Quantique-classique
un dictionnaire et quelques applications

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Quantum computing

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

$2^{100} >$ Avogadro

Quantum Information

transport qubits

discriminate states

(Gedenken) Experiments

rubidium $\sim$ small bacteria

time $\sim$ 2 seconds

$\Downarrow$

macro/micro $\neq$ classical/quantum

Three motivations

towards quantum optimal transport

numerical schemes uniform at the transition quantum-classical

filling the gap in regularity between quantum and classical

Three ideas

CM $\rightsquigarrow$ QM through a dictionary

strong $\rightsquigarrow$ weak topologies

Cauchy-Kowalevski $\rightsquigarrow$ Gronwall

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 :

structure of optimal couplings

Semiclassical approximation with low regularity :

direct "distance" between quantum and classical objects

Gronwall instead of Calderon-Vaillancourt

Time splitting algorithm uniform in $\hbar$:

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

Quantum Empirical Measures :

mean-field approximation uniform in $\hbar$

An exercise : how to metrize the space of quantum states

quantum information : how to distinguish two states ?

$$\psi_q(x) = (\pi\varepsilon)^{-d/4} e^{-\frac{(x-q)^2}{2\varepsilon}}$$

QUESTION : which "distance" between ψ_{q_1} and ψ_{q_2} ?

$$\left\|\frac{\psi_{q_1}-\psi_{q_2}}{\sqrt{2}}\right\|_{L^2(\mathbb{R}^d)} = \sqrt{1-e^{-\frac{|q_1-q_2|^2}{2\varepsilon}}} \underset{\varepsilon \text{ small}}{\sim} (1-\delta^{\text{Kroneker}}_{q_1,q_2})$$

$$\underset{\varepsilon\to 0}{\to} \quad \text{discrete (trivial) topology on space}$$

$$\left\|\frac{\psi_{q_1}-\psi_{q_2}}{\sqrt{2}}\right\|_{L^2(\mathbb{R}^d)} = \||\psi_{q_1}\rangle\langle\psi_{q_1}| - |\psi_{q_2}\rangle\langle\psi_{q_2}|\|_{HS}, \quad \boxed{|\psi\rangle\langle\psi|\phi = (\psi,\phi)\psi}$$

states in QM : (density matrix) $R>0, \operatorname{Tr} R = 1$, e.g (pure) $R = |\psi\rangle\langle\psi|$

Quantum Wassertein : $\text{MK}(|\psi_{q_1}\rangle\langle\psi_{q_1}|, |\psi_{q_2}\rangle\langle\psi_{q_2}|) = |q_1-q_2|$

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 $\to$ modern "optimal transport version"

$\pi \in \mathcal{P}(\mathbb{R}^{2n})$ coupling of $\mu, \nu \in \mathcal{P}(\mathbb{R}^n)$: $\int \pi(x,y)dy = \mu(x), \int \pi(x,y)dx = \nu(y)$

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

It's a distance !

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

more on the support of the optimal coupling (Knott-Smith : $\pi_{optimal} = \delta(x - T(y))\mu(x)$)

Wasserstein distances II. Brenier Theorem

Kantorovitch duality

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

μ,ν don't charge finite $(d-1)$-Hausdorff measure sets : $\sup = \max$, $\exists\ a_{\text{opt}}, b_{\text{opt}}$.

$$W_2(\mu,\nu)^2 = \int c\pi_{\text{opt}} = \int a_{\text{opt}} d\mu + \int b_{\text{opt}} d\nu = W_2(\mu,\nu)^2 \Rightarrow$$

$$\begin{aligned} (c(x,y) - a_{\text{opt}}(x) - b_{\text{opt}}(y)) &\geq 0 \\ \pi_{\text{opt}}(dx,dy)(c(x,y) - a_{\text{opt}}(x) - b_{\text{opt}}(y)) &= 0 \end{aligned}$$

Brenier Theorem : the support of π_{opt} is contained in the graph $y = x - \nabla a_{\text{opt}}$:

$$(y - \nabla\widetilde{a}_{\text{opt}}(x))\pi_{\text{opt}}(x,y) = 0, \qquad \widetilde{a}_{\text{opt}}(x) := \frac{1}{2}x^2 - a_{\text{opt}}(x)$$

