HAMILTONIAN EVOLUTION OF MONOKINETIC MEASURES WITH ROUGH MOMENTUM PROFILE

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ABSTRACT. Consider in the phase space $\mathbf{R}_x^N \times \mathbf{R}_\xi^N$ a probability density carried by the graph of a vector field U^{in} on $\mathbf{R}^N$, i.e. a Radon measure of the form $\mu^{in} = \rho^{in}(x)\delta(\xi - U^{in}(x))$. Let Φ_t be a Hamiltonian flow on $\mathbf{R}_N \times \mathbf{R}^N$. In this paper, we study the structure of the transported measure $\mu(t) := \Phi_t \# \mu^{in}$ and of its integral in the ξ variable denoted $\rho(t)$. In particular, we (a) provide estimates on the number of folds in $\operatorname{supp}(\mu(t)) = \Phi_t($ graph of $U^{in})$, (b) establish a decomposition of $\mu(t)$ into a "regular" component whose integral in the ξ variable is absolutely continuous with respect to the Lebesgue measure $\mathscr{L}^N$, (c) discuss the possibility of atoms for the measure $\rho(t)$ and (d) construct an example in which $\rho(t)$ is singular with respect to $\mathscr{L}^N$ and diffuse. We conclude our study by explaining how our results can be applied to the classical limit of the Schrödinger equation by using the formalism of Wigner measures. Our results hold for initial momentum profiles U^{in} less regular than C^1, for which the usual notion of caustic is not relevant. The proofs of these results is based on the area formula of geometric measure theory.

1. INTRODUCTION

The subject of this article is the propagation of a certain class of positive Radon measures by Hamiltonian flows.

Let $H \equiv H(x, \xi)$ be a Hamiltonian of class C^2 on $T^*\mathbf{R}^N = \mathbf{R}_x^N \times \mathbf{R}_\xi^N$. Assume that the system of Hamilton's equations

$$\left\{\begin{aligned} \dot{X}_t &= \nabla_\xi H(X_t, \Xi_t)\,, \qquad & X_0(x,\xi) &= x\,, \\ \dot{\Xi}_t &= -\nabla_x H(X_t, \Xi_t)\,, \qquad & \Xi_0(x,\xi) &= \xi\,, \end{aligned}\right. \tag{1}$$

generates a global flow

$$\Phi_t(x,\xi) = (X_t(x,\xi), \Xi_t(x,\xi))\,. \tag{2}$$

Let μ^{in} be a monokinetic measure on $\mathbf{R}_x^N \times \mathbf{R}_\xi^N$ i.e. a Radon measure of the form

$$\mu^{in}(x,\xi) = \rho^{in}(x)\delta_{U^{in}(x)}(\xi) \tag{3}$$

where U^{in} is a vector field on $\mathbf{R}^N$ and $\rho^{in} \in L^1(\mathbf{R}^N)$. Define

$$\mu(t) = \Phi_t \# \mu^{in} \tag{4}$$

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the push-forward of μ^{in} under Φ_t. Equivalently, $\mu(t) \in C_b(\mathbf{R}_+; w - \mathcal{M}(\mathbf{R}^N \times \mathbf{R}^N))$ is the unique weak solution of the Liouville equation

$$\left\{\begin{aligned} &\partial_t \mu + \{H, \mu\} = 0\,, \\ &\mu\big|_{t=0} = \mu^{in}\,, \end{aligned}\right. \tag{5}$$

where $\{\cdot,\cdot\}$ designates the Poisson bracket

$$\{f, g\} = \nabla_\xi f \cdot \nabla_x g - \nabla_x f \cdot \nabla_\xi g\,.$$

Our purpose is to study the structure of $\mu(t)$ and to deduce from it some information on its support

$$\operatorname{supp}(\mu(t)) \subset \Lambda_t := \Phi_t(\{(y, U^{in}(y)) \,|\, y \in \mathbf{R}^N\})\,.$$

While Λ_t is the image under Φ_t of the graph of U^{in}, it is not in general the graph of a vector field on $\mathbf{R}^N$ for all values of t.

When $U^{in} = \nabla S^{in}$ is a smooth gradient field on $\mathbf{R}^N$, then Λ_t is the union of graphs of $x \mapsto \nabla_x S_j(t, x)$, where S_j is a solution of the Hamilton-Jacobi equation

$$\partial_t S(t, x) + H(x, \nabla_x S(t, x)) = 0 \tag{6}$$

defined on some open set of $\mathbf{R}_t \times \mathbf{R}^N$. The graphs of $\nabla_x S_j$ are glued along submanifolds of Λ_t where the restriction of the canonical projection

$$\Pi : T^*\mathbf{R}^N = \mathbf{R}^N_x \times \mathbf{R}^N_\xi \ni (x, \xi) \mapsto x \in \mathbf{R}^N$$

is not smooth: see §8 in [5] and §46-47 in [6]. A natural question is to compute, or at least estimate, the number of solutions S_j of the Hamilton-Jacobi equation needed to obtain Λ_t.

Equivalently, the restriction to Λ_t of the canonical projection Π is in general not one-to-one for all t. The question above reduces to estimating the number $\mathcal{N}(t, x)$ of points in Λ_t whose image under Π is x. Thus, the function $\mathcal{N}$ describes the number of folds in Λ_t induced by the Hamiltonian dynamics Φ_t on the graph of U^{in} — even when U^{in} is not a gradient field.

Another natural question is to study the structure of the push-forward $\rho(t)$ of $\mu(t)$ under the canonical projection Π — equivalently, of the first marginal of the measure $\mu(t)$ in the product space $\mathbf{R}^N_x \times \mathbf{R}^N_\xi$. As we shall see, both questions are intimately related.

The mathematical problem described above appears in a great variety of contexts. It appeared first in the theory of geometric optics, in the works of Fermat and Huygens: see for instance chapter VII in [15], chapter III in [11] and chapter 12 §2 in [13]. It appears in the classical limit of quantum mechanics: see for instance chapter VII in [16] or [25]— we shall give more details on this case below.

