Velocity Averaging
and Quantum Kinetic Theory

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In memory of Claude Bardos (1940-2026)

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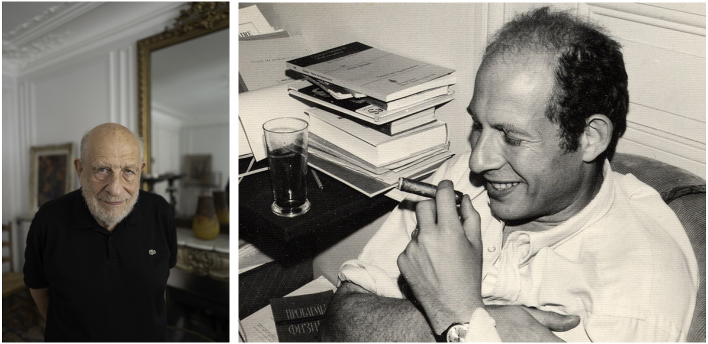

Figure: Left: at home, after being awarded the Maxwell Prize (2019), right: at École normale supérieure in 1963

What is Velocity Averaging?

Let $f^{in} \in L^2_{x,v}$ while $S \in L^\infty((0,T);L^2_{x,v})$. Let f be the solution of

$$\begin{cases} (\partial_t + v \cdot \nabla_x) f(t,x,v) = S(t,x,v)\,, & x, v \in \mathbf{R}^d \\ f(0,x,v) = f^{in}(x,v) \end{cases}$$

•For each $v \neq 0$, singularities in f^{in} and S are propagated by the characteristic flow $(x,v) \mapsto (x+tv,v)$: the solution f is not more regular than the data f^{in} and S (the operator $\partial_t + v \cdot \nabla_x$ is hyperbolic).

•Agoshkov [DAN1984] and G-Perthame-Sentis [CRAS1985], and then G-Lions-P-S [JFA1988] observed that **velocity averages**, i.e.

$$\rho[\phi](t,x) := \int_{\mathbf{R}^d} f(t,x,v)\phi(v)dv\,, \qquad \phi \in C_c(\mathbf{R}^d)$$

are **more regular** than f itself.

Applications of velocity averaging include

(a) the global existence of weak solutions of the Vlasov-Maxwell system for all bounded initial data of finite mass and energy [DiPerna-Lions 1989]

(b) the global existence of renormalized (i.e. mild) solutions of the Boltzmann equation for a hard sphere gas for all initial data of finite mass, energy and entropy [DiPerna-Lions 1989]

(c) the hydrodynamic limit of renormalized solutions of the Boltzmann equation to Leray solutions of the Navier-Stokes equations [G-Saint-Raymond 2004, 2009]

QUESTION Does velocity averaging apply to quantum dynamics?

The Schrödinger and the Wigner Equations

Let $\psi^{in} \in L^2(\mathbf{R}^d)$ satisfy $\|\psi^{in}\|_{L^2(\mathbf{R}^d)} = 1$. Let $\psi \equiv \psi(t,x)$ satisfy

$$\partial_t \psi = \tfrac{i\hbar}{2}\Delta_x \psi\,, \qquad \psi\Big|_{t=0} = \psi^{in}$$

The **Wigner transform** of ψ is

$$W_\hbar\{\psi\}(t,x,\xi) := \tfrac{1}{(2\pi)^d}\int_{\mathbf{R}^d} e^{-i\xi\cdot y}\psi(t,x+\tfrac{\hbar}{2}y)\overline{\psi(t,x-\tfrac{\hbar}{2}y)}dy$$

and satisfies the **Wigner equation**

$$(\partial_t + \xi\cdot\nabla_x)W_\hbar = 0$$

QUESTION Does velocity averaging apply to $W_\hbar$? Is is true that

$$\rho(t,x) = |\psi(t,x)|^2 = \int_{\mathbf{R}^d} W_\hbar(t,x,\xi)d\xi$$

is more regular that ψ **uniformly in** $\hbar \ll 1$? Applications to NLS?