Classical to quantum : a (simple but efficient) dictionary

warning : QM lives on an underlying phase space so $n \to 2d$

QM in a nutshel

$$
\begin{array}{rcl}
\text{functions } a(z) \text{ on } \mathbb{R}^{2d} & \longrightarrow & \text{operators } A \text{ on } L^2(\mathbb{R}^d, dx) \\
\text{positive functions} & \longrightarrow & \text{positive operators} \\
z := (q,p) \in \mathbb{R}^{2d} & \longrightarrow & Z := (x, -i\hbar\nabla_x) \text{ on } L^2(\mathbb{R}^d, dx) \\
\int_{\mathbb{R}^{2d}} a(z)dz & \longrightarrow & \operatorname{tr} A \\
\int_{\mathbb{R}^{2d}} c(z_1,z_2)dz_2 & \longrightarrow & \operatorname{tr}_2(C) \text{ on } L^2(\mathbb{R}^d) \\
\int_{\mathbb{R}^{2d}} a_1(z)a_2(z)dz & \longrightarrow & \operatorname{tr}(A_1A_2) \\
a(z_1) & \longrightarrow & A \otimes I \text{ on } L^2(\mathbb{R}^d) \otimes L^2(\mathbb{R}^d) \\
b(z_2) & \longrightarrow & I \otimes B \text{ on } L^2(\mathbb{R}^d) \otimes L^2(\mathbb{R}^d) \\
 & . & \\
\{z, a\} & \longrightarrow & \frac{1}{i\hbar}[Z, A]
\end{array}
$$

Quantum Wasserstein

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

Quantum Wassertein between R, S density matrices

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

$$\mathrm{MK}_\hbar(R,S) = \inf_{\substack{\Pi \\ \text{coupling} \\ R \text{ and } S}} \operatorname{tr}\left((x_1-x_2)^2 - \hbar^2(\nabla_{x_1}-\nabla_{x_2})^2\right)\Pi$$

It is not a distance ! (e.g. $\mathrm{MK}_\hbar(R,R)$ is not $=0$ for all R) but

it (almost) dominates weak topologies

Definition : $d_M(R,S) := \sup_{\substack{\|\mathcal{D}_x^\alpha \mathcal{D}_{\hbar\nabla}^\beta F\|_{TR}\leq 1 \\ |\alpha|,|\beta|\leq M}} |\operatorname{tr}(F(R-S))|, \quad M\in\mathbb{N}$

$(\mathcal{D}_x = \frac{1}{i\hbar}[x,\cdot],\ \mathcal{D}_{\hbar\nabla} = \frac{1}{i\hbar}[\hbar\nabla,\cdot])$

it is a distance !

$$\sim d_M^{classical}(\mu,\nu) := \sup_{\substack{\|\partial_x^\alpha \partial_\xi^\beta f\|_{L^\infty}\leq 1 \\ |\alpha|,|\beta|\leq M}} \left|\int(\mu-\nu)f(x,\xi)dxd\xi\right|$$

$$d_{[d/2]+2}(R,S) \leq \mathrm{MK}_\hbar(R,S) + D_d\sqrt{\hbar}$$

$$d_1(R,S) \leq \mathrm{MK}_\hbar(R,S) + D'_d\sqrt{\hbar}\left(1+\frac{\|R\|_{HS}+\|S\|_{HS}}{(2\pi\hbar)^d}\right)$$

Towards Quantum Transport (through Brenier Theorem)

How to "quantize" $(z_2 - \nabla\widetilde{a}_{\mathrm{opt}}(z_1))\pi_{\mathrm{opt}}(z_1, z_2) = 0$? $\quad (z = (q, p))$

Use again the dictionary :

- $\mu, \nu \to R, S$, $\pi_{\mathrm{opt}} \to \Pi_{\mathrm{opt}}$, $z_1 \to Z_1 = (x, -i\hbar\nabla_x) \otimes I$ (same for z_2), $\widetilde{a}_{\mathrm{opt}} \to \widetilde{A}_{\mathrm{opt}}$
- but what becomes ∇a ? (no ∇ in the dictionary)

$$\nabla a := \begin{pmatrix} \nabla_q a \\ \nabla_p a \end{pmatrix} = \begin{pmatrix} \{-p, a\} \\ \{q, a\} \end{pmatrix} \qquad \{f, g\} := \partial_q f \partial_p g - \partial_p f \partial_q g$$

$$\nabla a := \begin{pmatrix} \{-p, a\} \\ \{q, a\} \end{pmatrix} \xrightarrow{\textit{dictionary}} \nabla^{\mathrm{Q}} A := \begin{pmatrix} \frac{1}{i\hbar}[i\hbar\nabla_x, A] \\ \frac{1}{i\hbar}[x, A] \end{pmatrix}$$