In both examples above, the fact that U^{in} is a gradient field is important. There are however other types of physical models leading to the same mathematical problem even when U^{in} is not a gradient field. Indeed, the Maxwell distribution with density ρ, bulk velocity U and temperature θ, i.e.

$$\frac{\rho(x)}{(2\pi\theta)^{N/2}} e^{-|\xi - U(x)|^2/2\theta}$$

converges weakly to the monokinetic measure $\rho(x)\delta_{U(x)}(\xi)$ as $\theta \to 0^+$. The propagation of this class of measures by the flow Φ_t generated by the free Hamiltonian $H(x, \xi) := \frac{1}{2}|\xi|^2$, i.e. $\Phi_t(x, \xi) = (x + t\xi, \xi)$ can be viewed as the kinetic theory of pressureless gases, and appears for instance in a cosmological model due to Zeldovich [27, 9, 8, 7]. When U^{in} is a gradient field, the Liouville equation (5) can therefore be viewed as a kinetic formulation of the Hamilton-Jacobi equation (6).

While the classical mathematical theory of geometric optics or of the semi-classical limit of quantum mechanics is centered on the geometry of Λ_t in the case where both the Hamiltonian H and $U^{in} = \nabla S^{in}$ are smooth, our approach of the mathematical problem stated above is centered on the propagation of the monokinetic measure $\rho(x)\delta_{U^{in}(x)}(\xi)$ by the Hamiltonian flow. Besides, our analysis on the propagation problem is focussed on mathematical methods and results in which the initial momentum profile U^{in} is not required to be everywhere differentiable — so that Λ_t is not even a C^1-manifold. Likewise, the Hamiltonian nature of the dynamics is of limited importance in our analysis, and there is no need for the momentum profile U^{in} to be a gradient — or, equivalently, for Λ_t to be a Lagrangian submanifold of $T^*\mathbf{R}^N$.

However, we assume that the vector field generating the dynamics is at least of class C^1 — or equivalently that the Hamiltonian H is at least of class C^2 on $\mathbf{R}^N_x \times \mathbf{R}^N_\xi$ — so that the existence, uniqueness and regularity of the flow Φ_t results from the classical Cauchy-Lipschitz theory. The classical limit of quantum dynamics with rough potentials, for which the existence and uniqueness of the classical Hamiltonian flow does not follow from the Cauchy-Lipschitz theory, has been recently studied in [2]. Our viewpoint in the present paper is different and in some sense complementary: we focus our attention to the special class of monokinetic measures and to their propagation by smooth Hamiltonian flows, but obtain detailed information on the structure of the propagated measure $\mu(t)$ even for rough initial momentum profiles U^{in}.

The outline of the paper is as follows. In section 2 are gathered our assumptions on the Hamiltonian H with some elementary estimates on the flow Φ_t that are crucial in the sequel. Section 3 is focussed on the problem of estimating the number of folds in the support Λ_t of the propagated measure $\mu(t)$, while the structure of $\mu(t)$ itself is studied in section 5. Section 4 gathers together a few examples showing that the results in section 3 are sharp. In section 6, we study different exceptional sets that appear naturally in connection with the structure of the projected measure $\rho(t) := \Pi\#\mu(t)$, and explain how these sets are related to the traditional notion of "caustic" — introduced by Tschirnhaus in the 17th century in the context of geometric optics). Section 7 discusses various applications of the theory presented in sections 3-5, with an emphasis on the classical limit of quantum mechanics.

2. On the Hamiltonian flow

Let $H \equiv H(x, \xi) \in \mathbf{R}$ be a C^2 function on $\mathbf{R}^N \times \mathbf{R}^N$ satisfying the following assumptions: there exists $\kappa > 0$, and a function $h \in C(\mathbf{R}; \mathbf{R}_+)$ that is sublinear at infinity, i.e.

$$\frac{h(r)}{r} \to 0 \quad \text{as } r \to +\infty$$

such that

$$\begin{aligned} &|\nabla_\xi H(x,\xi)| \le \kappa(1 + |\xi|) \\ &|\nabla_x H(x,\xi)| \le h(|x|) + \kappa|\xi| \\ &|\nabla^2 H(x,\xi)| \le \kappa \end{aligned} \tag{7}$$

for all $(x,\xi)\in\mathbf{R}^N\times\mathbf{R}^N$.

Lemma 2.1. *Any Hamiltonian $H\in C^2(\mathbf{R}^N\times\mathbf{R}^N)$ satisfying (7) generates a global Hamiltonian flow Φ_t on $\mathbf{R}^N\times\mathbf{R}^N$. The map*

$$\mathbf{R}\times\mathbf{R}^N\times\mathbf{R}^N\ni(t,x,\xi)\mapsto\Phi_t(x,\xi)\in\mathbf{R}^N\times\mathbf{R}^N$$

is of class C^1. Moreover, for each $\eta>0$, there exists $C_\eta>0$ such that

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

for each $x,\xi\in\mathbf{R}^N$, and

$$|D\Phi_t(x,\xi)-\mathrm{Id}_{\mathbf{R}^N\times\mathbf{R}^N}|\le e^{\kappa|t|}-1$$

for all $t\in\mathbf{R}$.

Proof. By (7), one has the following a priori estimates, with the notation (2).

First

$$|X_t(x,\xi)-x|\le\int_0^t|\nabla_\xi H(\Phi_s(x,\xi))|ds\le\kappa t+\kappa\int_0^t|\Xi_s(x,\xi)|ds$$

and

$$\begin{aligned}|\Xi_t(x,\xi)|&\le|\xi|+\int_0^t|\nabla_x H(\Phi_s(x,\xi))|ds\\&\le|\xi|+\kappa\int_0^t|\Xi_s(x,\xi)|ds+\int_0^t h(X_s(x,\xi))ds\,.\end{aligned}$$

By Gronwall's inequality, for all $0\le s\le t$

$$|\Xi_s(x,\xi)|\le\left(|\xi|+\int_0^t h(X_\tau(x,\xi))d\tau\right)e^{\kappa s}\,,\tag{8}$$

so that

$$\begin{aligned}|X_t(x,\xi)-x|&\le\kappa t+\kappa\int_0^t e^{\kappa s}ds\left(|\xi|+\int_0^t h(X_\tau(x,\xi))d\tau\right)\\&\le\kappa t+e^{\kappa t}\left(|\xi|+\int_0^t h(X_\tau(x,\xi))d\tau\right)\,.\end{aligned}$$

