]\otimes I+I\otimes\mathcal{T}[b_n])T^{\frac12})\\&=(2\pi\hbar)^{-2d}\operatorname{tr}_{\mathfrak{H}\otimes\mathfrak{H}}(T^{\frac12}\mathcal{T}[a_n\otimes1+1\otimes b_n]T^{\frac12})\\&\le(2\pi\hbar)^{-2d}\operatorname{tr}_{\mathfrak{H}\otimes\mathfrak{H}}(T^{\frac12}\mathcal{T}[|q-q'|^2+|p-p'|^2]T^{\frac12})\end{aligned}$$

Now, one has

$$\mathcal{T}[|q-q'|^2+|p-p'|^2] = (2\pi\hbar)^{2d}(C_\hbar + 2d\hbar I_{\mathfrak{H}\otimes\mathfrak{H}})$$

Thus, for all $T \in \mathcal{C}(R,S)$, one has

$$\mathcal{W}_2(\mathcal{H}[R],\mathcal{H}[S])^2 = \lim_{n\to\infty}(2\pi\hbar)^{-d}\left(\mathrm{tr}_{\mathfrak{H}}(\mathcal{T}[a_n]R) + \mathrm{tr}_{\mathfrak{H}}(\mathcal{T}[b_n]S)\right)$$
$$\leq \mathrm{tr}_{\mathfrak{H}\otimes\mathfrak{H}}(T^{\frac{1}{2}}(C_\hbar + 2d\hbar I_{\mathfrak{H}\otimes\mathfrak{H}})T^{\frac{1}{2}}) = \mathrm{tr}_{\mathfrak{H}\otimes\mathfrak{H}}(T^{\frac{1}{2}}C_\hbar T^{\frac{1}{2}}) + 2d\hbar$$

Minimizing the r.h.s. in $T \in \mathcal{C}(R,S)$ leads to

$$\mathcal{W}_2(\mathcal{H}[R],\mathcal{H}[S])^2 \leq \mathfrak{d}(R,S)^2 + 2d\hbar$$

q.e.d.

(1) Start from

$$\mathcal{T}[|q-q'|^2+|p-p'|^2]=(2\pi\hbar)^{2d}(C_\hbar+2d\hbar I_{\mathfrak{H}\otimes\mathfrak{H}})$$

(2) For each $T\in\mathcal{C}(R,S)$, write

$$\begin{aligned}\operatorname{tr}_{\mathfrak{H}\otimes\mathfrak{H}}\left(T^{\frac{1}{2}}C_\hbar T^{\frac{1}{2}}\right)+2d\hbar\geq\tfrac{1}{(2\pi\hbar)^d}\operatorname{tr}_{\mathfrak{H}\otimes\mathfrak{H}}\left(T\mathcal{T}\left[\tfrac{|q-q'|^2+|p-p'|^2}{1+\epsilon|q-q'|^2+\epsilon|p-p'|^2}\right]\right)\\=\int_{\mathbf{R}^{4d}}\mathcal{H}[T](q,p,q',p')\tfrac{|q-q'|^2+|p-p'|^2}{1+\epsilon|q-q'|^2+\epsilon|p-p'|^2}dqdpdq'dp'\end{aligned}$$

(3) Conclude by monotone convergence, after observing that $\mathcal{H}[T]$ is a coupling of $\mathcal{H}[R]$ and $\mathcal{H}[S]$

Question structure of couplings for rank-1 density operators?

Lemma 2 Let $R \in \mathcal{D}(\mathfrak{H})$. Then

$$\operatorname{rank}(R) = 1 \implies \begin{cases} \mathcal{C}(f, R) = \{fR\}, & f \in \mathcal{P}(\mathbf{R}^d \times \mathbf{R}^d) \\ \mathcal{C}(R, S) = \{R \otimes S\}, & S \in \mathcal{D}(\mathfrak{H}) \end{cases}$$

Remark Rank-1 density operators=quantum analogues of Dirac mass

$$\mathcal{C}(\mu, \delta_z) = \{\mu \otimes \delta_z\} \quad \text{for all } \mu \in \mathcal{P}(\mathbf{R}^d \times \mathbf{R}^d)$$

Obviously Lemma 2 $\implies$ Theorem 1 (3)

Proof Since $\operatorname{rank}(R) = 1$, it is of the form $R = |\phi\rangle\langle\phi|$ with $\|\phi\|_{\mathfrak{H}} = 1$

$$\begin{aligned} \operatorname{tr}(((I - R) \otimes I)Q((I - R) \otimes I)) &= \operatorname{tr}(Q((I - R)^2 \otimes I)) \\ &= \operatorname{tr}(Q((I - R) \otimes I)) = \operatorname{tr}(R(I - R)) = 0 \\ &\implies ((I - R) \otimes I)Q((I - R) \otimes I) = 0 \end{aligned}$$