Mixed Quantum States

Density operator For $(\psi_j)_{j\ge1}$, orthonormal system in $\mathfrak{H} := L^2(\mathbf{R}^d)$

$$R(X,Y) := \sum_{j\ge1} \lambda_j \psi_j(X)\overline{\psi_j(Y)}\,, \qquad \sum_{j\ge1} \lambda_j = 1 \text{ and } \lambda_j \ge 0$$

Integral kernel of an operator on $L^2(\mathbf{R}^d)$ also denoted by R

$$R\phi(X) := \int_{\mathbf{R}^d} R(X,Y)\phi(Y)dY$$

The operator R satisfies

$$R = R^* \ge 0\,, \quad \text{and} \quad \underbrace{\|R\|}_{\sup_{j\ge1}\lambda_j} \le \sqrt{\operatorname{Tr}(R^2)} \le \underbrace{\operatorname{Tr}(R)}_{\sum_{j\ge1}\lambda_j} = 1$$

Wigner transform of R

$$W_\hbar[R](x,\xi) = \sum_{j\ge1} \lambda_j W_\hbar\{\psi_j\}(x,\xi)$$

Quantum Dynamics of Mixed States

Quantum Hamiltonian: set $\mathcal{H} := -\frac{\hbar^2}{2}\Delta_x + V(x) = \mathcal{H}^*$ on $L^2(\mathbf{R}^d)$. By Stone's theorem, $\mathcal{H}$ generates a quantum dynamics on $L^2(\mathbf{R}^d)$

$$U(t) := \exp(-\tfrac{it}{\hbar}\mathcal{H}) = U(-t)^*$$

For each density operator R^{in} on $L^2(\mathbf{R}^d)$, set $R(t) := U(t)R^{in}U(t)^*$, whose integral kernel $R(t, X, Y)$ solves the **von Neumann equation**

$$\partial_t R = \tfrac{i\hbar}{2}(\Delta_X - \Delta_Y)R + \frac{V(X)-V(Y)}{i\hbar}R$$

while $w_\hbar(t,x,\xi) := W_\hbar[R(t)](x,\xi)$ solves the **Wigner equation**

$$\begin{cases}(\partial_t + \xi\cdot\nabla_x)w_\hbar = K[V]\star_\xi w_\hbar\,, \quad K[V] := \frac{\mathcal{F}_{y\to\xi}[V(x+\frac{\hbar y}{2}) - V(x-\frac{\hbar y}{2})]}{(2\pi)^d i\hbar} \\ w_\hbar\Big|_{t=0} = W_\hbar[R^{in}]\end{cases}$$

Quantum Velocity Averaging: Mixed States

THM 1. Let $R_\hbar^{in}$ be a density operator on $L^2(\mathbf{R}^d)$ satisfying

$$\operatorname{Tr}((R_\hbar^{in})^2)=\int_{\mathbf{R}^{2d}}|R_\hbar^{in}(X,Y)|^2dXdY\le(2\pi\hbar)^dC_{in}^2$$

Let $0\le V\in\operatorname{Lip}(\mathbf{R}^d)$ and let $R_\hbar\equiv R_\hbar(t,X,Y)$ be the solution of

$$\partial_tR_\hbar=\tfrac{i\hbar}{2}(\Delta_X-\Delta_Y)R_\hbar+\frac{V(X)-V(Y)}{i\hbar}R_\hbar\,,\quad R_\hbar\Big|_{t=0}=R_\hbar^{in}$$

Then, for each $\phi\in C_c^1(\mathbf{R}^d)$, the density function

$$\rho_\hbar[\phi](t,x):=\int_{\mathbf{R}^d}W_\hbar[R_\hbar(t)](x,\xi)\phi(\xi)d\xi$$

belongs to $H^{1/4}((0,T)\times\mathbf{R}_x^d)$ with a uniform bound

$$\sup_{0<\hbar<1}\left\|\left(I+(-\Delta_{t,x})^{1/8}\right)\rho_\hbar[\phi]\right\|_{L^2((0,T)\times\mathbf{R}_x^d)}<+\infty$$