Since h is sublinear at infinity, we have, for every $R>0$

$$h(r)\le\mathbf{1}_{[0,R]}(r)\sup_{0\le r\le R}h(r)+\mathbf{1}_{(R,+\infty)}(r)r\sup_{r>R}\frac{h(r)}{r}\eta\le M_R+rm_R\,,\tag{9}$$

where

$$M_R=\sup_{0\le r\le R}h(r)\quad\text{ and }m_R=\sup_{r>R}\frac{h(r)}{r}\,,$$

so that

$$m_R\to0\quad\text{ as }R\to+\infty\,.$$

Therefore

$$\begin{aligned}|X_t(x,\xi)-x|&\le(\kappa+M_Re^{\kappa t})t+e^{\kappa t}|\xi|+m_Re^{\kappa t}\int_0^t|X_s(x,\xi)|ds\\&\le(\kappa+M_Re^{\kappa t})t+e^{\kappa t}|\xi|+m_Re^{\kappa t}|x|+m_Re^{\kappa t}\int_0^t|X_s(x,\xi)-x|ds\,.\end{aligned}$$

By Gronwall's inequality,
(10)
$$|X_t(x,\xi)-x| \le ((\kappa+M_Re^{\kappa t})t+e^{\kappa t}|\xi|+m_Re^{\kappa t}|x|)e^{tm_Re^{\kappa t}}$$
$$\le \kappa te^{tm_Re^{\kappa t}}+M_Rte^{t(\kappa+m_Re^{\kappa t})}+|\xi|e^{t(\kappa+m_Re^{\kappa t})}+m_R|x|e^{t(\kappa+m_Re^{\kappa t})}\,.$$

The same estimates hold for $-T\le t\le 0$ after substituting $|t|$ to t.

In view of (10)-(8), for each $(x,\xi)\in\mathbf{R}^N\times\mathbf{R}^N$, the trajectory $(x,\xi)\mapsto\Phi_t(x,\xi)$ cannot escape to infinity in finite time, and is therefore globally defined.

Besides, since $m_R\to 0$ as $R\to+\infty$, the estimate (10) obviously implies the first inequality in the lemma with

$$\eta := m_Re^{T(\kappa+m_Re^{\kappa T})} \quad \text{ and } C_\eta := (1+\kappa T+M_RT)e^{T(\kappa+m_Re^{\kappa T})}\,.$$

Since $H\in C^2(\mathbf{R}^N\times\mathbf{R}^N)$, the map $(t,x,\xi)\mapsto\Phi_t(x,\xi)$ is of class C^1 on its domain of definition $\mathbf{R}\times\mathbf{R}^N\times\mathbf{R}^N$. Differentiating the Hamilton equations (1) with respect to the initial condition, one finds that

$$\begin{cases} \dot{DX_t} = +\nabla^2_{x,\xi}H(\Phi_t)\cdot DX_t+\nabla^2_{\xi,\xi}H(\Phi_t)\cdot D\Xi_t\,,\\ \dot{D\Xi_t} = -\nabla^2_{x,x}H(\Phi_t)\cdot DX_t-\nabla^2_{x,\xi}H(\Phi_t)\cdot D\Xi_t\,,\end{cases}$$

so that

$$|D\Phi_t-\mathrm{Id}_{\mathbf{R}^N\times\mathbf{R}^N}|\le\kappa\int_0^{|t|}|D\Phi_s|ds\,.$$

The second inequality in the lemma follows from Gronwall's inequality. □

3. On the number of folds in Λ_t

Let $U^{in}\in C(\mathbf{R}^N;\mathbf{R}^N)$ satisfy the condition

$$\frac{|U^{in}(y)|}{|y|}\to 0 \quad \text{ as } |y|\to 0\,. \tag{11}$$

The present section is focussed on the structure of the set Λ_t in the introduction, defined as

$$\Lambda_t := \Phi_t(\{(y,U^{in}(y))\,|\,y\in\mathbf{R}^N\})\,,\quad t\in\mathbf{R}\,. \tag{12}$$

Consider the map

$$F_t:\,\mathbf{R}^N\ni y\mapsto F_t(y)=X_t(y,U^{in}(y))\in\mathbf{R}^N\,. \tag{13}$$

Whenever U^{in} is differentiable at y, the map F_t is also differentiable at y by the chain rule; for any such y, define absolute value of the Jacobian determinant

$$J_t(y)=|\det(DF_t(y))|\,. \tag{14}$$

We also introduce the set

$$\begin{aligned} C &:= \{(t,x)\in\mathbf{R}\times\mathbf{R}^N\,|\,F_t^{-1}(\{x\})\cap J_t^{-1}(\{0\})\neq\varnothing\}\,,\\ C_t &:= \{x\in\mathbf{R}^N\,|\,(t,x)\in C\}\,.\end{aligned} \tag{15}$$

For want of a better terminology and by analogy with geometric optics, C will be referred to as the "caustic" set.

Proposition 3.1. *Under the conditions above, for each $t \in \mathbf{R}$, the map F_t is proper and onto. Moreover*

$$\sup_{|t|\le T} \frac{|F_t(y)-y|}{|y|} \to 0 \quad \text{as } |y| \to \infty\,. \tag{16}$$

The proof of this proposition and the next one will use the following topological argument.

Lemma 3.2. *Let $g : \mathbf{R}^N \to \mathbf{R}^N$ be a continuous map satisfying the following condition: for some $R > 0$*

$$(g(x)|x) > 0 \quad \text{for all } x \in \mathbf{R}^N \text{ such that } |x| = R\,.$$

Then
a) there exists $x \in \mathbf{R}^N$ such that $|x| \le R$ and $g(x) = 0$;
b) if g is of class C^1 on $\mathbf{R}^N$ and 0 is a regular value of g, then $g^{-1}(\{0\}) \cap B(0,R)$ is finite and $\#(g^{-1}(\{0\}) \cap B(0,R))$ is odd.