Next, we deduce from the Cauchy-Schwarz inequality that

$$\begin{aligned}&|\langle\psi_1\otimes\psi_2|(R\otimes I)Q((I-R)\otimes I)\psi_1'\otimes\psi_2'\rangle|^2\\ \le&\langle\psi_1'\otimes\psi_2'|((I-R)\otimes I)Q((I-R)\otimes I)\psi_1'\otimes\psi_2'\rangle\\ &\times\langle\psi_1\otimes\psi_2|(R\otimes I)Q(R\otimes I)\psi_1\otimes\psi_2\rangle\end{aligned}$$

Hence

$$\begin{aligned}(R\otimes I)Q((I-R)\otimes I)=0=&((R\otimes I)Q((I-R)\otimes I))^*\\ =&((I-R)\otimes I)Q(R\otimes I)\\ \Longrightarrow&\;Q=(R\otimes I)Q(R\otimes I)\end{aligned}$$

so that $Q=R\otimes T$ where

$$\langle\psi|T|\psi'\rangle:=\langle\phi\otimes\psi|Q|\phi\otimes\psi'\rangle$$

Finally, $T=S$, since, for all $A\in\mathcal{L}(\mathfrak{H})$, one has

$$\operatorname{tr}(SA)=\operatorname{tr}(Q(I\otimes A))=\operatorname{tr}((R\otimes T)(I\otimes A))=\operatorname{tr}(TA)$$

q.e.d.

Quiz 5: Coupling Probability Densities with Pure States

Complete the proof of Lemma 2 in the case $\mathcal{C}(f, R)$ with R a rank-1 density operator.

QUANTUM OT IS CHEAPER

E. Caglioti, F. Golse, T. Paul: J. Statistical Phys. **181** (2020), 149–162

With $d = 1$ and $0 < a < b$, set

$$\mu := \tfrac{1}{2}(\delta_{+a,0} + \delta_{-a,0}) \text{ and } \nu := \tfrac{1}{2}(\delta_{+b,0} + \delta_{-b,0}) \in \mathcal{P}_2(\mathbf{R} \times \mathbf{R})$$

Proposition 3

(1) One has

$$\mathfrak{d}(\mathcal{T}[\mu], \mathcal{T}[\nu])^2 = \mathcal{W}_2(\mu, \nu)^2 + 2\hbar$$

(2) For $\rho_1, \rho_2 \in \mathcal{P}_2(\mathbf{R}^{2d})$ with optimal coupling Π for $\mathcal{W}_2$, one has

$$\mathfrak{d}(\mathcal{T}[\rho_1], \mathcal{T}[\rho_2])^2 = \mathcal{W}_2(\rho_1, \rho_2)^2 + 2d\hbar$$
$$\iff \mathcal{T}[\Pi] \in \mathcal{C}(\mathcal{T}[\rho_1], \mathcal{T}[\rho_2]) \text{ optimal for } \mathfrak{d}$$

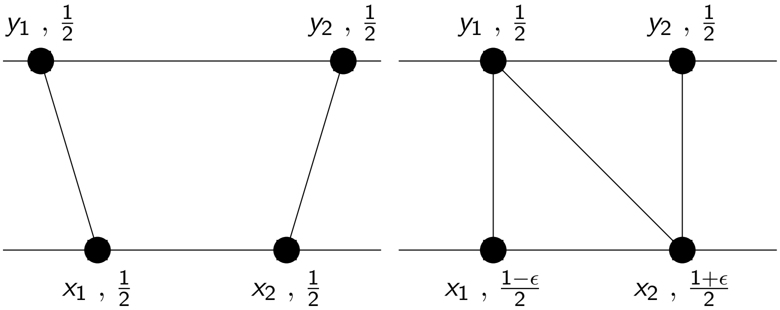

Figure: Left: equal masses; Right: unequal mass case

For $0 < \epsilon < 1$, set

$$\mu = \tfrac{1}{2}(\delta_{+a,0} + \delta_{-a,0}) \text{ and } \rho_\epsilon = \tfrac{1+\epsilon}{2}\delta_{+a,0} + \tfrac{1-\epsilon}{2}\delta_{-a,0} \in \mathcal{P}_2(\mathbf{R}\times\mathbf{R})$$

Proposition 4
For each $\epsilon \in (0,1)$, one has

$$\mathfrak{d}(\mathcal{T}[\mu], \mathcal{T}[\rho_\epsilon])^2 < \mathcal{W}_2(\mu, \rho_\epsilon)^2 + 2\hbar$$

Idea of the proof Optimal coupling(s) in the unequal mass case

$$T = \sum_{k,l,m,n\in\{\pm\}} \tau_{klmn}|k,l\rangle\langle m,n| \qquad \text{with } |k,l\rangle = |ka,0\rangle \otimes |lb,0\rangle$$

$$= \underbrace{\sum_{k,l\in\{\pm\}} \tau_{klkl}|k,l\rangle\langle k,l|}_{\text{Toeplitz coupling}} + \underbrace{\sum_{(k,l)\neq(m,n)\in\{\pm\}} \tau_{klmn}|k,l\rangle\langle m,n|}_{\text{nonclassical contribution}}$$

Remarks

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.

Quiz 6: Husimi Characterizes the Operator

(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.)