Quantizations of the quadratic Monge-Kantorovitch distance

Thierry PAUL
CNRS et Centre de Mathématiques Laurent Schwartz
École Polytechnique

Wavelets and Beyond
A celebration for Alexandre Grossmann and Yves Meyer
June 14 2019

Quantum computing

Quantum computing

Q-computer with 100 qubits $\rightarrow$ one mole of gaz

Quantum computing

Q-computer with 100 qubits $\rightarrow$ one mole of gaz

2^{100} >Avogadro

Quantum computing

Q-computer with 100 qubits $\rightarrow$ one mole of gaz

2^{100} $>$Avogadro

Quantum Information

Quantum computing

Q-computer with 100 qubits $\rightarrow$ one mole of gaz

2^{100} >Avogadro

Quantum Information

discriminate states

Quantum computing

Q-computer with 100 qubits $\rightarrow$ one mole of gaz

2^{100} >Avogadro

Quantum Information

discriminate states

(Gedenken) Experiments :

Quantum computing

Q-computer with 100 qubits $\rightarrow$ one mole of gaz

2^{100} >Avogadro

Quantum Information

discriminate states

(Gedenken) Experiments :

rubidium $\sim$ small bacteria

Quantum computing

Q-computer with 100 qubits $\rightarrow$ one mole of gaz

2^{100} >Avogadro

Quantum Information

discriminate states

(Gedenken) Experiments :

rubidium $\sim$ small bacteria

time $\sim$ 2 seconds

Quantum computing

Q-computer with 100 qubits $\rightarrow$ one mole of gaz

2^{100} >Avogadro

Quantum Information

discriminate states

(Gedenken) Experiments :

rubidium $\sim$ small bacteria

time $\sim$ 2 seconds

$\Downarrow$

macro/micro $\neq$ classical/quantum

How to metrize the space of quantum states ?

other than in Lebesgue, Schatten norms

Quantum analogue of Wasserstein distances.

quantization of Wasserstein

Toward quantum optimal transport.

stricture of optimal couplings

Time splitting algorithm unifnorm in $\hbar$.

$i\hbar\partial_t \ldots \Rightarrow \frac{\Delta t}{\hbar}$

Semiclassical approximation with low regularity.

direct "distance" between quantum and classical objects

Gronwall instead of Calderon-Vaillancourt

An exercise : how to metrize the space of quantum states

quantum information : how to distinguish two states ?

coherent states (Gabor) : for $z = (p, q) \in \mathbb{R}^{2d}$,

$$\psi_z(x) = (\pi\hbar)^{-d/4} e^{-\frac{(x-q)^2}{2\hbar}} e^{i\frac{p.x}{\hbar}}$$

Notations : $\psi_z \sim |\,\psi_z\rangle \sim |\,z\rangle,\ |\,\psi\rangle\langle\psi\,| = \mathbb{P}^{\perp}_{\psi}$

An exercise : how to metrize the space of quantum states

quantum information : how to distinguish two states ?

coherent states (Gabor) : for $z = (p, q) \in \mathbb{R}^{2d}$,

$$\psi_z(x) = (\pi\hbar)^{-d/4} e^{-\frac{(x-q)^2}{2\hbar}} e^{i\frac{p.x}{\hbar}}$$

Notations : $\psi_z \sim |\psi_z\rangle \sim |z\rangle, \ |\psi\rangle\langle\psi| = \mathbb{P}^{\perp}_{\psi}$

states in QM : (density matrix) $R > 0, \mathrm{Tr}\, R = 1$

e.g (pure) $R = |\psi\rangle\langle\psi|, \ \psi \in L^2(\mathbb{R}^d)$

An exercise : how to metrize the space of quantum states

quantum information : how to distinguish two states ?

coherent states (Gabor) : for $z = (p, q) \in \mathbb{R}^{2d}$,

$$\psi_z(x) = (\pi\hbar)^{-d/4} e^{-\frac{(x-q)^2}{2\hbar}} e^{i\frac{p.x}{\hbar}}$$

Notations : $\psi_z \sim |\,\psi_z\rangle \sim |\,z\rangle,\ |\,\psi\rangle\langle\psi\,| = \mathbb{P}^{\perp}_{\psi}$

states in QM : (density matrix) $R > 0, \operatorname{Tr} R = 1$

e.g (pure) $R = |\,\psi\rangle\langle\psi\,|,\ \psi \in L^2(\mathbb{R}^d)$

QUESTION : "distance" between $|\,z_1\rangle\langle z_1\,|$ and $|\,z_2\rangle\langle z_2\,|$, for $z_1, z_2 \in \mathbb{R}^{2d}$?

An exercise : how to metrize the space of quantum states

quantum information : how to distinguish two states ?

coherent states (Gabor) : for $z = (p, q) \in \mathbb{R}^{2d}$,

$$\psi_z(x) = (\pi\hbar)^{-d/4} e^{-\frac{(x-q)^2}{2\hbar}} e^{i\frac{p.x}{\hbar}}$$

Notations : $\psi_z \sim |\psi_z\rangle \sim |z\rangle, \ |\psi\rangle\langle\psi| = \mathbb{P}^{\perp}_{\psi}$

states in QM : (density matrix) $R > 0, \mathrm{Tr}\, R = 1$

e.g (pure) $R = |\psi\rangle\langle\psi|, \ \psi \in L^2(\mathbb{R}^d)$

QUESTION : "distance" between $|z_1\rangle\langle z_1|$ and $|z_2\rangle\langle z_2|$, for $z_1, z_2 \in \mathbb{R}^{2d}$?