Proof. Consider the homotopy $G \in C([0,1] \times \mathbf{R}^N; \mathbf{R}^N)$ defined by

$$G(t,x) = tx + (1-t)g(x)\,.$$

One has

$$G(t,x) \ne 0 \quad \text{whenever } t \in [0,1] \text{ and } |x| = R\,.$$

Indeed, $G(1,x) = x \ne 0$ if $|x| = R > 0$; besides, if $t \in [0,1[$ and $G(t,x) = 0$, one has

$$g(x) = -\frac{t}{1-t}x \quad \text{so that } (g(x)|x) = -\frac{t}{1-t}|x|^2 = -\frac{t}{1-t}R^2 < 0$$

for all $x \in \mathbf{R}^N$ such that $|x| = R$, which contradicts our assumption.

By the homotopy invariance of the degree (see Properties 7, 8 and Theorem 12.7 in chapter 12, §A of [24])

$$d(g, B(0,R), 0) = d(I, B(0,R), 0) = 1\,.$$

This implies a). Moreover, if g is of class C^1 on $\mathbf{R}^N$ and 0 is a regular value of g, all the elements of $g^{-1}(\{0\})$ are isolated points by the implicit function theorem, so $g^{-1}(\{0\}) \cap \overline{B(0,R)}$ is finite. Besides (see Property 2 in chapter 12, §A of [24])

$$d(g, B(0,R), 0) = \sum_{x \in g^{-1}(\{0\}) \cap B(0,R)} \operatorname{sign}(\det Dg(x)) = 1\,.$$

Therefore, there exists an integer $m \in \mathbf{N}$ such that

$$\#\{x \in B(0,R) \,|\, g(x) = 0 \text{ and } \det(Dg(x)) > 0\} = m+1$$
$$\#\{x \in B(0,R) \,|\, g(x) = 0 \text{ and } \det(Dg(x)) < 0\} = m$$

so that $\#(g^{-1}(\{0\}) \cap B(0,R)) = 2m+1$, which proves b). □

Proof of Proposition 3.1. By the first inequality in Lemma 2.1 and the condition (11 on U^{in}, for each $\eta > 0$, one has

$$\varlimsup_{|y|\to+\infty} \sup_{|t|\le T} \frac{|F_t(y)-y|}{|y|} \le \eta\,,$$

so that (16) holds.

Because of (16), the continuous map F_t satisfies

$$(F_t(y) - x|y) = |y|^2 + o(|y|^2) \quad \text{as } |y| \to +\infty \tag{17}$$

so that F_t is onto by applying Lemma 3.2 to the map $g : y \mapsto F_t(y) - x$. On the other hand

$$|F_t(y)| \to +\infty \quad \text{ as } |y| \to +\infty$$

so that F_t is proper. □

By Proposition 3.1, we know that, for each $(t, x) \in \mathbf{R} \times \mathbf{R}^N$, the equation $F_t(y) = x$ has at least one solution $y \in \mathbf{R}^N$ when U^{in} is a continuous vector field sublinear at infinity, i.e. satisfying (11). In the next proposition, we study the number $\mathcal{N}(t, x)$ of solutions of this equation in the case where U^{in} is of class C^1 at least. Equivalently, $\mathcal{N}(t, x)$ is the number of intersections of the manifold Λ_t with $T_x^*\mathbf{R}^N \simeq \{x\}\times\mathbf{R}^N$. Therefore, the integer-valued function $\mathcal{N}$ measures the number of folds in the manifold Λ_t resulting from the interaction of the Hamiltonian flow Φ_t with the initial profile U^{in}.

Proposition 3.3. *[Smooth case] Assume that (11) holds for $U^{in} \in C^1(\mathbf{R}^N, \mathbf{R}^N)$ and that*

$$|DU^{in}(y)| = O(1) \quad \text{ as } |y| \to +\infty\,.$$

a) For each $t \in \mathbf{R}$, one has $\mathscr{L}^N(C_t) = 0$.
b) The set C is closed in $\mathbf{R} \times \mathbf{R}^N$.
c) For each $(t, x) \in \mathbf{R} \times \mathbf{R}^N \setminus C$, the set $F_t^{-1}(\{x\})$ is finite, and henceforth denoted by

$$\{y_j(t, x)\,,\ j = 1, \ldots, \mathcal{N}(t, x)\}\,.$$

The integer $\mathcal{N}$ is a constant function of (t, x) in each connected component of $\mathbf{R} \times \mathbf{R}^N \setminus C$ and, for each $j \geq 1$, the map y_j is of class C^1 on each connected component of $\mathbf{R} \times \mathbf{R}^N \setminus C$ where $\mathcal{N} \geq j$.
d) There exists $a < 0 < b$ such that $C\cap((a, b)\times\mathbf{R}^N) = \varnothing$ and $\mathcal{N} = 1$ on $(a, b)\times\mathbf{R}^N$.
e) $\mathcal{N}(t, x)$ is odd for each $(t, x) \in \mathbf{R} \times \mathbf{R}^N \setminus C$.

Proof. If $U^{in} \in C^1(\mathbf{R}^N)$, the map F_t is of class C^1 from $\mathbf{R}^N$ to $\mathbf{R}^N$, being the composition of C^1 maps. Since C_t is the set of critical values of F_t, one has $\mathscr{L}^N(C_t) = 0$ by Sard's Theorem (in the equal dimension case), which proves a).

Pick any sequence $(t_n, x_n) \in C$ such that $(t_n, x_n) \to (t, x)$ in $\mathbf{R}\times\mathbf{R}^N$ as $n \to \infty$. By definition of C, there exists y_n such that $F_{t_n}(y_n) = x_n$. Since the sequences t_n and x_n converge, they are both bounded. Let $T = \sup_n |t_n|$; assume that the sequence y_n is unbounded; if so there exists a subsequence y_{n_l} such that $|y_{n_l}| \to \infty$. By (16)

$$|x_{n_l} - y_{n_l}| = |F_{t_{n_l}}(y_{n_l}) - y_{n_l}| \leq \sup_{|t|\leq T} |F_t(y_{n_l}) - y_{n_l}| = o(|y_{n_l}|)$$

so that $|x_{n_l}| \sim |y_{n_l}|$ as $n_l \to +\infty$. Since this contradicts the fact that the sequence x_n is bounded, we conclude that the sequence y_n is bounded. Therefore, there exists a convergent subsequence y_{n_k} of y_n; call y its limit as $n_k \to +\infty$. Passing to the limit in both relations

$$F_{t_{n_k}}(y_{n_k}) = x_{n_k} \quad \text{ and } J_{t_{n_k}}(y_{n_k}) = |\det(\nabla F_{t_{n_k}}(y_{n_k}))| = 0\,,$$

we conclude that (t, x, y) satisfies

$$F_t(y) = x \quad \text{ and } J_t(y) = 0$$

and therefore that $(t, x) \in C$, which proves b).