- only ambiguity, ordering : $(Z \otimes I - I \otimes \nabla^{\mathrm{Q}} A)\Pi_{\mathrm{opt}}$, $\Pi_{\mathrm{opt}}(Z \otimes I - I \otimes \nabla^{\mathrm{Q}} A)$?

QM prefers symmetry : $\Pi_{\mathrm{opt}}^{\frac{1}{2}}(Z \otimes I - I \otimes \nabla^{\mathrm{Q}}\widetilde{A})\Pi_{\mathrm{opt}}^{\frac{1}{2}} = 0 \qquad \Pi_{\mathrm{opt}}^{\frac{1}{2}}\exists$ in QM

Quantum Kantorowitch duality and quantum transport

Theorem (Caglioti, Golse, P.)

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

sup $\to$ max is painful $A_{\mathrm{opt}}, B_{\mathrm{opt}}$ are defined 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.)

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

$$\boxed{\exists A_{opt},\ B_{opt}}$$

Define $\widetilde{A} := \frac{1}{2} H_0 - A_{\text{opt}}, \quad H_0 = -\hbar^2 \Delta + x^2$ on $L^2(\mathbb{R}^d)$

Theorem (Caglioti, Golse, P.)

$\ker(R) = \ker(S) = \{0\}$, $\mathrm{tr}(H_0^{1+\epsilon}(R+S)) < \infty$, A_{opt} **bounded** on $L^2(\mathbb{R}^d) \Longrightarrow$

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

i.e., let $\mathbb{P}$ projector on the image of Π_{opt}, $Q' := \frac{1}{i\hbar}[-i\hbar\nabla, \widetilde{A}]$ and $P' = \frac{1}{i\hbar}[x, \widetilde{A}]$, then

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

$$\text{“on” the image of } \Pi_{opt},\ \binom{Q}{P} \mapsto \nabla^Q \widetilde{A}$$

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

An $\mathbb{SNCF}$ type alternative view oui !

Analogy with geodesics : instead of fixing the two points R, S

look at optimal coupling Π

Instead of R, S, take for granted $A = A^*, B = B^*$ bounded with

$$C - A \otimes I - I \otimes B \geq 0 \text{ on } Dom(C)$$

Then any trace 1 positive $\Pi \in \mathcal{L}(\ker(C - A \otimes I - I \otimes B))$
is an optimal coupling of its marginals

$$R := \operatorname{Tr}_2 \Pi \text{ and } S := \operatorname{Tr}_1 \Pi.$$

hints of the proof

$$\begin{array}{lrcl}
(\textit{constraints}) & A\otimes I + B\otimes I & \leq & C \\
 & & \Updownarrow & \\
 & C - A\otimes I - I\otimes B & \geq & 0 \\
(\textit{optimality}) & \text{with} \quad \mathrm{tr}\,(\Pi(C - A\otimes I - I\otimes B)) & = & 0 \\
(\textit{positivity}) & & \Downarrow & \\
 & \Pi^{\frac{1}{2}}(C - A\otimes I - I\otimes B)\Pi^{\frac{1}{2}} & = & 0 \\
(\textit{positivity}) & & \Downarrow & \\
 & \Pi^{\frac{1}{2}}(C - A\otimes I - I\otimes B) = (C - A\otimes I - I\otimes B)\Pi^{\frac{1}{2}} & = & 0 \\
(\textit{action of the derivation } \frac{1}{i\hbar}[\cdot, P\otimes I]) & & \Downarrow & \\
 & \frac{1}{i\hbar}[C - A\otimes I - I\otimes B, P\otimes I]\Pi^{\frac{1}{2}} + (C - A\otimes I - I\otimes B)\frac{1}{i\hbar}[\Pi^{\frac{1}{2}}, P\otimes I] & = & 0 \\
(\textit{left multiplication by } \Pi^{\frac{1}{2}}) & ([C, P\otimes I] = I\otimes Q + [H_o, P]\otimes I) & \Downarrow & \\
 & \Pi^{\frac{1}{2}}(I\otimes Q - \frac{1}{i\hbar}[\widetilde{A}, P]\otimes I)\Pi^{\frac{1}{2}} & = & 0
\end{array}$$

