Propagation of Monokinetic Measures with Rough Momentum Profiles I

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Quantum Systems:
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Statement of the problem

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

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

where

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

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

$$\dot{X} = D_\xi H(X, \Xi), \quad \dot{\Xi} = -D_x H(X, \Xi)$$
I.e. $t \mapsto \Phi_t(x, \xi) = \text{solution of } (H) \text{ s.t. } (x, \xi) \text{ at } \Phi_0(x, \xi) = (x, \xi)$

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

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

denoted $\nu = T \# \mu$

Propagated measure: with Hamiltonian flow $\Phi_t$, we define

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

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

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

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 \( t \in \mathbb{R} \)? 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 \( \rho^{in} \) 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 \( x \in \mathbb{R}^N \):

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

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

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

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

\[
W_\epsilon[a^{in} e^{S^{in}/\epsilon}](x, \xi) \rightarrow a^{in}(x)^2 \delta_{\nabla_x S^{in}(x)}(\xi)
\]
Thm (Lions-Paul '93): Assume $a_{in} \in L^2(\mathbb{R}^N)$ and $S_{in} \in W^{1,1}_{loc}(\mathbb{R}^N)$
Let $V \in C^2(\mathbb{R}^N)$ 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

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

Then

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

and

(b) \begin{align*}
\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{align*}
Hamiltonian propagation of Wigner measure

Hence

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

with \((X_t, \Xi_t) = \text{flow generated by Hamiltonian of classical mechanics} \quad H(x, \xi) := \frac{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 \(\mathbb{R} \times \mathbb{R}^N\) — not limited by caustic onset

See also Gérard-Markowich-Mauser-Poupaud CPAM’97 for other PDEs.
Proper Hamiltonian flows

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

\[(H) \quad \begin{cases} |
\nabla_\xi H(x, \xi)| \leq \kappa (1 + |\xi|), \\
\n\nabla_x H(x, \xi)| \leq h(|x|) + \kappa |\xi| \end{cases} \]

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.

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

b) for each $t > 0$, one has $|D\Phi_t(x, \xi) - I| \leq e^{\kappa |t|} - 1$
The dynamics in configuration space

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

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

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

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

Lemma: The map $F_t$ satisfies the following properties

- $F_t(y) = y + o(|y|)$ as $|y| \to \infty$ for all $t \in \mathbb{R}$ $\Rightarrow$ $F_t$ is proper
- $\text{deg}(F_t, B(0,R), x) = 1$ for $x \in \mathbb{R}^N$ and $R \gg 1$ $\Rightarrow$ $F_t$ is onto
Rough (non $C^1$) momentum profiles $U^{in}$

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

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

(Variant of) Rademacher’s thm: $\mathcal{L}^N(E) = 0$ where

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

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):

\[C_t := \{x \in R^N \mid F_t^{-1}(\{x\}) \cap (Z_t \cup E) \neq \emptyset\}\]
**Thm A:** Assume Hamiltonian \( H \) satisfies condition \((H)\) and that momentum profile \( U^{in} \) satisfies \((SL+DU)\). Then

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

(b) the following conditions are equivalent

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

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

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

(d) under the equivalent conditions in (b)

\[
\mu(t, x, \cdot) = \sum_{F_t(y)=x} \frac{\rho^{in}(y)}{J_t(y)} \delta_{\Xi_t}(y, U^{in}(y)) \quad \text{for a.e. } x \in \mathbb{R}^N
\]
Outside caustic fiber, $\mu(t) = \text{a.e. finite sum of monokinetic measures}$

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

More than an analogy: if $a_k \in L^2(\mathbb{R}^N)$ and $S_k \in W^{1,1}_{\text{loc}}(\mathbb{R}^N)$, 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 $\mathcal{S}'(\mathbb{R}^N \times \mathbb{R}^N)$ as $\epsilon \to 0$ provided that $\nabla S_1(x) \ldots, \nabla S_n(x)$ linearly independent for a.e. $x \in \mathbb{R}^N$
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

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

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 $\mathcal{L}^N(C_t) = 0$ for all $t \in \mathbb{R}$.

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

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

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

$$\mathcal{H}^1(\{(t, y) \text{ s.t. } |t| \leq T & F_t(y) = x\}) < \infty$$
Solving for $y$ the equation $F_t(y) = x$: smooth ($C^1$) case

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

**Thm B’:** Assume Hamiltonian $H$ satisfies (H) and momentum profile $U^{in} \in C_b^1(\mathbb{R}^N, \mathbb{R}^N)$ satisfies (SL)

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

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

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

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

(e) Set $F_t^{-1}(\{x\}) := \{y_j(t, x) \mid j = 1, \ldots, \mathcal{N}(t, x)\}$ 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 $\Lambda_t$

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

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

Therefore

$$
\Lambda_t \cap (\{x\} \cap \mathbb{R}^N) = \{(x, \Xi_t(y, U^{in}(y))) \mid F_t(y) = x\}
$$

$$
\Rightarrow \#(\Lambda_t \cap (\{x\} \cap \mathbb{R}^N)) \leq \mathcal{N}(t, x)
$$

