Propagation of Monokinetic Measures with Rough Momentum Profiles I

François Golse

Ecole Polytechnique
Centre de Mathématiques Laurent Schwartz

Quantum Systems:
A Mathematical Journey from Few to Many Particles

May 16th 2013 CSCAMM, University of Maryland.

Work in collaboration with Claude Bardos,
Peter Markowich and Thierry Paul

Statement of the problem

Def: Monokinetic probability measure in the 1-particle phase space $\mathbf{R}^N_x \times \mathbf{R}^N_\xi$, with density ρ^{in} and momentum profile $U^{in} \equiv U^{in}(x) \in \mathbf{R}^N$

$$\mu^{in}(x, d\xi) := \rho^{in}(x)\delta_{U^{in}(x)}(\xi)$$

where

$$\rho^{in} \geq 0 \text{ a.e.,} \quad \text{and} \int_{\mathbf{R}^N} \rho^{in}(x)dx = 1$$

Hamiltonian flow $\Phi_t : \mathbf{R}^N_x \times \mathbf{R}^N_\xi \ni (x, \xi) \mapsto (X, \Xi)(t; x, \xi) \in \mathbf{R}^N_x \times \mathbf{R}^N_\xi$ generated by Hamiltonian system

$$(H) \qquad \dot{X} = D_\xi H(X, \Xi)\,, \quad \dot{\Xi} = -D_x H(X, \Xi)$$

I.e. $t \mapsto \Phi_t(x,\xi) =$ solution of (H) s.t. (x,ξ) at $\Phi_0(x,\xi) = (x,\xi)$

If $T : X \to Y$ is measurable and μ is a probability measure on X, define a probability measure ν on Y by

$$\nu(B) := \mu(T^{-1}(B)), \quad \text{denoted } \nu = T\#\mu$$

Propagated measure: with Hamiltonian flow Φ_t, we define

$$\mu(t) := \Phi_t\#\mu^{in}$$

Space marginal of $\mu(t)$: with the notation $\Pi : (x,\xi) \mapsto x$, we set

$$\rho(t) := \Pi\#\mu(t) = F_t\#(\rho^{in}\mathscr{L}^N) \quad \text{i.e. } \rho(t,\cdot) = \int_{\mathbf{R}^N} \mu(t,\cdot,d\xi)$$

Statement of problem III

To study the structure of the propagated phase space probability measure $\mu(t)$ and of its space marginal $\rho(t)$ for all $t \in \mathbf{R}$

For instance

•Is $\mu(t)$ still a monokinetic measure? if not

•Is $\mu(t)$ representable in terms of monokinetic measures?

•Is $\rho(t)$ a probability density for all $t \in \mathbf{R}$? if not

•What can be said of the singular component of $\rho(t)$?

Moreover, we are interested in answering these questions under the most general regularity assumptions possible on ρ^{in} and U^{in}.

Earlier research in this direction: Gasser-Markowich ('94), Sparber-Markowich-Mauser ('03)...

Motivation: classical limit of Schrödinger's equation

Classical limit of Schrödinger's equation for $x \in \mathbf{R}^N$:

$$i\epsilon\partial_t\psi_\epsilon + \tfrac{1}{2}\epsilon^2\Delta_x\psi_\epsilon = V(x)\psi_\epsilon\,, \quad \psi_\epsilon(0,x) = a^{in}(x)e^{iS^{in}(x)/\epsilon}$$

Wigner function at scale ϵ: for each wave function $\Psi \in L^2(\mathbf{R}^N)$

$$W_\epsilon[\Psi](x,\xi) := \tfrac{1}{(2\pi)^N}\int_{\mathbf{R}^N} \Psi(x+\tfrac{1}{2}\epsilon y)\overline{\Psi(x-\tfrac{1}{2}\epsilon y)}e^{-i\xi\cdot y}dy$$