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

$$(\tfrac{1}{2}(x-y)^2 - a(x) - b(y))\Pi(dx, dy) = 0$$

but $\frac{1}{2}(x-y)^2 - a(x) - b(y) \geq 0$ so it cancels on $\sup(\Pi)$ at **second order** so

$$\frac{\partial}{\partial x}\left((\tfrac{1}{2}(x-y)^2 - a(x) - b(y))\Pi(dx, dy)\right) =$$

$$(y - \nabla\tilde{a}(x))\Pi(dxdy) + (\tfrac{1}{2}(x-y)^2 - a(x) - b(y))\partial_x\Pi(dx, dy) =$$

$$(y - \nabla\tilde{a}(x))\Pi(dxdy) + 0 = 0 \qquad \text{QED}$$

very simple (new) “moral” proof of Brenier Theorem.

more by iterating derivations at quantum level

Quantum optimal transport is cheaper

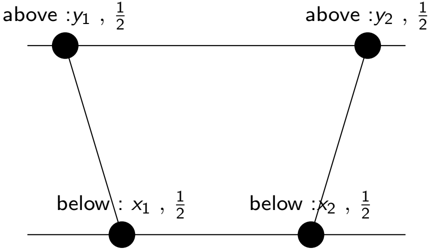

FIGURE: equal masses

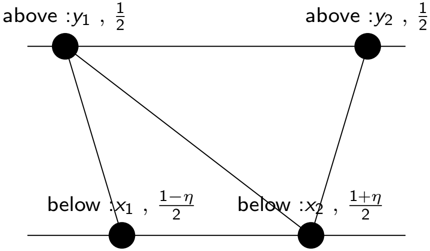

FIGURE: different masses

C : $$W_2(\tfrac{1-\eta}{2}\delta_{x_1} + \tfrac{1+\eta}{2}\delta_{x_2}, \tfrac{1}{2}\delta_{y_1} + \tfrac{1}{2}\delta_{y_2}) = C_{classical}$$

Q : $$\mathrm{MK}_\hbar(\tfrac{1-\eta}{2}|\,\psi_{x_1}\rangle\langle\psi_{x_1}\,| + \tfrac{1+\eta}{2}|\,\psi_{x_2}\rangle\langle\psi_{x_2}\,|, \tfrac{1}{2}|\,\psi_{y_1}\rangle\langle\psi_{y_1}\,| + \tfrac{1}{2}|\,\psi_{y_2}\rangle\langle\psi_{y_2}\,|) = C_{quantum}$$

$\eta = 0$ (equal masses) $$C_{quantum} = C_{classical}$$

$\eta > 0$ (non equal masses) $$C_{quantum} < C_{classical}$$

due to quantum terms without classical counterparts

Inverse dictionary : Wigner

For D density matrix : $D \geq 0,\ \operatorname{tr} D = 1$:

$$\text{Wigner : } W_\hbar[D](q,p) := \int D(q+\hbar\tfrac{\eta}{2}, q-\hbar\tfrac{\eta}{2}) e^{ip\eta} d\eta \quad (D(x,y) \text{ int. ker. of } D)$$

$$\text{inverted by : } D(x,y) = \int W_\hbar[D](\tfrac{x+y}{2}, p) e^{i\frac{p(x-y)}{\hbar}} \frac{dp}{(2\pi\hbar)^d}$$

$W_\hbar[D]$ is not positive *but* $e^{\frac{\hbar}{4}\Delta} W_\hbar[D] \geq 0$

$$\Rightarrow \lim_{\hbar\to 0} W_\hbar[D] \geq 0 \text{ (as measure)}$$

$$\boxed{\underset{\hbar=0}{\text{classical}} \overset{Wigner}{\leftrightarrow} \underset{\hbar>0}{\text{quantum}}}$$

$$\dot{R} = \frac{1}{i\hbar}[H, R]$$

$$\boxed{R^{in}} \quad \underset{evolution}{\overset{quantum}{\longrightarrow}} \quad \boxed{R(t)}$$

Wigner $\updownarrow$ $\qquad\qquad$ $\updownarrow$ *Wigner* ?