In strong Schatten class $\|T\|_p^p = \mathrm{Tr}(T^*T)^{p/2}$ (e.g. Trace ($p = 1$), HS ($p = 2$)) :

An exercise : how to metrize the space of quantum states

quantum information : how to distinguish two states ?

coherent states (Gabor) : for $z = (p, q) \in \mathbb{R}^{2d}$,

$$\psi_z(x) = (\pi\hbar)^{-d/4} e^{-\frac{(x-q)^2}{2\hbar}} e^{i\frac{p.x}{\hbar}}$$

Notations : $\psi_z \sim |\psi_z\rangle \sim |z\rangle, \ |\psi\rangle\langle\psi| = \mathbb{P}^{\perp}_{\psi}$

states in QM : (density matrix) $R > 0, \mathrm{Tr}\, R = 1$

e.g (pure) $R = |\psi\rangle\langle\psi|, \ \psi \in L^2(\mathbb{R}^d)$

QUESTION : "distance" between $|z_1\rangle\langle z_1|$ and $|z_2\rangle\langle z_2|$, for $z_1, z_2 \in \mathbb{R}^{2d}$?

In strong Schatten class $\|T\|_p^p = \mathrm{Tr}(T^*T)^{p/2}$ (e.g. Trace ($p = 1$), HS ($p = 2$)) :

$$\big\| |z_1\rangle\langle z_1| - |z_2\rangle\langle z_2| \big\|_p = 2^{\frac{1}{p}} \sqrt{1 - e^{-\frac{|z_1 - z_2|^2}{2\hbar}}}$$

An exercise : how to metrize the space of quantum states

quantum information : how to distinguish two states ?

coherent states (Gabor) : for $z = (p, q) \in \mathbb{R}^{2d}$,

$$\psi_z(x) = (\pi\hbar)^{-d/4} e^{-\frac{(x-q)^2}{2\hbar}} e^{i\frac{p.x}{\hbar}}$$

Notations : $\psi_z \sim |\,\psi_z\rangle \sim |\,z\rangle, \ |\,\psi\rangle\langle\psi\,| = \mathbb{P}^{\perp}_{\psi}$

states in QM : (density matrix) $R > 0, \mathrm{Tr}\, R = 1$

e.g (pure) $R = |\,\psi\rangle\langle\psi\,|, \ \psi \in L^2(\mathbb{R}^d)$

QUESTION : "distance" between $|\,z_1\rangle\langle z_1\,|$ and $|\,z_2\rangle\langle z_2\,|$, for $z_1, z_2 \in \mathbb{R}^{2d}$?

In strong Schatten class $\|T\|_p^p = \mathrm{Tr}(T^*T)^{p/2}$ (e.g. Trace ($p = 1$), HS ($p = 2$)) :

$$\big\|\,|\,z_1\rangle\langle z_1\,| - |\,z_2\rangle\langle z_2\,|\,\big\|_p \quad = \quad 2^{\frac{1}{p}}\sqrt{1 - e^{-\frac{|z_1 - z_2|^2}{2\hbar}}} \underset{\hbar \text{ small}}{\sim} 2^{1/p}\ \delta^{\text{Kroneker}}_{z_1, z_2}$$

An exercise : how to metrize the space of quantum states

quantum information : how to distinguish two states ?

coherent states (Gabor) : for $z = (p, q) \in \mathbb{R}^{2d}$,

$$\psi_z(x) = (\pi\hbar)^{-d/4} e^{-\frac{(x-q)^2}{2\hbar}} e^{i\frac{p.x}{\hbar}}$$

Notations : $\psi_z \sim |\psi_z\rangle \sim |z\rangle, \; |\psi\rangle\langle\psi| = \mathbb{P}^{\perp}_{\psi}$

states in QM : (density matrix) $R > 0, \mathrm{Tr}\, R = 1$

e.g (pure) $R = |\psi\rangle\langle\psi|, \; \psi \in L^2(\mathbb{R}^d)$

QUESTION : "distance" between $|z_1\rangle\langle z_1|$ and $|z_2\rangle\langle z_2|$, for $z_1, z_2 \in \mathbb{R}^{2d}$?

In strong Schatten class $\|T\|_p^p = \mathrm{Tr}(T^*T)^{p/2}$ (e.g. Trace ($p = 1$), HS ($p = 2$)) :

$$\big\| |z_1\rangle\langle z_1| - |z_2\rangle\langle z_2| \big\|_p = 2^{\frac{1}{p}} \sqrt{1 - e^{-\frac{|z_1 - z_2|^2}{2\hbar}}} \underset{\hbar \text{ small}}{\sim} 2^{1/p} \, \delta^{\text{Kroneker}}_{z_1, z_2}$$

$$\underset{\hbar \to 0}{\longrightarrow} \text{ discrete (trivial) topology on phase space}$$

An exercise : how to metrize the space of quantum states

quantum information : how to distinguish two states ?

coherent states (Gabor) : for $z = (p, q) \in \mathbb{R}^{2d}$,

$$\psi_z(x) = (\pi\hbar)^{-d/4} e^{-\frac{(x-q)^2}{2\hbar}} e^{i\frac{p.x}{\hbar}}$$

Notations : $\psi_z \sim |\,\psi_z\rangle \sim |\,z\rangle, \ |\,\psi\rangle\langle\psi\,| = \mathbb{P}^{\perp}_{\psi}$

states in QM : (density matrix) $R > 0, \mathrm{Tr}\, R = 1$

e.g (pure) $R = |\,\psi\rangle\langle\psi\,|, \ \psi \in L^2(\mathbb{R}^d)$

QUESTION : “distance” between $|\,z_1\rangle\langle z_1\,|$ and $|\,z_2\rangle\langle z_2\,|$, for $z_1, z_2 \in \mathbb{R}^{2d}$?