Case of WKB ansatz: for $a^{in} \in L^2(\mathbf{R}^N)$ and $S^{in} \in W^{1,1}_{loc}(\mathbf{R}^N)$

$$W_\epsilon[a^{in}e^{S^{in}/\epsilon}](x,\xi) \to a^{in}(x)^2\delta_{\nabla_x S^{in}(x)}(\xi)$$

Thm (Lions-Paul '93): Assume $a^{in} \in L^2(\mathbf{R}^N)$ and $S^{in} \in W^{1,1}_{loc}(\mathbf{R}^N)$
Let $V \in C^2(\mathbf{R}^N)$ satisfy, for some $\alpha > N/2$, the condition

$$V(x) = o(|x|) \text{ and } V^-(x) = o(|x|^{-\alpha}) \quad \text{as } |x| \to \infty$$

Set

$$\psi_\epsilon(t,\cdot) := e^{-i\frac{t}{\epsilon}\left(-\frac{\epsilon^2}{2}\Delta_x + V(x)\right)} a^{in} e^{iS^{in}/\epsilon}$$

Then

(a) $\quad W_\epsilon[\psi_\epsilon] \to \mu \geq 0 \quad$ in $\mathcal{S}'(\mathbf{R}^N_x \times \mathbf{R}^N_\xi)$ as $\epsilon \to 0^+$

and

(b) $$\begin{cases} \partial_t \mu + \xi \cdot \nabla_x \mu - \nabla_x V(x) \cdot \nabla_\xi \mu = 0 \\ \mu\big|_{t=0} = a^{in}(x)^2 \delta_{\nabla_x S^{in}(x)}(\xi) \end{cases}$$

Hamiltonian propagation of Wigner measure

Hence

$$\mu(t) = (X_t, \Xi_t)\#\mu^{in} \quad \text{with } \mu^{in}(x,\xi) := a^{in}(x)^2 \delta_{\nabla_x S^{in}(x)}(\xi)$$

with (X_t, Ξ_t)=flow generated by Hamiltonian of classical mechanics

$$H(x,\xi) := \tfrac{1}{2}|\xi|^2 + V(x)$$

Propagation of Wigner measure for WKB ansatz requires much less regularity of V, and of S^{in} and a^{in} than the WKB method

Propagation of Wigner measure for WKB ansatz is global on $\mathbf{R} \times \mathbf{R}^N$ — not limited by caustic onset

See also Gérard-Markowich-Mauser-Poupaud CPAM'97 for other PDEs.

Hamiltonian $H(x,\xi)$ satisfies, for some $\kappa{>}0$ and $h(r){=}o(r)$ at ∞

$$(H) \qquad \begin{cases} |\nabla_\xi H(x,\xi)| \le \kappa(1+|\xi|)\,, & |D^2 H(x,\xi)| \le \kappa \\ |\nabla_x H(x,\xi)| \le h(|x|) + \kappa|\xi| \end{cases}$$

Prop: Under assumptions (H), Hamiltonian H generates a global flow $\Phi_t = (X_t, \Xi_t)$ that is C^1 in all its variables. Besides

a) for each $T, \eta > 0$ there exists $C_{T,\eta} > 0$ s.t.

$$\sup_{|t|\le T} |X_t(x,\xi) - x| \le C_{T,\eta}(1+|\xi|) + \eta|x|$$

b) for each $t > 0$, one has $|D\Phi_t(x,\xi) - I| \le e^{\kappa|t|} - 1$

The dynamics in configuration space

Assume initial momentum profile $U^{in} \in C(\mathbf{R}^N; \mathbf{R}^N)$ satisfies

$$(SL) \qquad |U^{in}(x)| = o(|x|) \quad \text{as } |x| \to \infty$$

With the Hamiltonian flow $\Phi_t = (X_t, \Xi_t)$, define the map

$$F_t : \mathbf{R}^N \ni y \mapsto X_t(y, U^{in}(y)) \in \mathbf{R}^N$$

Lemma: The map F_t satisfies the following properties

- $F_t(y) = y + o(|y|)$ as $|y| \to \infty$ for all $t \in \mathbf{R}$ $\Rightarrow$ F_t is proper
- $\deg(F_t, B(0,R), x) = 1$ for $x \in \mathbf{R}^N$ and $R \gg 1$ $\Rightarrow$ F_t is onto