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

$$
\mathcal{N}(t, x) = n \text{ for all } (t, x) \in O_n \Rightarrow
$$

$$
\Lambda \cap (O_n \times \mathbb{R}^N) = \bigcup_{j=1}^{n}\{(t, x, \Xi_t(y_j(t, x), U^{in}(y_j(t, x))) \mid (t, x) \in O_n\}
$$
Example of $\Lambda_t$: free dynamics of cubic lagrangian

Free flow $H(x, \xi) = \frac{1}{2} \xi^2$ in space dimension $N = 1$

initial profile $U^{\text{in}}$ 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)

\[ \int_{B(0,2R)} J_t(y) dy = \int_{\mathbb{R}^N} \#(F_t^{-1}(\{x\}) \cap (\overline{B(0,2R)})) dx \]

\[ \geq \int_{B(0,R)} \#(F_t^{-1}(\{x\}) \cap (\overline{B(0,2R)})) dx \]

\[ = \int_{B(0,R)} \mathcal{N}(t,x) dx \]

By Bienaymé-Chebyshiev’s inequality

\[ \mathcal{L}^N(\{x \in \overline{B(0,R)} \text{ s.t. } \mathcal{N}(t,x) \geq n\}) \leq \frac{1}{n} \int_{B(0,2R)} J_t(y) dy \]
By the estimate on the gradient $|D\Phi_t|$ of the Hamiltonian flow

$$\left|D_x X_t(y, U_{in}(y))\right| \leq e^{\kappa|t|}, \quad \left|D_\xi X_t(y, U_{in}(y))\right| \leq (e^{\kappa|t|} - 1)$$

so that, by Hadamard’s inequality

$$J_t(y) = \left|\det(D_x X_t(y, U_{in}(y)) + D_\xi X_t(y, U_{in}(y))DU_{in}(y))\right| \leq (e^{\kappa|t|} + (e^{\kappa|t|} - 1)|DU_{in}(y)|)^N$$

Therefore

$$\mathcal{L}^N(\{x \in \overline{B(0, R)} \text{ s.t. } \mathcal{N}(t, x) \geq n\}) \leq \frac{e^{\kappa N|t|}}{n} \left\|1 + |DU_{in}|\right\|_{L^N(\overline{B(0, R)})}^N$$
Proof of (c): consider the map

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

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

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

with

\[ \begin{align*}
V(t, y) &= \nabla_\xi H(\Phi_t(y, U^{in}(y))) \\
M(t, y) &= D_x X_t(y, U^{in}(y)) + D_\xi X_t(y, U^{in}(y)) D U^{in}(y).
\end{align*} \]

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

$$K_m := F^{-1}(\overline{B(0, m)})$$

$$K'_m := \{ y \in \mathbb{R}^N \mid \text{there exists } t \in [-T, T] \text{ s.t. } (t, y) \in K_m \}$$

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

$$\|VV^T + MM^T\|_{L^{N/2}(K_m)}^{N/2} \leq 2^{N/2-1} \|V\|_{L^{\infty}(K_m)}^N \mathcal{L}^{N+1}(K_m)$$

$$+ 2^{N/2} T \|M\|_{L^N(K'_m)}^N < \infty$$
By the co-area formula (Maly-Swanson-Ziemer ’02), for each $m > 0$

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

In particular, for each $m > 0$

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

so that

$$
\mathcal{H}^1(F^{-1}(\{x\})) < \infty \quad \text{for a.e. } x \in \mathbb{R}^N
$$
Proof of (a): using the bound on the counting function in Thm B

\[ \mathcal{L}^N(\{x \text{ s.t. } |x| \leq R \text{ and } N(t, x) = \infty\}) = 0 \]

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 \( Z_t := J^{-1}_t(\{0\}) \), define a positive measurable function \( b \) by the formula

\[ b(y) = \frac{\rho^{in}(y)}{J_t(y)} \text{ if } y \in P_t, \quad \text{and } b(y) = 0 \text{ if } y \notin P_t \]
Therefore

\[
\langle \mu(t), \chi \rangle = \int \chi(F_t(y), \Xi_t(y, U^{in}(y))) b(y) J_t(y) dy
\]

\[
= \int \left( \sum_{y \in F_t^{-1}(\{x\})} b(y) \psi(x, \Xi_t(y, U^{in}(y))) \right) dx
\]

\[
= \int \left( \sum_{y \in F_t^{-1}(\{x\})} b(y) \langle \delta_{\Xi_t(y, U^{in}(y))}, \psi(x, \cdot) \rangle \right) dx
\]

by the area formula, so that

\[
\mu(t, x, \cdot) = \sum_{y \in F_t^{-1}(\{x\})} b(y) \delta_{\Xi_t(y, U^{in}(y))}
\]
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 $L_{loc}^{N,1}$ gradient.

In the complement of the caustic fiber, a Lebesgue-negligible 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.