In strong Schatten class $\|T\|_p^p = \mathrm{Tr}(T^*T)^{p/2}$ (e.g. Trace ($p = 1$), HS ($p = 2$)) :

$$\big\| |\,z_1\rangle\langle z_1\,| - |\,z_2\rangle\langle z_2\,| \big\|_p = 2^{\frac{1}{p}} \sqrt{1 - e^{-\frac{|z_1 - z_2|^2}{2\hbar}}} \underset{\hbar \text{ small}}{\sim} 2^{1/p} \, \delta^{\text{Kroneker}}_{z_1, z_2}$$

$\underset{\hbar \to 0}{\longrightarrow}$ discrete (trivial) topology on phase space

Quantum Wassertein :

$$\mathrm{MK}_\hbar(|\,z_1\rangle\langle z_1\,|, |\,z_2\rangle\langle z_2\,|)^2 = |z_1 - z_2|^2 + 2d\hbar$$

Wasserstein distances I.

Monge problem : $\min_{T:\mathbb{R}^n \to \mathcal{B}^n} \int C(x, T(x))\mu(dx), \quad \mu \in \mathcal{P}(\mathbb{R}^n)$ probablity, $\quad C(x, y) =$ cost

e.g. $C(x, T(x)) = |x - T(x)|^2$

Wasserstein distances I.

Monge problem : $\min_{T:\mathbb{R}^n \to \mathcal{B}^n} \int C(x, T(x))\mu(dx), \quad \mu \in \mathcal{P}(\mathbb{R}^n)$ probablity, $\quad C(x, y) =$ cost

e.g. $C(x, T(x)) = |x - T(x)|^2$
not well defined, leads to modern "optimal transport version"

Wasserstein distances I.

Monge problem : $\min_{T:\mathbb{R}^n \to \mathcal{B}^n} \int C(x, T(x))\mu(dx)$, $\mu \in \mathcal{P}(\mathbb{R}^n)$ probablity, $C(x,y) =$ cost

e.g. $C(x, T(x)) = |x - T(x)|^2$
not well defined, leads to modern "optimal transport version"

coupling : for $\mu, \nu \in \mathcal{P}(\mathbb{R}^n)$, $\pi \in \mathcal{P}(\mathbb{R}^{2n})$ such that

$$\int \pi(x,y)dy = \mu(x), \int \pi(x,y)dx = \nu(y)$$

Wasserstein distances I.

Monge problem : $\min_{T:\mathbb{R}^n \to \mathcal{B}^n} \int C(x, T(x))\mu(dx)$, $\mu \in \mathcal{P}(\mathbb{R}^n)$ probablity, $C(x, y) =$ cost

e.g. $C(x, T(x)) = |x - T(x)|^2$
not well defined, leads to modern "optimal transport version"

coupling : for $\mu, \nu \in \mathcal{P}(\mathbb{R}^n)$, $\pi \in \mathcal{P}(\mathbb{R}^{2n})$ such that

$$\int \pi(x, y) dy = \mu(x), \int \pi(x, y) dx = \nu(y)$$

Definition of Wasserstein metric of order 2

$$W_2^2(\mu, \nu) = \min_{\substack{\pi \text{ coupling} \\ \mu \text{ and } \nu}} \int (x - y)^2 \pi(dx, dy)$$

Wasserstein distances I.

Monge problem : $\min_{T:\mathbb{R}^n \to \mathcal{B}^n} \int C(x, T(x))\mu(dx)$, $\mu \in \mathcal{P}(\mathbb{R}^n)$ probablity, $C(x, y) =$ cost

e.g. $C(x, T(x)) = |x - T(x)|^2$
not well defined, leads to modern "optimal transport version"

coupling : for $\mu, \nu \in \mathcal{P}(\mathbb{R}^n)$, $\pi \in \mathcal{P}(\mathbb{R}^{2n})$ such that

$$\int \pi(x, y)dy = \mu(x), \int \pi(x, y)dx = \nu(y)$$

Definition of Wasserstein metric of order 2

$$W_2^2(\mu, \nu) = \min_{\substack{\pi \ \text{coupling} \\ \mu \ \text{and} \ \nu}} \int (x - y)^2 \pi(dx, dy)$$

It's a distance !

Wasserstein distances I.