Rough (non C^1) momentum profiles U^{in}

Assume initial momentum profile $U^{in} \in C(\mathbf{R}^N; \mathbf{R}^N)$ satisfies

$$\begin{cases} |U^{in}(x)| = o(|x|) \quad \text{as } |x| \to \infty & \text{(SL)} \\ DU^{in} \in L^{N,1}_{loc}(\mathbf{R}^N) & \text{(DU)} \end{cases}$$

(Variant of) **Rademacher's thm:** $\mathscr{L}^N(E) = 0$ where

$$E := \{y \in \mathbf{R}^N \mid U^{in} \text{ not differentiable}\}$$

Jacobian:

$$J_t(y) := |\det(DF_t(y))|, \quad P_t := J_t^{-1}((0,\infty)), \quad Z_t := J_t^{-1}(\{0\})$$

Caustic fiber (for rough momentum profiles):

$$C_t := \{x \in \mathbf{R}^N \mid F_t^{-1}(\{x\}) \cap (Z_t \cup E) \neq \varnothing\}$$

Structure of $\mu(t)$ and $\rho(t)$ outside caustic fiber

Thm A: Assume Hamiltonian H satisfies condition (H) and that momentum profile U^{in} satisfies (SL+DU). Then

(a) for a.e. $x \in \mathbf{R}^N$ and all $t \in \mathbf{R}$, the set $F_t^{-1}(\{x\})$ is finite

(b) the following conditions are equivalent

$$\rho(t)(C_t) = 0 \Leftrightarrow \rho(t)(\mathbf{R}^N \setminus C_t) = 1 \Leftrightarrow \rho^{in} = 0 \text{ a.e. on } Z_t$$

(c) under the equivalent conditions in (b), $\rho(t) \ll \mathscr{L}^N$ and

$$\rho(t,x) := \frac{d\rho(t)}{d\mathscr{L}^N}(x) = \sum_{F_t(y)=x} \frac{\rho^{in}(y)}{J_t(y)} \quad \text{for a.e. } x \in \mathbf{R}^N$$

(d) under the equivalent conditions in (b)

$$\mu(t,x,\cdot) = \sum_{F_t(y)=x} \frac{\rho^{in}(y)}{J_t(y)} \delta_{\Xi_t(y,U^{in}(y))} \quad \text{for a.e. } x \in \mathbf{R}^N$$

Structure of $\mu(t)$ outside caustic fiber

Outside caustic fiber, $\mu(t) =$ a.e. finite sum of monokinetic measures

Analogy with $\psi_\epsilon \simeq$ locally finite sum of WKB ansatz away from caustic

More than an analogy: if $a_k \in L^2(\mathbf{R}^N)$ and $S_k \in W^{1,1}_{loc}(\mathbf{R}^N)$, then

$$W_\epsilon \left[\sum_{k=1}^{n} a_k e^{iS_k/\epsilon} \right] (x, \cdot) \to \sum_{k=1}^{n} a_k(x)^2 \delta_{\nabla S_j(x)}$$

in $\mathcal{S}'(\mathbf{R}^N \times \mathbf{R}^N)$ as $\epsilon \to 0$ provided that $\nabla S_1(x) \ldots, \nabla S_n(x)$ linearly independent for a.e. $x \in \mathbf{R}^N$

Solving for y the equation $F_t(y) = x$

Counting function: we define $\mathcal{N}(t,x) := \#F_t^{-1}(\{x\})$

The counting function measures the complexity of the structure of the propagated measure $\mu(t)$

If momentum profile U^{in} satisfies (SL) then

$$M_T(R) := \sup_{\substack{|y|\geq R\\ |t|\leq T}} |F_t(y) - y|/|y| \to 0 \text{ as } R \to \infty$$

Let $R_T^* > 0$ satisfy $M_T(R_T^*) < \frac{1}{2}$; then, for all $R > 2R_T^*$ one has

$$|x| \leq R \text{ and } F_t(y) = x \Rightarrow |y| \leq 2R$$

(Indeed $|y| > 2R > R_T^* \Rightarrow |F_t(y) - y| \leq \frac{1}{2}|y| \Rightarrow |F_t(y)| \geq \frac{1}{2}|y| > R$.)