Remark: Uniform L^2 Bound on Wigner Functions

Using Plancherel's theorem & integrating by substitution shows that

$$\int_{\mathbf{R}^{2d}} |W_\hbar[R^{in}]_\hbar(x,\xi)|^2 dx d\xi = \int_{\mathbf{R}^{2d}} |R^{in}_\hbar(X,Y)|^2 \frac{dXdY}{(2\pi\hbar)^d} = \frac{\operatorname{Tr}\big((R^{in}_\hbar)^2\big)}{(2\pi\hbar)^d}$$

Besides

$$\lambda_{\hbar,j} \geq 0\,, \quad \sum_{j\geq 1} \lambda_{\hbar,j} = 1\,, \quad \sum_{j\geq 1} \lambda_{\hbar,j}^2 = (2\pi\hbar)^d \underbrace{\|W_\hbar[R^{in}_\hbar]\|^2_{L^2}}_{\leq C^2_{in}}$$

By the Cauchy-Schwarz inequality, $\operatorname{rank}(R^{in}_\hbar) \to \infty$ as $\hbar \to 0$ since

$$1 = \left(\sum_{j\geq 1} \lambda_{\hbar,j}\right)^2 \leq \sum_{j\geq 1} \mathbf{1}_{\lambda_{\hbar,j}>0} \cdot \sum_{j\geq 1} \lambda_{\hbar,j}^2 \leq \operatorname{rank}(R^{in}_\hbar)(2\pi\hbar)^d C^2_{in}$$

Therefore, the assumptions of Thm1 exclude pure states!

Quantum Velocity Averaging: the Case of Pure States

THM 2. Let $\psi_\hbar \in C^1(\mathbf{R}^d;\mathbf{C}\setminus\{0\})$ s.t. $\|\psi_\hbar\|_{L^2(\mathbf{R}^d)} = 1$ for $\hbar \in (0,1)$ and $w_\hbar = W_\hbar\{\psi_\hbar\} \to w$ in $\mathcal{S}'(\mathbf{R}^d \times \mathbf{R}^d)$ as $\hbar \to 0$. Assume that

$$\hbar \left\|\nabla|\psi_\hbar|^2\right\|_{L^2(B(0,R))} \to 0 \quad \text{for all } R>0$$

and that

$$\begin{cases}\rho_\hbar = \int w_\hbar d\xi \ \to \int w d\xi \ =: \rho\\ J_\hbar = \int \xi w_\hbar d\xi \to \int \xi w d\xi \ =: J\end{cases} \qquad \text{strongly in } L^2(B(0,R))$$

while

$$\mathcal{E}_\hbar = \int \tfrac{|\xi|^2}{2} w_\hbar d\xi \to \int \tfrac{|\xi|^2}{2} w d\xi =: \mathcal{E} \qquad \text{weakly in } L^2(B(0,R))$$

Then

$$w = \rho(x)\delta(\xi - u(x))\,, \qquad \text{where } u(x) := \frac{\mathbf{1}_{\rho(x)>0}}{\rho(x)} J(x)$$

How is THM 2 related to Velocity Averaging?

Assumptions

•That $w_{\hbar_n} \to w$ in $\mathcal{S}'(\mathbf{R}^d \times \mathbf{R}^d)$ is proved in [P.-L. Lions -T. Paul '93]

•Weak convergence of $\mathcal{E}_{\hbar_n}$ is a **tightness** condition in ξ (decay of $w_{\hbar_n}$ for $|\xi| \to \infty$ **uniform** in $\hbar_n$)

•Strong convergence of $\rho_{\hbar_n}$ and $J_{\hbar_n}$ in L^2_{loc} = expected **conclusion** of a velocity averaging theorem.

Conclusion

That $w = \rho(x)\delta(\xi - u(x))$ shows that the averaging effect in ξ disappears as $\hbar \to 0$.