Monge problem : $\min_{T:\mathbb{R}^n \to \mathcal{B}^n} \int C(x, T(x))\mu(dx)$, $\mu \in \mathcal{P}(\mathbb{R}^n)$ probablity, $C(x, y) =$ cost

e.g. $C(x, T(x)) = |x - T(x)|^2$
not well defined, leads to modern "optimal transport version"

coupling : for $\mu, \nu \in \mathcal{P}(\mathbb{R}^n)$, $\pi \in \mathcal{P}(\mathbb{R}^{2n})$ such that

$$\int \pi(x, y)dy = \mu(x), \int \pi(x, y)dx = \nu(y)$$

Definition of Wasserstein metric of order 2

$$W_2^2(\mu, \nu) = \min_{\substack{\pi \ \ coupling \\ \mu \ \ and \ \ \nu}} \int (x - y)^2 \pi(dx, dy)$$

It's a distance !

e.g. $W_2(\mu, \mu) = 0$ for optimal coupling $\pi_{opt} = \delta(x - y)\mu(x)$ (and not $\mu \otimes \mu$!)

Wasserstein distances I.

Monge problem : $\min_{T:\mathbb{R}^n\to\mathcal{B}^n} \int C(x, T(x))\mu(dx)$, $\mu \in \mathcal{P}(\mathbb{R}^n)$ probablity, $C(x,y) =$ cost

e.g. $C(x, T(x)) = |x - T(x)|^2$
not well defined, leads to modern "optimal transport version"

coupling : for $\mu, \nu \in \mathcal{P}(\mathbb{R}^n)$, $\pi \in \mathcal{P}(\mathbb{R}^{2n})$ such that

$$\int \pi(x,y)dy = \mu(x), \int \pi(x,y)dx = \nu(y)$$

Definition of Wasserstein metric of order 2

$$W_2^2(\mu,\nu) = \min_{\substack{\pi \ \mathit{coupling} \\ \mu \ \mathit{and} \ \nu}} \int (x-y)^2 \pi(dx,dy)$$

It's a distance !

e.g. $W_2(\mu,\mu) = 0$ for optimal coupling $\pi_{opt} = \delta(x-y)\mu(x)$ (and not $\mu \otimes \mu$!)
In fact Knott-Smith : $\exists T / \ \pi_{opt} = \delta(x - T(y))\mu(x)$ so that

$$W_2^2(\mu,\nu) = \int (x - T(x))^2 \mu(dx) \Leftrightarrow \text{ Monge problem.}$$

Wasserstein distances II. Brenier Theorem

more on the support of the optimal coupling (Knott-Smith)

Kantorovitch duality

$$W_2(\mu,\nu)^2 = \sup_{\substack{a,b/\ \forall x,y,\\ a(x)+b(y)\leq c(x,y)}} \int_{\mathbb{R}^n} a d\mu + \int_{\mathbb{R}^n} b d\nu.$$

if μ,ν don't charge sets of finite $(d-1)$-Hausdorff measure, $\sup = \max$:

$\exists\ a_{\text{opt}}, b_{\text{opt}}$.

Brenier Theorem : the support of $\pi_{\text{opt}}^{\mu,\nu}$ is contained in the graph of $\nabla \tilde{a}_{\text{opt}}$ where $\widetilde{a}_{\text{opt}}(x) := \frac{1}{2}x^2 - a_{\text{opt}}(x)$. In other words

$$(y - \nabla\widetilde{a}_{\text{opt}}(x))\pi_{\text{opt}}(x,y) = 0.$$

Classical to quantum : a (simple but efficient) dictionary

warning : QM lives on phase space (*habemus Alex*) so $n \to 2d$

QM in a nutshel

$$
\begin{array}{rcl}
\text{functions } a(z) \text{ on } \mathbb{R}^{2d} & \longrightarrow & \text{operators } A \text{ on } L^2(\mathbb{R}^d, dx) \\
\text{positive functions} & \longrightarrow & \text{positive operators} \\
z := (q,p) \in \mathbb{R}^{2d} & \longrightarrow & Z := (x, -i\hbar\nabla_x) \text{ on } L^2(\mathbb{R}^d, dx) \\
\int_{\mathbb{R}^{2d}} a(z)dz & \longrightarrow & \operatorname{tr} A \\
\int_{\mathbb{R}^{2d}} a(z)a'(x)dz & \longrightarrow & \operatorname{tr}(AA') \\
a(z_1) & \longrightarrow & A \otimes I \text{ on } L^2(\mathbb{R}^d) \otimes L^2(\mathbb{R}^d) \\
b(z_2) & \longrightarrow & I \otimes B \text{ on } L^2(\mathbb{R}^d) \otimes L^2(\mathbb{R}^d) \\
\int_{\mathbb{R}^{2d}} c(z_1,z_2)dz_2 & \longrightarrow & \operatorname{tr}_2(C) \text{ on } L^2(\mathbb{R}^d) \text{ defined by} \\
 & & \operatorname{Tr}_{L^2(\mathbb{R}^d)}(\operatorname{tr}_2(C)A) = \operatorname{tr}_{L^2(\mathbb{R}^d)\otimes L^2(\mathbb{R}^d)}((A \otimes I)),\ \forall A \\
 & . & \\
 & . & \\
 & . & \\
\{z, a\} & \longrightarrow & \frac{1}{i\hbar}[Z, A]
\end{array}
$$