Estimates on the set $F_t^{-1}(\{x\})$: rough (non C^1) case

Thm B: Assume Hamiltonian H satisfies (H) and momentum profile U^{in} satisfies (SL+DU). Let $T > 0$ and $R_T^* > 0$ s.t. $M_T(R_T^*) < \frac{1}{2}$.

(a) The caustic fibers satisfy $\mathscr{L}^N(C_t) = 0$ for all $t \in \mathbf{R}$.

(b) For each $t \in [-T, T]$ and each $R > 2R_T^*$

$$\mathscr{L}^N(\{x \text{ s.t. } |x| \leq R \;\&\; \mathcal{N}(t,x) \geq n\}) \leq \frac{e^{\kappa N|t|}}{n} \|1+|Du^{in}|\,\|^N_{L^N(B(0,2R))}$$

(c) For a.e. $x \in \mathbf{R}^N$

$$\mathscr{H}^1(\{(t,y) \text{ s.t. } |t| \leq T \;\&\; F_t(y) = x\}) < \infty$$

Solving for y the equation $F_t(y) = x$: smooth (C^1) case

Caustic: define $C := \{(t,x) \in \mathbf{R} \times \mathbf{R}^N \text{ s.t. } x \in C_t\}$

Thm B': Assume Hamiltonian H satisfies (H) and momentum profile $U^{in} \in C^1_b(\mathbf{R}^N, \mathbf{R}^N)$ satisfies (SL)

(a) The caustic C is closed in $\mathbf{R} \times \mathbf{R}^N$.

(b) The integer $\mathcal{N}(t,x)$ is odd for each $(t,x) \in \mathbf{R} \times \mathbf{R}^N \setminus C$.

(c) There exists $a<0<b$ s.t. $a<t<b \Rightarrow C_t = \varnothing$ and $\mathcal{N}(t,x) = 1$.

(d) The integer-valued counting function $\mathcal{N}$ is constant on each connected component of $\mathbf{R} \times \mathbf{R}^N \setminus C$

(e) Set $F_t^{-1}(\{x\}) := \{y_j(t,x) \,|\, j = 1, \ldots, \mathcal{N}(t,x)\}$ for all $x \notin C_t$; then each map $y_j \in C^1(\mathcal{O}_j)$, where $\mathcal{O}_j := \{(t,x) \text{ s.t. } \mathcal{N}(t,x) \geq j\}$.

The manifold Λ_t

For each $t \in \mathbf{R}$, we define

$$\Lambda_t := \Phi_t(\{(x,\xi) \text{ s.t. } \xi = U^{in}(x)\}) \quad \Lambda := \{(t,x,\xi) \,|\, (x,\xi) \in \Lambda_t\}$$

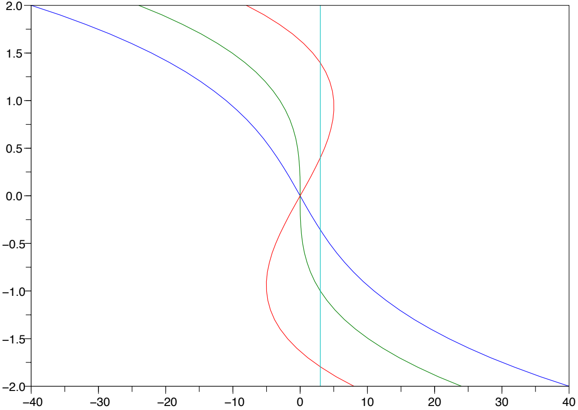
Therefore

$$\Lambda_t \cap (\{x\} \cap \mathbf{R}^N) = \{(x, \Xi_t(y, U^{in}(y))) \,|\, F_t(y) = x\}$$
$$\Rightarrow \#(\Lambda_t \cap (\{x\} \cap \mathbf{R}^N)) \leq \mathcal{N}(t,x)$$