In the case of pure states, **the conclusions of velocity averaging prevent applying velocity averaging!**

Example (WKB) If $\psi_\hbar(x) = a(x)e^{i\frac{S(x)}{\hbar}}$, then $w = a(x)^2\delta(\xi - \nabla S(x))$

Pure States and Wigner Functions

Question Criterion for $w \equiv w(x,\xi) \in L^2(\mathbf{R}_x^d \times \mathbf{R}_\xi^d)$ to be the Wigner transform of a pure state=rank-one orthogonal projection in $L^2(\mathbf{R}^d)$?

LEMMA 3. Let $R =$density operator on $L^2(\mathbf{R}^d)$. Assume that

$$\mathcal{F}_{\xi\to y} W_\hbar[R] : \mathbf{R}_x^d \times \mathbf{R}_y^d \to \mathbf{C} \setminus \{0\} \text{ is of class } C^1$$

Then, for all $j,k = 1,\dots,d$

$$\operatorname{rank}(R) = 1 \iff \begin{cases} \frac{4}{\hbar^2}\partial_{y_j}\left(\frac{\partial_{y_k}\mathcal{F}_{\xi\to y}W_\hbar[R]}{\mathcal{F}_{\xi\to y}W_\hbar[R]}\right) = \partial_{x_j}\left(\frac{\partial_{x_k}\mathcal{F}_{\xi\to y}W_\hbar[R]}{\mathcal{F}_{\xi\to y}W_\hbar[R]}\right) \\ \partial_{y_j}\left(\frac{\partial_{x_k}\mathcal{F}_{\xi\to y}W_\hbar[R]}{\mathcal{F}_{\xi\to y}W_\hbar[R]}\right) = \partial_{x_j}\left(\frac{\partial_{y_k}\mathcal{F}_{\xi\to y}W_\hbar[R]}{\mathcal{F}_{\xi\to y}W_\hbar[R]}\right) \end{cases}$$

in the sense of distributions on $\mathbf{R}^d \times \mathbf{R}^d$

Main Idea in LEMMA 3

In space dimension $d = 1$: if $R(X, Y) \equiv \psi(X)\overline{\psi(Y)}$, then

$$\mathcal{F}_{\xi\to y} W_\hbar[R](x, y) = \psi(x + \tfrac{\hbar}{2}y)\overline{\psi(x - \tfrac{\hbar}{2}y)}$$

Taking the ln leads to the d'Alembert formula

$$\begin{aligned}\ln \mathcal{F}_{\xi\to y} W_\hbar[R](x, y) =& \ln \psi(x + \tfrac{\hbar}{2}y) + \ln \overline{\psi(x - \tfrac{\hbar}{2}y)}\\ =& a(x + \tfrac{\hbar}{2}y) + b(x - \tfrac{\hbar}{2}y)\end{aligned}$$

for the general solution at time y of the wave equation with speed $\frac{\hbar}{2}$

$$\left(\tfrac{4}{\hbar^2}\partial_y^2 - \partial_x^2\right) \ln \mathcal{F}_{\xi\to y} W_\hbar[R](x, y) = 0$$

Care must be exercised with the branches of $\ln \mathcal{F}_{\xi\to y} W_\hbar[R]$...

RMK Similar observation by Tatarskii (1983) in the original variables $X = x + \frac{\hbar}{2}y$ and $Y = x - \frac{\hbar}{2}y$...