Quantum Wasserstein

$$\begin{array}{rcl} \mu,\nu \in \mathcal{P}(\mathbb{R}^{2d}) & \longrightarrow & \text{density matrices } (R,S>0, \mathrm{tr}=1) \\ \pi & \longrightarrow & \Pi > 0.\, \mathrm{tr}\,\Pi = 1 \text{ on } L^2(\mathbb{R}^{2d}) \\ & & \text{coupling } R \text{ and } S \text{ i.e. } \mathrm{tr}_2\,\Pi = R, \mathrm{tr}_1\,\Pi = S \\ c=(z_1-z_2)^2 & \longrightarrow & C = (x_1-x_2)^2 + (-i\hbar\nabla_{x_1} - (-i\hbar\nabla_{x_2}))^2 \\ & & = -\hbar^2\Delta_{x_1-x_2} + (x_1-x_2)^2 \text{ (coupling harmonic oscillator)} \\ \int_{\mathbb{R}^{2d}\times\mathbb{R}^{2d}} c\pi & \longrightarrow & \mathrm{tr}\,(C\Pi) \end{array}$$

Quantum Wassertein between R, S density matrices

$$\mathrm{MK}_\hbar(R,S) = \inf_{\substack{\Pi \\ \text{coupling } R \text{ and } S}} \mathrm{tr}\,(C\Pi)$$

not a distance (e.g. $\geq 2d\hbar = \inf\, \mathit{spectrum}(C)$) but

- if one defines $\widetilde{W}[R](z) = \langle z\,|R|\,z\rangle, \widetilde{W}[S](z) = \langle z\,|R|\,z\rangle$, then

$$W_2(\widetilde{W}[R], \widetilde{W}[S])^2 - 2d\hbar \leq \mathrm{MK}_\hbar(R,S)^2$$

- if R, S are Töplitz, i.e. $R = \int_{\mathbb{R}^{2d}} \mu(z)|\,z\rangle\langle z\,|dz,\ S = \int_{\mathbb{R}^{2d}} \nu(z)|\,z\rangle\langle z\,|dz$, then

$$W_2(\widetilde{W}[R], \widetilde{W}[S])^2 - 2d\hbar \leq \mathrm{MK}_\hbar(R,S)^2 \leq W_2(\mu,\nu)^2 + 2d\hbar$$

Towards Quantum Transport

Motivation in quantum information

Question : what becomes Brenier theorem in quantum mechanics ?

$$\Updownarrow$$

How to "quantize" $(z_2 - \nabla\widetilde{a}_{\text{opt}}(z_1))\pi_{\text{opt}}(z_1, z_2) = 0.$?

Use again the dictionary :

- $\mu, \nu \to R, S$
- $\pi_{\text{opt}} \to \Pi_{\text{opt}}$
- $z_1, z_2 \to Z_1 = (x, -i\hbar\nabla_x) \otimes I, Z_2 = I \otimes (x, -i\hbar\nabla_x)$
- $\widetilde{a}_{\text{opt}} \to \widetilde{A}_{\text{opt}}$

But what becomes ∇a ? (no ∇ in the dictionary)

$\nabla a = \nabla_z a = \nabla_{\binom{q}{p}} a$ therefore $\nabla a = \{J\binom{q}{p}, a\}$, $J = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}$, *i.e.* $\nabla a = \binom{\{-p,a\}}{\{q,a\}}$.
which quantizes as

$$\nabla a \to \begin{pmatrix} \frac{1}{i\hbar}[i\hbar\nabla_x, A] \\ [x, A] \end{pmatrix} := \nabla^Q A$$

The only ambiguity which remains is the ordering :

$$(Z \otimes I - I \otimes \nabla^Q A)\Pi_{\text{opt}} \text{ or } \Pi_{\text{opt}}(Z \otimes I - I \otimes \nabla^Q A) ?$$

QM prefer symmetry : it will be

$$(\Pi_{\text{opt}})^{\frac{1}{2}}(Z \otimes I - I \otimes \nabla^Q \widetilde{A})(\Pi_{\text{opt}})^{\frac{1}{2}} = 0$$

$(\Pi_{\text{opt}})^{\frac{1}{2}}$ exists only in quantum mechanics.

Quantum Kantorowitch duality and quantum transport

Theorem (Caglioti, Golse, P.)

$$\mathrm{MK}_\hbar(R,S) = \sup_{\substack{A,B \text{ bounded on } L^2(\mathbb{R}^d) \\ A\otimes I + I\otimes B \le C}} \mathrm{tr}\,(AR + BS)$$

sup $\to$ max is painful $A_{\text{opt}}, B_{\text{opt}}$ act on a ... Gelfand triple.
For $\ker B = \{0\}$, $\mathcal{J}(B) := \{\psi,\ (\psi, B^{-1}\psi) < \infty\} \subset L^2(\mathbb{R}^d)$,

$$\mathcal{J}(B) \subset L^2(\mathbb{R}^d) \subset \mathcal{J}(B)' = \{\psi,\ (\psi, B\psi) < \infty\}.$$

Theorem (Caglioti, Golse, P.)

$$\mathrm{MK}_\hbar(R,S) = \max_{\substack{A\colon\ \mathcal{J}(R)\to\mathcal{J}(R)' \\ B\colon\ \mathcal{J}(S)\to\mathcal{J}(S)' \\ A\otimes I + I\otimes B \le C}} \mathrm{tr}\,(AR + BS)$$