For $(t,x) \in \mathbf{R}\times\mathbf{R}^N \setminus C$, all the solutions of the equation $F_t(y) - x = 0$ are isolated by the implicit function theorem. The set of all such points, $F_t^{-1}(\{x\})$, is therefore compact since F_t is proper. By the implicit function theorem, the integer $\mathcal{N}$ is a locally constant function of $(t,x) \in \mathbf{R}\times\mathbf{R}^N \setminus C$, and is therefore constant on each connected component of $\mathbf{R}\times\mathbf{R}^N \setminus C$. Let $j \in \mathbf{N}^*$, and let Ω be a connected component of $\mathbf{R}\times\mathbf{R}^N \setminus C$; by the implicit function theorem $y_j \in C^1(\Omega)$. This proves c).

Assume $\inf\{t > 0 \,|\, C_t \neq \varnothing\} = 0$. Then, there exists (t_n, x_n, y_n) such that

$$t_n \to 0^+\,, \quad F_{t_n}(y_n) = x_n\,, \qquad \text{and } J_{t_n}(y_n) = 0\,.$$

Assume that a subsequence y_{n_k} of the sequence y_n is bounded. Up to extraction of a subsequence, one can assume that $y_{n_k} \to y$, so that $0 = J_{t_{n_k}}(y_{n_k}) \to J_0(y)$. But since $F_t = \mathrm{Id}_{\mathbf{R}^N}$, one has $J_0(y) = 1$. Therefore $|y_n| \to +\infty$. By the second inequality in Lemma 2.1

$$\begin{aligned}
&|D_x X_{t_n}(y_n, U^{in}(y_n)) - \mathrm{Id}_{\mathbf{R}^N}| \le e^{\kappa|t_n|} - 1\,,\\
&|D_\xi X_{t_n}(y_n, U^{in}(y_n)) \cdot DU^{in}(y_n)| = O\left(e^{\kappa|t_n|} - 1\right)\,,
\end{aligned}$$

so that

$$\begin{aligned}
0 = J_{t_n}(y_n) &= |\det(D_x X_{t_n}(y_n, U^{in}(y_n)) + D_\xi X_{t_n}(y_n, U^{in}(y_n)) \cdot DU^{in}(y_n))|\\
&\to |\det(\mathrm{Id}_{\mathbf{R}^N})| = 1 \qquad \text{as } n \to \infty\,.
\end{aligned}$$

Thus the assumption $t_n \to 0$ leads to a contradiction. Therefore,

$$\inf\{t > 0 \,|\, C_t \neq \varnothing\} = b > 0\,.$$

By the same token,

$$\sup\{t < 0 \,|\, C_t \neq \varnothing\} = a < 0\,.$$

Thus $(a,b)\times\mathbf{R}^N$ is contained in the connected component of $\{0\}\times\mathbf{R}^N$ in $\mathbf{R}\times\mathbf{R}^N\setminus C$. Since $F_0 = \mathrm{Id}_{\mathbf{R}^N}$, one has $\mathcal{N}(0,x) = 1$ for all $x \in \mathbf{R}^N$, and since $\mathcal{N}$ is constant on each connected component of $\mathbf{R}\times\mathbf{R}^N \setminus C$, one concludes $\mathcal{N} = 1$ on $(a,b)\times\mathbf{R}^N$, which proves d).

If $(t,x) \in \mathbf{R}\times\mathbf{R}^N \setminus C$, the point x is a regular value of F_t. Since F_t is proper, $F_t^{-1}(\{x\})$ is compact, and therefore bounded. Pick $R > 0$ such that

$$F_t^{-1}(\{x\}) \subset B(0,R)\,.$$

By (17) and Lemma 3.2 b) applied to the map $g:\, y \mapsto F_t(y) - x$

$$\#F_t^{-1}(\{x\}) = \#(F_t^{-1}(\{x\}) \cap B(0,R)) \text{ is odd}\,,$$

which proves e). $\square$

When U^{in} is not of class C^1, the arguments used to prove Proposition 3.3 are no longer valid. However one can still obtain some information on the number $\mathcal{N}(t,x)$ of solutions y of the equation $F_t(y) = x$ by a completely different method, involving the area — or co-area formula.

Assume that $U^{in} \in C(\mathbf{R}^N;\mathbf{R}^N)$ satisfies (11) and that its gradient (in the sense of distributions) DU^{in} satisfies the condition

$$\partial_l U_k^{in}\big|_\Omega \in L^{N,1}(\Omega) \text{ for each bounded open } \Omega \subset \mathbf{R}^N\,, \tag{18}$$

for all $k, l = 1, \ldots, N$. We recall that a measurable function $f : \Omega \to \mathbf{R}$ belongs to the Lorentz space $L^{N,1}(\Omega)$ if

$$\int_0^\infty \left(\mathscr{L}^N(\{x \in \Omega \,|\, |f(x)| \geq \lambda\})\right)^{1/N} d\lambda < \infty\,.$$

By Theorem B in [14], the vector field U^{in} is differentiable a.e. on $\mathbf{R}^N$. Let E be the $\mathscr{L}^N$-negligible set defined as

$$E := \{y \in \mathbf{R}^N \,|\, U^{in} \text{ is not differentiable at } y\}\,. \tag{19}$$

By the chain rule, the absolute value of the Jacobian determinant

$$\begin{aligned} J_t(y) = |\det(D_x X_t(y, U^{in}(y)) + D_\xi X_t(y, U^{in}(y)) DU^{in}(y))| \\ \text{is defined for all } (t, y) \in \mathbf{R} \times (\mathbf{R}^N \setminus E)\,. \end{aligned} \tag{20}$$