Smooth case: let $O_n \subset \mathbf{R}^N \setminus C$ be a connected component, then

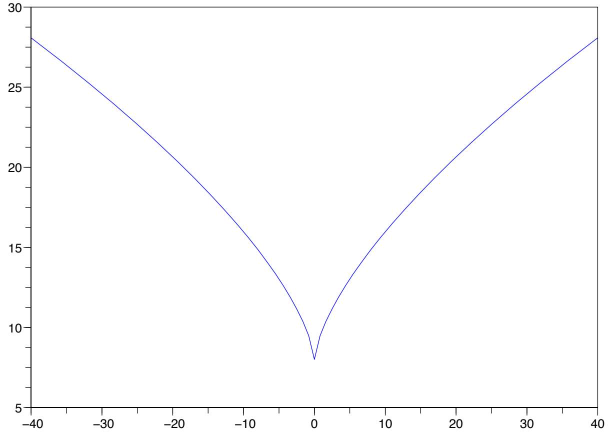
$$\mathcal{N}(t,x) = n \text{ for all } (t,x) \in O_n \Rightarrow$$
$$\Lambda \cap (O_n \times \mathbf{R}^N) = \bigcup_{j=1}^{n} \{(t, x, \Xi_t(y_j(t,x)), U^{in}(y_j(t,x)) \,|\, (t,x) \in O_n\}$$

Example of Λ_t: free dynamics of cubic lagrangian



Free flow $H(x,\xi) = \frac{1}{2}\xi^2$ in space dimension $N = 1$
initial profile U^{in} inverse of $y \mapsto -8y - 3y^3$, time $t = 0, 8, 16$

Example of caustic



Caustic (simple cusp) in case of cubic lagrangian

Proof of (b): apply area formula (Maly-Swanson-Ziemer '02)

$$\int_{\overline{B(0,2R)}} J_t(y)dy = \int_{\mathbf{R}^N} \#(F_t^{-1}(\{x\}) \cap (\overline{B(0,2R)}))dx$$
$$\geq \int_{\overline{B(0,R)}} \#(F_t^{-1}(\{x\}) \cap (\overline{B(0,2R)}))dx$$
$$= \int_{\overline{B(0,R)}} \mathcal{N}(t,x)dx$$

By Bienaymé-Chebyshev's inequality

$$\mathscr{L}^N(\{x \in \overline{B(0,R)} \text{ s.t. } \mathcal{N}(t,x) \geq n\}) \leq \frac{1}{n} \int_{\overline{B(0,2R)}} J_t(y)dy$$

By the estimate on the gradient $|D\Phi_t|$ of the Hamiltonian flow

$$|D_x X_t(y, U^{in}(y))| \le e^{\kappa|t|}\,, \qquad |D_\xi X_t(y, U^{in}(y))| \le (e^{\kappa|t|} - 1)$$

so that, by Hadamard's inequality

$$\begin{aligned} J_t(y) &= |\det(D_x X_t(y, U^{in}(y)) + D_\xi X_t(y, U^{in}(y)) DU^{in}(y))| \\ &\le (e^{\kappa|t|} + (e^{\kappa|t|} - 1)|DU^{in}(y)|)^N \end{aligned}$$

Therefore

$$\mathscr{L}^N(\{x \in \overline{B(0,R)} \text{ s.t. } \mathcal{N}(t,x) \ge n\}) \le \frac{e^{\kappa N|t|}}{n} \|1+|DU^{in}|\|^N_{L^N(B(0,R))}$$