Define the harmonic oscillator $H_0 = -\hbar^2\Delta + x^2$ on $L^2(\mathbb{R}^d)$ and

$$\widetilde{A} := H_0 - A_{opt}$$

Theorem (Caglioti, Golse, P.)
Let $\ker(R) = \ker(S) = \{0\}$ and $\operatorname{tr}(H_0^{1+\epsilon}R) < \infty,\ \operatorname{tr}(H_0^{1+\epsilon}S) < \infty$.
Then, for any optimal coupling Π of R and S

$$\Pi^{\frac{1}{2}}(Z \otimes I - I \otimes \nabla^Q \widetilde{A})\Pi^{\frac{1}{2}} = 0$$

In other words, let $\mathbb{P}$ be the projector on the image of the optimal coupling of R and S, define $Q' := \frac{1}{i\hbar}[-i\hbar\nabla, \widetilde{A}], P' = \frac{1}{i\hbar}[x, \widetilde{A}]$

$$\mathbb{P}\left(Q \otimes I - I \otimes Q'\right)\mathbb{P} = 0$$

$$\mathbb{P}\left(P \otimes I - I \otimes P'\right)\mathbb{P} = 0$$

Ehrenfest interpretation : $\operatorname{tr}(QR) = \operatorname{tr}(Q'S),\ \operatorname{tr}(PR) = \operatorname{tr}(P'S)$.

proof (hints)

$$\begin{aligned}
Z\otimes Z-\widetilde{A}\otimes I-I\otimes\widetilde{B} &\geq 0 \text{ and}\\
\mathrm{tr}\,(\Pi(Z\otimes Z-\widetilde{A}\otimes I-I\otimes\widetilde{B}) &= 0\Longrightarrow\\
\Pi^{\frac{1}{2}}(Z\otimes Z-\widetilde{A}\otimes I-I\otimes\widetilde{B})\Pi^{\frac{1}{2}} &= 0\Longrightarrow\\
\Pi^{\frac{1}{2}}(Z\otimes Z-\widetilde{A}\otimes I-I\otimes\widetilde{B})=(Z\otimes Z-\widetilde{A}\otimes I-I\otimes\widetilde{B})\Pi^{\frac{1}{2}} &= 0\Longrightarrow\\
\frac{1}{i\hbar}[Z\otimes Z-\widetilde{A}\otimes I-I\otimes\widetilde{B},P\otimes I]\Pi^{\frac{1}{2}}+(Z\otimes Z-\widetilde{A}\otimes I-I\otimes\widetilde{B})\frac{1}{i\hbar}[\Pi^{\frac{1}{2}},P\otimes I] &= 0\Longrightarrow\\
\Pi^{\frac{1}{2}}(I\otimes Q-\frac{1}{i\hbar}[\widetilde{A},P]\otimes I)\Pi^{\frac{1}{2}} &= 0
\end{aligned}$$

At classical level derivation $\frac{1}{i\hbar}[\cdot,P]\to\frac{\partial}{\partial x}$: no action on *measures*.

$$(xy-\tilde{a}(x)-\tilde{b}(y))\Pi(dx,dy)=0$$

but $(xy-\tilde{a}(x)-\tilde{b}(y))\geq 0$ so it cancels on sup(Π) at **second order** so

$$\frac{\partial}{\partial x}(xy-\tilde{a}(x)-\tilde{b}(y))\Pi(dx,dy)=(y-\nabla\tilde{a}(x))\Pi(dxdy)+0=0 \qquad \text{QED}$$

very simple (new) proof of Brenier Theorem.

Semiclassical approximation : old and news

Semiclassical situations are nowadays experimental.
Several strategies, several type of results :

- weak convergence of Wigner, no rate of convergence **but no ansatz on initial data** P.L. Lions, P., BV regularity Ambrosio, Figalli, et al (including P.) $\Rightarrow$ the diPerna-Lions flow is the limit of the classical one.
- strong approximation with precise remainders, **but strong ansatz on initial data** (WKB, coherent states, pseudodiff....) regularity consuming because of Calderon-Vaillancourt
- difficulty of estimating because schizophrenic comparisons between two different paradigms.

Semiquantum Wasserstein

- estimates directly the "distance" between classical and quantum solution
- Gronwald type startegy (instead of Cauche-Kovaleswka for microlocal analysis)
- Gronwald $\Rightarrow$ need to (semiclassical) estimates only initial data, and no)($\hbar^\infty$) term.

Gives also $\hbar$-independent estimates for numerical schemes.

Semiquantum Wasserstein

for R (quantum) density matrix and ν (classical) probability density, a coupling is

$$\mathbb{P}^{R,\nu} : (p,q) \mapsto \mathbb{P}^{R,\nu}(p,q) \in \mathcal{L}(L^2(\mathbb{R}^d)) \ a.e. \text{ such that}$$

- $\mathbb{P}^{R,\nu}(p,q) > 0$ a.e. and $\int_{\mathbb{R}^{2d}} \operatorname{tr} \mathbb{P}^{R,\nu}(p,q)dpdq = 1$
- $\int_{\mathbb{R}^{2d}} \mathbb{P}^{R,\nu}(p,q)dpdq = R$
- $\operatorname{tr} \mathbb{P}^{R,\nu}(p,q) = \nu(p,q)$