Removing the Non-Vanishing Condition on ψ

For D =derivation on a commutative unital Banach algebra $\mathcal{A}$, set

$$T[D]f := fD^2f - (Df)^2$$

Lemma 4. One has

$$\begin{array}{ll} (a) & \|f-1\|<1 \implies T[D](f)=f^2 D \ln f \\ (b) & T[D](fg) = T[D](f)g^2 + f^2 T[D](g) \end{array}$$

Apply this to Wigner functions of pure states — in dimension $d = 1$ with the notation

$$T_x := T[\partial_x]\,, \qquad T_y := T[\partial_y]$$

Lemma 3 if $\psi \neq 0$, or Lemma 4 in general imply that, for $\psi \in H^2(\mathbf{R})$

$$T_y \mathcal{F}_{\xi\to y} W_\hbar\{\psi\}(x,y) = \tfrac{\hbar^2}{4} T_x \mathcal{F}_{\xi\to y} W_\hbar\{\psi\}(x,y)$$

Specialize this identity to $y = 0$ observing that

$$\begin{aligned} \rho(x) &= |\psi(x)|^2 = \mathcal{F}_{\xi\to y} W_\hbar\{\psi\}(x,0) \\ J(x) &= \int_{\mathbf{R}} \xi W_\hbar\{\psi\}(x,\xi)d\xi = -i\partial_y \mathcal{F}_{\xi\to y} W_\hbar\{\psi\}(x,0) \\ \mathcal{E}(x) &= \int_{\mathbf{R}} \frac{\xi^2}{2} W_\hbar\{\psi\}(x,\xi)d\xi = -\partial_y^2 \mathcal{F}_{\xi\to y} W_\hbar\{\psi\}(x,0) \end{aligned}$$

This leads to the following **key identity**

$$\begin{aligned} J(x)^2 - 2\rho(x)\mathcal{E}(x) &= T_y \mathcal{F}_{\xi\to y} W_\hbar\{\psi\}(x,0) \\ &= \frac{\hbar^2}{4} T_x \mathcal{F}_{\xi\to y} W_\hbar\{\psi\}(x,0) \\ &= \frac{\hbar^2}{4} \left(\rho(x)\partial_x^2\rho(x) - (\partial_x\rho(x))^2\right) \\ &= \frac{\hbar^2}{8} \left(\partial_x^2(\rho(x)^2) - 4(\partial_x\rho(x))^2\right) \end{aligned}$$

Proof of THM 2, $d = 1$

Apply this identity to $\psi_\hbar$ as in THM 2

$$J_\hbar^2 - 2\rho_\hbar \mathcal{E}_\hbar = \tfrac{1}{8}\partial_x^2 \underbrace{(\hbar^2 \rho_\hbar^2)}_{\to 0 \text{ in } L^1} - \tfrac{1}{2} \underbrace{\hbar^2 (\partial_x \rho_\hbar)^2}_{\to 0 \text{ in } L^1} \to 0 \quad \text{in } \mathcal{D}'(\mathbf{R}_x)$$

$$\downarrow$$

$$J^2 - 2\rho\,\mathcal{E} \quad \text{in weak } L^1(\mathbf{R}^d) \text{ as } \hbar \to 0$$

Hence

$$J^2 = \left(\int_{\mathbf{R}} \xi w d\xi\right)^2 = \int_{\mathbf{R}} w d\xi \int_{\mathbf{R}} \xi^2 w d\xi = 2\rho\mathcal{E}$$

Since $w \geq 0$ [P.-L. Lions -T. Paul Rev. Mat. Iberoam. '93], this is an equality case in the Cauchy-Schwarz inequality.
Hence w is a probability measure with 0 variance. ☐

A Detour: Madelung's QHD (1926)

In 1926, E. Madelung observed an analogy between the quantum dynamics of pure states and hydrodynamics.

Let $\psi \equiv \psi(t,x) \in \mathbf{C}$ be a solution of the free Schrödinger equation

$$\partial_t \psi(t,x) = \tfrac{i\hbar}{2}\partial_x^2 \psi(t,x)\,, \qquad x \in \mathbf{R}$$

Then $w(t,x,\xi) := W_\hbar\{\psi(t,\cdot)\}(x,\xi)$ satisfies

$$\partial_t w(t,x,\xi) + \xi \partial_x w(t,x,\xi) = 0$$

In particular

$$\partial_t \underbrace{\int w(t,x,\xi)d\xi}_{=\rho} + \partial_x \underbrace{\int \xi w(t,x,\xi)d\xi}_{=J} = 0$$

$$\partial_t \underbrace{\int \xi w(t,x,\xi)d\xi}_{=J} + \partial_x \underbrace{\int \xi^2 w(t,x,\xi)d\xi}_{=2\mathcal{E}} = 0$$