Proof of (c): consider the map

$$F : [-T, T] \times \mathbf{R}^N \ni (t, y) \mapsto F(t, y) \in \mathbf{R}^N$$

Jacobian $DF(t, y)$ is the column-wise partitioned matrix

$$DF(t, y) = [V(t, y)\,,\; M(t, y)]\,, \quad |t| \leq T\,,\; y \in \mathbf{R}^N \setminus E$$

with

$$\begin{cases} V(t, y) = \nabla_\xi H(\Phi_t(y, U^{in}(y))) \\ M(t, y) = D_x X_t(y, U^{in}(y)) + D_\xi X_t(y, U^{in}(y)) DU^{in}(y)\,. \end{cases}$$

so that

$$DF(t, y) DF(t, y)^T = V(t, y) V(t, y)^T + M(t, y) M(t, y)^T$$

For each $m > 0$, both sets

$$K_m := F^{-1}(\overline{B(0,m)})$$
$$K'_m := \{y \in \mathbf{R}^N \mid \text{ there exists } t \in [-T,T] \text{ s.t. } (t,y) \in K_m\}$$

are compact since F_t is proper uniformly in $|t| \leq T$. Therefore

$$\|VV^T + MM^T\|^{N/2}_{L^{N/2}(K_m)} \leq 2^{N/2-1}\|V\|^N_{L^\infty(K_m)}\mathscr{L}^{N+1}(K_m) + 2^{N/2}T\|M\|^N_{L^N(K'_m)} < \infty$$

By the co-area formula (Maly-Swanson-Ziemer '02), for each $m > 0$

$$\int_{\mathbf{R}^N} \mathscr{H}^1(F^{-1}(\{x\}) \cap K_m) dx = \int_{K_m} \sqrt{\det(VV^T + MM^T)(t,y)} dt dy < \infty$$

In particular, for each $m > 0$

$$\mathscr{H}^1(F^{-1}(\{x\})) = \mathscr{H}^1(F^{-1}(\{x\}) \cap K_m) < \infty \quad \text{a.e. in } |x| \leq m$$

so that

$$\mathscr{H}^1(F^{-1}(\{x\})) < \infty \quad \text{for a.e. } x \in \mathbf{R}^N$$

Proof of Thm A

Proof of (a): using the bound on the counting function in Thm B

$$\mathscr{L}^N(\{x \text{ s.t. } |x| \le R \text{ and } \mathcal{N}(t,x) = \infty\}) = 0$$

Proofs of (c+d): by definition of $\mu(t) = \Phi_t \# \mu^{in}$

$$\langle \mu(t), \chi \rangle = \langle \mu^{in}, \chi \circ \Phi_t \rangle = \int \chi(F_t(y), \Xi_t(y, U^{in}(y)))\rho^{in}(y)dy$$

Since $\rho^{in} = 0$ a.e. on $Z_t := J_t^{-1}(\{0\})$, define a positive measurable function b by the formula

$$b(y) = \rho^{in}(y)/J_t(y) \text{ if } y \in P_t\,, \quad \text{ and } b(y) = 0 \text{ if } y \notin P_t$$

Therefore

$$\begin{aligned}\langle \mu(t), \chi \rangle &= \int \chi(F_t(y), \Xi_t(y, U^{in}(y)))b(y)J_t(y)dy \\ &= \int \left(\sum_{y \in F_t^{-1}(\{x\})} b(y)\psi(x, \Xi_t(y, U^{in}(y))) \right) dx \\ &= \int \left(\sum_{y \in F_t^{-1}(\{x\})} b(y)\langle \delta_{\Xi_t(y, U^{in}(y))}, \psi(x, \cdot) \rangle \right) dx\end{aligned}$$

by the area formula, so that

$$\mu(t, x, \cdot) = \sum_{y \in F_t^{-1}(\{x\})} b(y)\delta_{\Xi_t(y, U^{in}(y))}$$

Conclusion

We have obtained a detailed description of the propagation of monokinetic measures by proper Hamiltonian flows under the assumption that the initial momentum profile is sublinear at infinity with $L^{N,1}_{loc}$ gradient

In the complement of the caustic fiber, a Lebesgue-negligeable set, the propagated measure is an a.e. finite sum of monokinetic measures

We have obtained an estimate on the distribution of values of the number of terms in this sum

The proof of these results is based on the area formula from GMT