The semiquantum Wasserstien (Golse, P.) is

$$E_\hbar(R,\nu)^2 = \inf_{\substack{\mathcal{P}^{R,\nu} coupling \\ R \ and \ \nu}} \int_{\mathbb{R}^{2d}} \operatorname{tr}_{L^2(\mathbb{R}^d)} \Big((x_1-q)^2 + (-i\hbar\nabla_{x_1} - p)^2)\mathcal{P}^{R,\nu}(q,p)\Big) dpdq.$$

Same bounds than for $\mathrm{MK}_\hbar$: $W_2^2(\widetilde{W}[R],\nu) - \frac{1}{2}d\hbar \leq E_\hbar(R,\nu)^2$

and if R Töplitz $\quad W_2^2(\widetilde{W}[R],\nu) - \frac{1}{2}d\hbar \leq E_\hbar(R,\nu)^2 \leq W_2^2(\mu,\nu) + \frac{1}{2}d\hbar$

Triangular inequalities :

$$\begin{aligned} \mathsf{MK}_\hbar(R,S) &\leq E_\hbar(R,\rho)+E_\hbar(S,\rho) \\ E_\hbar(R,\nu) &\leq E_\hbar(R,\rho)+W_2(\rho,\nu) \end{aligned}$$

Semiclassical I. General propagation result à la Gronwall

Let $V \in C^{1,1}(\mathbb{R}^d)$ and let $S(t)$ and $\nu(t)$ solve respectively the

Semiclassical I. General propagation result à la Gronwall

Let $V \in C^{1,1}(\mathbb{R}^d)$ and let $S(t)$ and $\nu(t)$ solve respectively the

von Neumann equation, associated to Schrödinger $i\hbar\partial_t\psi = (-\hbar^2\Delta + V(x))\psi$

$$\partial_t S(t) = \frac{1}{i\hbar}[-\hbar^2\Delta + V(x), S(t)], \quad S(0) = S^{in}$$

Semiclassical I. General propagation result à la Gronwall

Let $V \in C^{1,1}(\mathbb{R}^d)$ and let $S(t)$ and $\nu(t)$ solve respectively the

von Neumann equation, associated to Schrödinger $i\hbar\partial_t\psi = (-\hbar^2\Delta + V(x))\psi$

$$\partial_t S(t) = \frac{1}{i\hbar}[-\hbar^2\Delta + V(x), S(t)], \quad S(0) = S^{in}$$

and Liouville equation, associated to $\Phi(t)$, flow of Hamiltonian $p^2 + V(q)$

$$\partial_t \nu(t) = \{p^2 + V(q), \nu(t)\}, \quad \nu(0) = \nu^{in}$$

Semiclassical I. General propagation result à la Gronwall

Let $V \in C^{1,1}(\mathbb{R}^d)$ and let $S(t)$ and $\nu(t)$ solve respectively the

von Neumann equation, associated to Schrödinger $i\hbar\partial_t\psi = (-\hbar^2\Delta + V(x))\psi$

$$\partial_t S(t) = \frac{1}{i\hbar}[-\hbar^2\Delta + V(x), S(t)], \quad S(0) = S^{in}$$

and Liouville equation, associated to $\Phi(t)$, flow of Hamiltonian $p^2 + V(q)$

$$\partial_t \nu(t) = \{p^2 + V(q), \nu(t)\}, \quad \nu(0) = \nu^{in}$$

Theorem (Golse, P.) *For all* $t \in \mathbb{R}$ *and* **any** S^{in}, ν^{in},

$$E_\hbar(S(t), \nu(t)) \leq e^{(1+Lip(\nabla V)^2)t} E_\hbar(S^{in}, \nu^{in}).$$

Semiclassical I. General propagation result à la Gronwall

Let $V \in C^{1,1}(\mathbb{R}^d)$ and let $S(t)$ and $\nu(t)$ solve respectively the

von Neumann equation, associated to Schrödinger $i\hbar\partial_t\psi = (-\hbar^2\Delta + V(x))\psi$

$$\partial_t S(t) = \frac{1}{i\hbar}[-\hbar^2\Delta + V(x), S(t)], \quad S(0) = S^{in}$$

and Liouville equation, associated to $\Phi(t)$, flow of Hamiltonian $p^2 + V(q)$

$$\partial_t \nu(t) = \{p^2 + V(q), \nu(t)\}, \quad \nu(0) = \nu^{in}$$

Theorem (Golse, P.) *For all $t \in \mathbb{R}$ and* **any** *S^{in}, ν^{in},*

$$E_\hbar(S(t), \nu(t)) \leq e^{(1+Lip(\nabla V)^2)t} E_\hbar(S^{in}, \nu^{in}).$$

Corollary *For all $t \in \mathbb{R}$ and* **any** *S^{in}*

$$W_2(\widetilde{W}[S(t)], \widetilde{W}[S^{in}]\#\Phi(t)) \leq e^{(1+Lip(\nabla V)^2)t} E_\hbar(S^{in}, \widetilde{W}[S^{in}]) + \frac{1}{2} d\hbar.$$