Henceforth, the notation $J_t^{-1}(\{0\})$ designates the set

$$J_t^{-1}(\{0\}) := \{y \in \mathbf{R}^N \setminus E \,|\, J_t(y) = 0\}\,, \tag{21}$$

and we shall also consider the set

$$Z_t := J_t^{-1}(\{0\}) \cup E\,. \tag{22}$$

Theorem 3.4. *[Rough case] Assume that $U^{in} \in C(\mathbf{R}^N; \mathbf{R}^N)$ satisfies (11) and (18).*
a) for all $t \in \mathbf{R}$, the function $J_t \in L^1_{loc}(\mathbf{R}^N)$;
b) for all $t \in \mathbf{R}$, there are finitely many solutions y of the equation

$$F_t(y) = x \tag{23}$$

for a.e. $x \in \mathbf{R}^N$ — in other words, $\mathcal{N}(t, x)$ is finite for a.e. $x \in \mathbf{R}^N$, for all $t \in \mathbf{R}$;
c) for each bounded $B \subset \mathbf{R}^N$, denote by $\mathcal{N}_B(t, x)$ the number of solutions $y \in B$ of (23); then, whenever B is bounded, for each $t \in \mathbf{R}$ and each $n \in \mathbf{N}$, one has

$$\begin{aligned} \mathscr{L}^N\left(\{x \in \mathbf{R}^N \,|\, \mathcal{N}_B(t, x) \geq n\}\right) &\leq \frac{1}{n}\int_B J_t(y)dy \\ &\leq \frac{1}{n} e^{N\kappa|t|} \|1 + (1 - e^{-\kappa|t|})\|DU^{in}\|^N_{L^N(B)}\,; \end{aligned}$$

d) let $t \in \mathbf{R}$; then for a.e. $x \in \mathbf{R}^N$, all solutions y of (23) satisfy

$$y \in \mathbf{R}^N \setminus E \text{ and } J_t(y) > 0\,;$$

e) for all $T > 0$

$$\mathscr{H}^1(\{(t, y) \in [-T, T] \times \mathbf{R}^N \,|\, F_t(y) = x\}) < +\infty$$

for a.e. $x \in \mathbf{R}^N$.

Remarks.
a) By the first statement in Proposition 3.1, $\mathcal{N}(t, x) = \mathcal{N}_{\mathbf{R}^N}(t, x) \geq 1$ for all $(t, x) \in \mathbf{R} \times \mathbf{R}^N$.
b) Even in the smooth case, i.e. assuming in addition that $U^{in} \in C^1(\mathbf{R}^N)$, statement c) in Theorem 3.4 provides information on the number of folds of Λ_t, that is the image under Φ_t of the graph of U^{in}, which seems to be new at the time of this writing.

Proof. By the second estimate in Lemma 2.1

$$|D_xX_t(y,U^{in}(y))+D_\xi X_t(y,U^{in}(y))\cdot DU^{in}(y)|\le e^{\kappa|t|}+(e^{\kappa|t|}-1)|DU^{in}(y)| \tag{24}$$

so that

$$\begin{aligned}J_t(y)&=|\det(D_xX_t(y,U^{in}(y))+D_\xi X_t(y,U^{in}(y))\cdot DU^{in}(y))|\\&\le e^{N\kappa|t|}(1+(1-e^{-\kappa|t|})|DU^{in}(y)|)^N\end{aligned} \tag{25}$$

by Hadamard's inequality. Since U^{in} satisfies (18) and since $L^{N,1}(\Omega)\subset L^N(\Omega)$, this inequality implies statement a).

Since the map F_t is proper by Proposition 3.1, the set $K_{t,R}=F_t^{-1}(\overline{B(0,R)})$ is compact for each $R>0$. By the area formula (see Theorem 3.4 in [20] and Theorem A in [14])

$$\int_{\mathbf{R}^N}\#(F_t^{-1}(\{x\})\cap K_{t,R})dx=\int_{K_{t,R}}J_t(y)dy<+\infty\,.$$

Therefore $\#F_t^{-1}(\{x\})<\infty$ for a.e. $x\in\overline{B(0,R)}$; since this is true for all $R\in\mathbf{N}$, one concludes that $\#F_t^{-1}(\{x\})<\infty$ for a.e. $x\in\mathbf{R}^N$, so that b) holds.

Let B be a measurable subset of $\mathbf{R}^N$; applying again the area formula shows that

$$\int_{\mathbf{R}^N}\mathcal{N}_B(t,x)dx=\int_B J_t(y)dy\,.$$

By the Bienaymé-Chebyshev inequality, for each $n\ge1$

$$\mathscr{L}^N\left(\{x\in\mathbf{R}^N\,|\,\mathcal{N}_B(t,x)\ge n\}\right)\le\frac{1}{n}\int_B J_t(y)dy\,,$$

which is precisely the first inequality in c). The second inequality follows from (25) and Hölder's inequality.

Let $n=1$ and $Z_t:=J_t^{-1}(\{0\})\cup E$. Let $B=Z_t\cap K_{t,R}$; the set B is measurable and bounded. Then

$$\int_B J_t(y)dy=0$$

since $J_t(y)=0$ for all $y\in B\setminus E$ and $\mathscr{L}^N(E)=0$. Applying c) shows that

$$\mathscr{L}^N(\{x\in\mathbf{R}^N\,|\,|x|\le R\text{ and }\mathcal{N}_{Z_t}(t,x)\ge1\})=0\,,$$

which entails d) by monotone convergence, letting $R\in\mathbf{N}$ tend to infinity.

Consider next the continuous map

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

In view of (16), $|F(t,y)|\to\infty$ as $|y|\to+\infty$ uniformly in $t\in[-T,T]$. Therefore, the set $K_R:=F^{-1}(\overline{B(0,R)})$ is compact for each $R>0$. Then, for each $t\in[-T,T]$ and each $y\in\mathbf{R}^N\setminus E$, the Jacobian $DF(t,y)$ is the column-wise partitioned matrix

$$DF(t,y)=[V(t,y)\,,\,M(t,y)]\,,$$

with

$$V(t,y)=\nabla_\xi H(\Phi_t(y,U^{in}(y)))$$

and

$$M(t,y):=D_xX_t(y,U^{in}(y))+D_\xi X_t(y,U^{in}(y))DU^{in}(y)\,.$$

Therefore,

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

so that, by the co-area formula (Theorem 1.3 in [21])

$$\begin{aligned}\int_{\mathbf{R}^N} &\mathscr{H}^1(F^{-1}(\{x\}) \cap K_R)dx \\ &= \int_{K_R} \sqrt{\det(V(t,y)V(t,y)^T + M(t,y)M(t,y)^T)}dtdy\,.\end{aligned}$$