$$\dot{W} = \{h, W\}$$

$$\boxed{W[R^{in}]} \quad \underset{evolution}{\overset{classical}{\longrightarrow}} \quad \boxed{W[R^{in}] \circ \Phi(t) \sim W[R(t)]?}$$

Semiclassical approximation : old and new *(fluctuat nec mergitur)*

Several strategies, several type of results :

- weak convergence of dynamics, no rate of convergence **no ansatz on initial data**
  $\Rightarrow$ the diPerna-Lions flow is the classical limit of the quantum one
- strong approximation with precise remainders, **but strong ansatz on initial data**
  $\Rightarrow$ regularity consuming because of Calderon-Vaillancourt
- schizophrenia of estimating : comparisons between two different paradigms

Semiquantum Wasserstein

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

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

Semiquantum Wasserstein (apply dictionary only on second half of the objects)

- μ (classical) probability density and S (quantum) density matrix
- coupling of μ and S : $\mathbb{P}(p,q) \in \mathcal{L}(L^2(\mathbb{R}^d))$ *for a.e.* $(p,q) \in \mathbb{R}^{2d}$
  - $\mathbb{P}(p,q) > 0$ a.e. and $\int_{\mathbb{R}^{2d}} \operatorname{tr} \mathbb{P}(p,q) dpdq = 1$
  - $\operatorname{tr} \mathbb{P}(p,q) = \mu(p,q)$, $\int_{\mathbb{R}^{2d}} \mathbb{P}(p,q) dpdq = S$
- cost $C(q,p) = (q-y)^2 + (p - (-i\hbar\nabla_y))^2 - d\hbar$ acting on $L^2(\mathbb{R}^d, dy)$

The semiquantum Wasserstien (Golse, P.) is

$$E_\hbar^2(\mu, S) = \inf_{\substack{P(p,q) \\ coupling \\ R\ \ and\ \ \nu}} \int_{\mathbb{R}^{2d}} \operatorname{tr}_{L^2(\mathbb{R}^d)} \left(C(q,p) \mathbb{P}(q,p) \right) dpdq.$$

Same bounds than for $\mathrm{MK}_\hbar$

$$
\begin{aligned}
d_{[d/2]+2}(R,S) &\leq E_\hbar(\mu,S) + D_d\sqrt{\hbar} \qquad\qquad W[R] := \mu \\
d_1(R,S) &\leq E_\hbar(\mu,S) + D'_d\sqrt{\hbar}\big(1 + \tfrac{\|R\|_{HS}+\|S\|_{HS}}{(2\pi\hbar)^d}\big)
\end{aligned}
$$

Triangular inequalities for the triplet $(W_2, E_\hbar, \mathrm{MK}_\hbar)$

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

Semiclassical I. General propagation result à la Gronwall

Let $V \in C^{1,1}(\mathbb{R}^d)$ and let $S(t)$ and $\mu(t)$ 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 $p^2 + V(q)$

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

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

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

Key idea of the proof :

1. Π^{in} coupling μ^{in} and $S^{in} \rightsquigarrow \Pi(t)$ coupling $\mu(t)$ and $S(t)$

   $\partial_t \Pi = \frac{1}{i\hbar}[-\hbar^2\Delta, \Pi] + \{p^2 + V(q), \Pi\}$

2. $|\partial_t \int \mathrm{tr}\, C\Pi(t)| \leq \int \mathrm{tr}\, C\pi(t) \Rightarrow \int \mathrm{tr}\, C\Pi(t) \leq e^{\lambda t} \int \mathrm{tr}\, C\Pi(0)$ (Gronwall)
3. choose Π optimal coupling of μ^{in} and S^{in}.

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$\rightsquigarrow$ Estimate $E_\hbar(\mu^{in}, S^{in})$

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$\rightsquigarrow$ Estimate $E_\hbar(?, S^{in})$

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$\rightsquigarrow$ Estimate $E_\hbar(e^{\hbar\Delta/4}W[R^{in}], S^{in})$

Question : get quantitative semiclassical approximation without specific ansatz ?

$H_j(x) := \hbar^{-\frac{d}{4}} h_j(\frac{x}{\sqrt{\hbar}}) e^{-\frac{x^2}{2\hbar}}$, h_j Hermite polynomials on $\mathbb{R}^d$, $j \in \mathbb{N}^d$.