Semiclassical I. General propagation result à la Gronwall

Let $V \in C^{1,1}(\mathbb{R}^d)$ and let $S(t)$ and $\nu(t)$ solve respectively the

von Neumann equation, associated to Schrödinger $i\hbar\partial_t\psi = (-\hbar^2\Delta + V(x))\psi$

$$\partial_t S(t) = \frac{1}{i\hbar}[-\hbar^2\Delta + V(x), S(t)], \quad S(0) = S^{in}$$

and Liouville equation, associated to $\Phi(t)$, flow of Hamiltonian $p^2 + V(q)$

$$\partial_t \nu(t) = \{p^2 + V(q), \nu(t)\}, \quad \nu(0) = \nu^{in}$$

Theorem (Golse, P.) *For all* $t \in \mathbb{R}$ *and* **any** S^{in}, ν^{in},

$$E_\hbar(S(t), \nu(t)) \leq e^{(1+Lip(\nabla V)^2)t} E_\hbar(S^{in}, \nu^{in}).$$

Corollary *For all* $t \in \mathbb{R}$ *and* **any** S^{in}

$$W_2(\widetilde{W}[S(t)], \widetilde{W}[S^{in}]\#\Phi(t)) \leq e^{(1+Lip(\nabla V)^2)t} E_\hbar(S^{in}, \widetilde{W}[S^{in}]) + \frac{1}{2}d\hbar.$$

Estimate $E_\hbar(S^{in}, \widetilde{W}[S^{in}])$.

Semiclassical I. General propagation result à la Gronwall

Let $V \in C^{1,1}(\mathbb{R}^d)$ and let $S(t)$ and $\nu(t)$ solve respectively the

von Neumann equation, associated to Schrödinger $i\hbar\partial_t\psi = (-\hbar^2\Delta + V(x))\psi$

$$\partial_t S(t) = \frac{1}{i\hbar}[-\hbar^2\Delta + V(x), S(t)], \quad S(0) = S^{in}$$

and Liouville equation, associated to $\Phi(t)$, flow of Hamiltonian $p^2 + V(q)$

$$\partial_t \nu(t) = \{p^2 + V(q), \nu(t)\}, \quad \nu(0) = \nu^{in}$$

Theorem (Golse, P.) *For all $t \in \mathbb{R}$ and* **any** S^{in}, ν^{in},

$$E_\hbar(S(t), \nu(t)) \leq e^{(1+Lip(\nabla V)^2)t} E_\hbar(S^{in}, \nu^{in}).$$

Corollary *For all $t \in \mathbb{R}$ and* **any** S^{in}

$$W_2(\widetilde{W}[S(t)], \widetilde{W}[S^{in}]\#\Phi(t)) \leq e^{(1+Lip(\nabla V)^2)t} E_\hbar(S^{in}, \widetilde{W}[S^{in}]) + \frac{1}{2}d\hbar.$$

Estimate $E_\hbar(S^{in}, \widetilde{W}[S^{in}])$.

Example : S^{in} **any** Töplitz $\Rightarrow E_\hbar(S^{in}, \widetilde{W}[S^{in}]) = \frac{1}{2}d\hbar$ **(no regularity)**.

Semiclassical II. Time Splitting uniform in $\hbar$

Problem : mesh Δt gives a priori error of size $\frac{\Delta t}{\hbar}$, when estimated in Schatten classes (or Sobolev).

How to get uniform in $\hbar$ error terms ?

Time splitting for von Neumann :

$$\begin{cases} S^0 = S^{in}, \\ \partial_t A(t) = \frac{1}{i\hbar}[-\hbar^2\Delta, A(t)], \quad A(0) = S^n, & n \in \mathbb{N} \\ \partial_t B(t) = \frac{1}{i\hbar}[V(x), B(t)], \quad B(0) = A(\Delta t), \\ S^{n+1} = B(\Delta t) \end{cases}$$

Theorem (Golse, Shi Jin, P.)For $\Delta t < \frac{1}{2}$ and any $n \in \mathbb{N}$,

$$W_2(\widetilde{W}[S^n], \widetilde{W}[S(n\Delta t)) \leq C\Delta t + \sqrt{\hbar}e^{Dn\Delta t}$$

Corollary Let $W_1(\mu,\nu) := \min_{\substack{\pi \ coupling \\ \mu \ and \ \nu}} \int \min(1, |x-y|)\pi(dx, dy)$. Then

$$W_1(\widetilde{W}[S^n], \widetilde{W}[S(n\Delta t)) \leq Ce^{Dn\Delta t}\Delta t^{\frac{1}{3}}, \quad C, D \text{ independent of } \hbar.$$

Semiclassical III. Semiclassical with low regularity

Question : how to get quantitative semiclassical approximation without specific ansatz on initial data ?

Answer :low regularity conditions on $W[S^{in}]$.

References

- F. Golse, C. Mouhot, T. P. : *On the Mean Field and Classical Limits of Quantum Mechanics*, Commun. Math. Phys. **343** (2016), 165–205.
- F. Golse, T. P : *The Schrödinger Equation in the Mean-Field and Semiclassical Regime*, Arch. Rational Mech. Anal. **223** (2017), 57–94.
- F. Golse, T. P. : *Wave Packets and the Quadratic Monge-Kantorovich Distance in Quantum Mechanics*, Comptes Rendus Mathematique **356** 177 - 197 (2018) .
- E. Caglioti, F. Golse, T. P. : *Towrads quantum transport*, preprint
- F. Golse, S. Jin, T. P. : *On the convergence of time splitting methods for the Schrödinger equation in the semiclassical regime*, preprint
- F. Golse, T. P. : *Low regularity semiclassical evolution*, in preparation

downloadable on `http://www.cmls.polytechnique.fr/perso/paul/`