By Lemma 2.1, $(t,x,\xi) \mapsto \Phi_t(x,\xi)$ is of class C^1 on $\mathbf{R}\times\mathbf{R}^N\times\mathbf{R}^N$, so that the map $(t,y) \mapsto V(t,y)$ is continuous on $\mathbf{R}\times\mathbf{R}^N$, and therefore bounded on the compact K_R. On the other hand, by (24)

$$\sup_{|t|\le T} |M(t,y)| \le e^{\kappa T} + (e^{\kappa T}-1)|DU^{in}(y)| \in L^N_{loc}(\mathbf{R}^N)\,,$$

since U^{in} satisfies (18). Denoting

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

that is compact in $\mathbf{R}^N$ (being the projection of the compact K_R on the second factor in $\mathbf{R}\times\mathbf{R}^N$), one has

$$\begin{aligned}\|VV^T + MM^T\|^{N/2}_{L^{N/2}(K_R)} &\le 2^{N/2-1}\|V\|^N_{L^\infty(K_R)}\mathscr{L}^{N+1}(K_R) + 2^{N/2}T\|M\|^N_{L^N(K'_R)} \\ &< \infty\,.\end{aligned}$$

Therefore $\mathscr{H}^1(F^{-1}(\{x\})\cap K_R) < +\infty$ is finite for a.e. $x \in \overline{B(0,R)}$, and since this is true for all $R \in \mathbf{N}$, one concludes that $\mathscr{H}^1(F^{-1}(\{x\})) < +\infty$ for a.e. $x \in \mathbf{R}^N$, which is statement e). □

Theorem 3.4 suggests considering the sets

$$C'_t = \{x \in \mathbf{R}^N \mid F_t^{-1}(\{x\}) \text{ is infinite}\} \tag{26}$$

for all $t \in \mathbf{R}$.

On the other hand, the definition of the caustic (15) in the smooth case should be modified as follows when the continuous vector field U^{in} is not of class C^1 but satisfies (11) and (18):

$$\begin{aligned} C_t &:= \{x \in \mathbf{R}^N \mid F_t^{-1}(\{x\}) \cap Z_t \neq \varnothing\}\,, \\ C &:= \bigcup_{t\in\mathbf{R}} C_t\,, \end{aligned} \tag{27}$$

where Z_t is defined in (22). Notice that this definition coincides with (15) whenever U^{in} is differentiable everywhere. However we do not know whether C or C_t are closed whenever U^{in} is not of class C^1.

The first part of statement c) in Proposition 3.3 is equivalent to the inclusion

$$C'_t \subset C_t \qquad \text{for all } t \in \mathbf{R}\,. \tag{28}$$

Statements b) and d) in Theorem 3.4 can be recast as follows

$$\mathscr{L}^N(C'_t) = 0 \text{ and } \mathscr{L}^N(C_t) = 0\,, \qquad \text{for all } t \in \mathbf{R}\,. \tag{29}$$

This is the analogue of statement a) in Proposition 3.3 in the case of a rough U^{in}. Notice that (29) is a consequence of the area formula while statement a) in Proposition 3.3 follows from Sard's theorem (see Remark 2.97 on pp. 103–104 in [3], discussing the relation between Sard's theorem and the co-area formula).

4. Some examples

While the notion of caustic C naturally occurs in studying the geometry of Λ_t in the smooth case, its relation to the number of solutions y of the equation $F_t(y) = x$ is slightly less obvious, as shown by the following examples. In all these examples, the Hamiltonian is

$$H(x, \xi) = \tfrac{1}{2}\xi^2$$

generating the free flow

$$\Phi_t : \mathbf{R} \times \mathbf{R} \ni (x, \xi) \mapsto (x + t\xi, \xi) \in \mathbf{R} \times \mathbf{R}\,.$$

Thus

$$F_t : \mathbf{R} \ni y \mapsto y + tU^{in}(y) \in \mathbf{R}\,.$$

The first example below shows that the set $F_t^{-1}(\{x\})$ may be finite even if $x \in C_t$. In other words, it may happen that the inclusion (28) is strict for all $t \in \mathbf{R}$.

Example 1. Set $N = 1$, and let U^{in} be real analytic on $\mathbf{R}$ and satisfy (11). Therefore F_t is real analytic on $\mathbf{R}$ for each $t \in \mathbf{R}$. For each $x \in \mathbf{R}$, the set $F_t^{-1}(\{x\})$ is the set of zeros of the analytic function $y \mapsto F_t(y) - x$. Since U^{in} satisfies (11), one has $F_t(y) \sim y$ as $|y| \to \infty$, so that, for each $t \in \mathbf{R}$, the function F_t is not a constant. Therefore the zeros of $y \mapsto F_t(y) - x$ are isolated for each $(t, x) \in \mathbf{R} \times \mathbf{R}$. Equivalently, the set $F_t^{-1}(\{x\})$ consists of isolated points. On the other hand, for each $(t, x) \in \mathbf{R}^2$, the set $F_t^{-1}(\{x\})$ is compact since F_t is proper by Proposition 3.1. Therefore the set $F_t^{-1}(\{x\})$ is finite for all $(t, x) \in \mathbf{R}^2$.

The next example shows that the set $F_t^{-1}(\{x\})$ may be infinite for infinitely many times t — in this case, for all t in a nonempty, open interval of $\mathbf{R}$.

Example 2. Set $N = 1$, and let U^{in} be defined by

$$U^{in}(z) := \begin{cases} \tanh(z)\sin(\ln|z|) & \text{if } z > 0\,, \\ 0 & \text{if } z = 0\,. \end{cases}$$

Clearly $U^{in} \in C^1(\mathbf{R}^*)$ and, for all $z \in \mathbf{R}^*$, one has

$$(U^{in})'(z) = (1 - \tanh^2(z))\sin(\ln|z|) + \frac{\tanh(z)}{z}\cos(\ln|z|)\,.$$

Observe that $(U^{in})'(z) = \sqrt{2}\sin(\ln|z| + \frac{\pi}{4}) + O(z^2)$ does not have a limit for $z \to 0$, so that $U^{in} \notin C^1(\mathbf{R})$. On the other hand

$$\sup_{z \in \mathbf{R}} |U^{in}(z)| = 1 \quad \text{and} \quad \sup_{z \neq 0} |(U^{in})'(z)| \leq 2$$

so that U^{in} is Lipschitz continuous on $\mathbf{R}$ and the map F_t is proper on $\mathbf{R}$.