Semiclassical II. Semiclassical with low regularity

let $0 < S^{in} = (\sqrt{S^{in}})^2$ satisfies the checkable conditions

$$
\begin{aligned}
|\langle H_{j'}\,|\sqrt{S^{in}}|\,H_j\rangle| &\leq C\hbar(1+\hbar|j|)^{-\frac{3}{2}-\epsilon}(1+|j'-j|)^{-1-\epsilon}\\
|\langle H_{j'}\,|[\Omega,\sqrt{S^{in}}]|\,H_j\rangle| &\leq \tau(\hbar)\hbar(1+\hbar|j|)^{-\frac{3}{2}-\epsilon}(1+|j'-j|)^{-1-\epsilon},\\
\Omega = \hbar^2\Delta,\ x^2,\ \hbar\nabla, x \quad &, \qquad \tau(\hbar) = o(1) \text{ as } \hbar \to 0.
\end{aligned}
$$

Theorem (Golse, P.) $\lambda = Lip(\nabla V)$,

$$
\sup_{\substack{Lip(f)\leq 1\\ \|\nabla f\|_{L^2}\leq 1}} \int (\underbrace{W[S(t)]}_{\substack{von\\ Neu\\ mann}} - \underbrace{W[S^{in}]\circ\Phi(t)}_{Liouville}) f(x,\xi)\,dx d\xi \leq Ce^{\lambda t}\max(\sqrt{\hbar}, \sqrt{\tau(\hbar)}).
$$

Corollary I Same conclusion when $W[S^{in}]$ has low regularity ($\sim C^5$).

Corollary II $S^{in} = (S_1^{in})^{\otimes N}$, regularity on S_1^{in} alone, independently of N

Corollary III no regularity needed for $(S_1^{in})^{(k)}$ polar Fourier, for $|k|$ large

Operator form : $W[\mathcal{S}(t) := W[S^{in}] \circ \Phi(t)$.

$$\sup_{\substack{\|\frac{1}{i\hbar}[x,F]\|_{TR},\|\frac{1}{i\hbar}[-i\hbar\nabla,F]\|_{TR}\leq 1\\ \|F\|_{HS}\leq 1\\ \|\frac{1}{i\hbar}[x,F]\|_{HS},\|\frac{1}{i\hbar}[-i\hbar\nabla,F]\|_{HS}\leq 1}} |\operatorname{tr}(F(S(t)-\mathcal{S}(t)))| \leq Ce^{\lambda t}\max(\sqrt{\hbar},\sqrt{\tau(\hbar)}).$$

Semiclassical III. Time Splitting uniform in $\hbar$

$$\text{Trotter formula } e^{M_1+M_2} = \text{“}\lim_{n\to\infty}\text{”}\left(e^{\frac{M_1}{n}}e^{\frac{M_2}{n}}\right)^n$$

$$\text{Time splitting } (\Delta t = \tfrac{t}{n}) \text{ for } i\hbar\partial_t S = [-\hbar^2\Delta + V(x), S]$$

$$\begin{cases} \partial_s A_n(s) = \frac{1}{i\hbar}[-\hbar^2\Delta, A_n(s)], & 0\le s\le \Delta t, \quad A_n(0) = S^n \qquad S^0 = S^{in}, \\ \partial_s B_n(s) = \frac{1}{i\hbar}[V(x), B_n(s)], & 0\le s\le \Delta t, \quad B_n(0) = A_n(\Delta t), \quad S^n = B_n(\Delta t) \end{cases}$$

Problem : mesh Δt gives error $\sim \frac{\Delta t}{\hbar}$ in Sobolev, Schatten top. : prob. when $\hbar << \Delta t$

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

Theorem (Golse, Shi Jin, P.) Let $\hbar \le \Delta t$, then $\exists C, D$ independent of $\hbar$ s. t.

$$d_{[d/2]+2}(S^{n+1}, S(n\Delta t)) \le C\Delta t e^{Dn\Delta t}$$

Corollary By optimization, $\forall\hbar, \forall\Delta t$,

$$d_{[d/2]+2}(S^{n+1}, S(n\Delta t)) \le Ce^{Dn\Delta t}\Delta t^{\frac{1}{3}} \qquad (\Delta t^{\frac{2}{3}} \text{ by Strang}).$$

Quantum Empirical Measures

What is a classical EM ?