The key identity in the proof of THM 2 gives a closure relation for $\mathcal{E}$

$$J^2 - 2\rho\mathcal{E} = \tfrac{\hbar^2}{4} T_x\rho = \tfrac{\hbar^2}{4}\rho\left(\partial_x^2\rho - 4(\partial_x\sqrt{\rho})^2\right)$$

leading to Madelung's QHD system

$$\begin{cases}\partial_t\rho + \partial_x J = 0\\ \partial_t J + \partial_x\left(\frac{J^2}{\rho}\right) = \frac{\hbar^2}{4}\partial_x\left(\partial_x^2\rho - 4(\partial_x\sqrt{\rho})^2\right) = \frac{\hbar^2}{4}\partial_x\left(\frac{T_x\rho}{\rho}\right)\end{cases}$$

THM 5. If $\psi \equiv \psi(t,x) \in C_b(\mathbf{R}_t; H^2(\mathbf{R}))$ is a solution of the (free) Schrödinger equation satisfying the condition

$$\psi \neq 0 \text{ a.e. on } \mathbf{R}_t \times \mathbf{R}_x$$

then, the following observables satisfy the Madelung QHD system

$$\rho := |\psi|^2 \quad \text{and} \quad J := \hbar\Im(\overline{\psi}\partial_x\psi)$$

Proof (sketch) Use the key identity in the proof of THM 2

$$2\rho_\hbar\mathcal{E}_\hbar - J_\hbar = \frac{\hbar^2}{4}\rho_\hbar\left(\partial_x^2\rho_\hbar - 4(\partial_x\sqrt{\rho_\hbar})^2\right)$$

Observe that $\mathcal{E}_\hbar, \partial_x^2\rho_\hbar \in L^1_{loc}(\mathbf{R}^2_{t,x})$, that $J_\hbar^2/\rho_\hbar \le \hbar^2|\nabla_x\psi_\hbar|^2$, and that $\partial_x\sqrt{\rho_\hbar} \in L^2_{loc}(\mathbf{R}^2_{t,x})$ (by Lions-Villani lemma [CRAS 1995] on the regularity of square roots), and divide both sides by $\rho_\hbar > 0$ a.e.

$\square$

Condition $\hbar^2\|\partial_x\rho\|^2_{L^2} \to 0$ The Euler equation in QHD is

$$\partial_t J_\hbar + \partial_x\left(\frac{J_\hbar^2}{\rho_\hbar} + \underbrace{\hbar^2\left((\partial_x\sqrt{\rho_\hbar})^2 - \tfrac{1}{4}\partial_x^2\rho_\hbar\right)}_{=\rho_\hbar\Pi_\hbar}\right) = 0$$

Introducing the quantum pressure tensor

$$\Pi_\hbar := -\frac{\hbar^2}{4}\frac{T_x\rho_\hbar}{\rho_\hbar} = -\frac{\hbar^2}{4}\partial_x^2 \ln\rho_\hbar$$

we see that, for all $R > 0$

$$\hbar^2\|\partial_x\rho\|^2_{L^2(B(0,R))} \to 0 \iff \rho_\hbar^2\Pi_\hbar \to 0 \text{ in } \mathcal{D}'(\mathbf{R}^2)$$

Conclusions

Summarizing, we have seen that

• Velocity averaging improves the regularity of observable densities (i.e. moments of the Wigner function in the momentum variable ξ) over the Wigner function for some convenient class of mixed states

• But velocity averaging is expected to fail in the case of pure states and in the semiclassical regime with vanishing quantum pressure

• This last result rests on a characterization of the Wigner function of pure states leading to a new (?) derivation of Madelung's quantum Euler equation