$$\mu_{Z_N}(z) = \frac{1}{N}\sum_{k=1}^{N}\delta(z - z_k)$$

I. as a "function" of $z = (q,p)$ parametrized by $Z_N := (z_1, \ldots, z_N)$

Φ_t flow of Hamiltonian $H_N = \sum_{i=1\ldots N} p_i^2 + \frac{1}{N}\sum_{i<j=1\ldots N} V(q_i - q_j)$

$\mu^t_{Z_N} := \mu_{\Phi_t(Z_n)}(z)$ solves Vlasov = one-particle Liouville where $V \to V * \mu$

$$\partial_t \mu^t_{Z_N}(q,p) = (2p.\nabla_q - \nabla_q V * \mu^t_{Z_N}.\nabla_p)\mu^t_{Z_N}(q,p),$$

$\rightsquigarrow$ Mean field limit : $\partial_t \rho_N(Z_N) = \{H_N, \rho_N\},\ \rho_N(t=0) = (\rho^{in})^{\otimes N} \Rightarrow$

$\lim_{N\to\infty}(\rho_{N;1}(z) := \int \rho(z, z_2, \ldots, z_N) dz_2 \ldots dz_N)$ solves Vlasov, $\rho_{N;1}(t=0) = \rho^{in}$

II. as a "function" $\mu(z; z_1, \ldots, z_N)$

the integral kernel of the operator

$$\rho(z_1, \ldots, z_N) \longrightarrow \rho_{N;1}(z) = \int \mu(z; z_1, \ldots, z_N)\rho(z_1, \ldots, z_N) dz_1 \ldots dz_N$$

Quantize ?

N particle density $\longrightarrow$ its first marginal.

apply $\downarrow$ dictionary

N part. dens. mat. D_N $\longrightarrow$ its first marginal $D_{N;1:} = \mathrm{Tr}_{\mathcal{H}^{N-1}} D$

$$W[D](z_1,\dots,z_N) \longrightarrow W[D_{N;1}](z) = W[D]_{N;1}(z) = \int \mu(z;z_1,\dots,z_N) W[D](z_1,\dots,z_N) dZ_N$$

the empirical measure μ is the integral kernel

of the same operator in classical and quantum mechanics

$$[\text{quantization}, \text{empirism}] = 0$$

$$\mathcal{M}^*(D_N) := D_{N;1}$$

propagation : $\mathcal{M}^*(t)(D_N) := \mathcal{M}^*(D_N(t))$

where $D_N(t)$ solves N body quantum evolution

$$i\hbar\partial_t D_N(t) = [-\hbar^2\Delta_N + \frac{1}{N}\sum_{i<j} V(x_i - x_j), D_N(t)]$$

equation for $\mathcal{M}(t)$ "contains" 1-particle non-linear Hartree

$$i\hbar\partial_t D = [-\hbar^2\Delta + V_D, D],\ \ V_D = V * D(x,x)$$

like EM solves Vlasov

Hartree = application of dictionary to Vlasov

Mean-field uniform in $\hbar$

Schrödinger	$\xrightarrow{N\to\infty}$	**Hartree**
$\hbar \to 0 \downarrow$	$\searrow$	$\downarrow \hbar \to 0$
Liouville	$\xrightarrow{N\to\infty}$	**Vlasov**

Independent large N and small $\hbar$ asymptotic limits

Theorem (Golse, P.) $\int |\hat{V}(\xi)|(1+|\xi|)^{d+6} d\xi < \infty$,

$D_N(t)$: N body linear evolution, $D_N(0) = (D^{in})^{\otimes N}$

$D(t)$: non linear Hartree evolution, $D(0) = D^{in}$

$$d_{d+5}(D_{N;1}(t) - D(t)) \leq C(t) N^{-1/2} \qquad \longrightarrow 0 \text{ as } N \to \infty$$

no dependence in $\hbar$ and for all initial D

$$\|W[D_{N;1}(t)] - W[D(t)]\|'_{d+5,\infty} \leq C(t) N^{-1/2}$$

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. : *Towards quantum transport*, preprint
- E. Caglioti, F. Golse, T. P. : *Quantum optimal transport is cheaper*, 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
- F. Golse, T. P. : *Empirical Measures and Quantum Mechanics : Applications to the Mean-Field Limit*, Communication in Mathematical Physics (2019).