Let $x = 0$; for each t such that $|t| > 1$, the set $F_t^{-1}(\{0\})$ is infinite.

Indeed, the set $F_t^{-1}(\{0\})$ obviously contains $z = 0$; besides, $F_t^{-1}(\{0\})$ contains also a decreasing sequence $y_n \to 0$ as $n \to +\infty$, which satisfies

$$\sin(\ln|y_n|) \to -1/t \qquad \text{as } n \to \infty\,.$$

Therefore $F_t^{-1}(\{0\})$ is countably infinite whenever $|t| > 1$.

Notice that, in example 2, whenever $T > 1$

$$\{(t, y) \in [-T, T] \times \mathbf{R} \,|\, F_t(y) = 0\} = ([-T, -1] \cup [1, T]) \times (\{0\} \cup \{y_n \,|\, n \geq 1\})$$

so that

$$\mathscr{H}^1(\{(t, y) \in [-T, T] \times \mathbf{R} \,|\, F_t(y) = 0\}) = +\infty\,.$$

In other words, the set of points x for which

$$\mathscr{H}^1(\{(t,y) \in [-T,T] \times \mathbf{R} \,|\, F_t(y) = x\}) = +\infty\,,$$

while $\mathscr{L}^1$-negligible by statement e) of Theorem 3.4, may be non empty.

There is another interesting observation in connection with Example 2. Observe that $0 \in C_t'$ and that

$$F_t^{-1}(\{0\}) = \{0\} \cup \{y_n \,|\, n \geq 1\}\,, \qquad \text{whenever } |t| > 1\,.$$

Nevertheless, for each $n \geq 1$

$$(U^{in})'(y_n) = \sin(\ln|y_n|) + \cos(\ln|y_n|) + O(|y_n|^2) \to -\frac{1}{t} + \sqrt{1 - \frac{1}{t^2}} \neq -\frac{1}{t}$$

if $|t| > 1$, and F_t is not differentiable at $y = 0$. Thus $y = 0$ is in the exceptional set E where the Lipschitz continuous function U^{in} is not differentiable, so that $0 \in C_t$ with the definition (27) although

$$F_t^{-1}(\{0\}) \cap J_t^{-1}(\{0\}) = \varnothing\,,$$

so that 0 would not belong to C_t had we kept the classical definition (15) in the case of non everywhere differentiable U^{in} profiles.

The next two examples show that $F_t^{-1}(\{x\})$ can even be uncountably infinite, even for a smooth profile U^{in}.

Example 3. Set $N = 1$, and let U^{in} be defined by

$$U^{in}(z) := \begin{cases} +1 & \text{if } z < -1\,, \\ -z & \text{if } |z| \leq 1\,, \\ -1 & \text{if } z > 1\,. \end{cases}$$

Consider the equation

$$F_t(y) := y + tU^{in}(y) = x$$

with unknown y; for $t < 1$, its solution is unique and given by

$$y = \begin{cases} x - t & \text{if } x < t - 1\,, \\ \dfrac{x}{1-t} & \text{if } |x| \leq 1 - t\,, \\ x + t & \text{if } x > 1 - t\,. \end{cases}$$

For $t = 1$, the solution is

$$y = \begin{cases} x - t & \text{if } x < 0\,, \\ \text{any } y \in [-1,1] & \text{if } x = 0\,, \\ x + 1 & \text{if } x > 0\,. \end{cases}$$

For $t > 1$, the solution is

$$y = \begin{cases} x - t & \text{if } x < 1 - t\,, \\ x - t\,,\ \dfrac{x}{1-t} \text{ and } x + t & \text{if } 1 - t \leq x \leq t - 1\,, \\ x + t & \text{if } x > t - 1\,. \end{cases}$$

Now $F_t^{-1}(\{x\})$ is finite for all $x \in \mathbf{R}$ whenever $t \neq 1$, while $F_1^{-1}(\{0\}) = [-1,1]$.

Example 4. In the previous example, U^{in} is Lipschitz continuous but not of class C^1. Yet the same phenomenon can be observed by smoothing U^{in} near $z = \pm 1$. Regularize U^{in} and obtain $U^{in}_\epsilon \in C^\infty(\mathbf{R})$ so that

$$\operatorname{supp}(U^{in}_\epsilon - U^{in}) \subset [-1-\epsilon, -1+\epsilon] \cup [1-\epsilon, 1+\epsilon]\,, \quad \text{and}$$
$$U^{in}_\epsilon \le U^{in} \text{ on } [-1-\epsilon, -1+\epsilon] \text{ and } U^{in} \le U^{in}_\epsilon \text{ on } [1-\epsilon, 1+\epsilon]\,.$$

In that case

$$F_1^{-1}(\{0\}) = [-1+\epsilon, 1-\epsilon]\,.$$

Indeed, since $U^{in}_\epsilon \le U^{in}$ on $[-1-\epsilon, -1+\epsilon]$, all the points on the graph of U^{in}_ϵ with abscissa in $(-1-\epsilon, -1+\epsilon)$ will reach $x = 0$ after $t = 1$. The same is true of the points on the graph of U^{in}_ϵ with abscissa in $(1-\epsilon, 1+\epsilon)$. Thus the regularization does not affect the dynamics of the points with abscissa in $(-1+\epsilon, 1-\epsilon)$ for all $t \in [0, 1]$, and in particular for $t = 1$.

5. On the structure of $\mu(t)$

Throughout this section, we assume that $U^{in} \in C(\mathbf{R}^N; \mathbf{R}^N)$ satisfies the sublinearity condition (11) at infinity and the regularity condition (18).

Consider a monokinetic measure μ^{in} of the form (3) with $\rho^{in} \in L^1(\mathbf{R}^N)$, whose action on a test function $\chi \in C_b(\mathbf{R}^N \times \mathbf{R}^N)$ is given by the formula

$$\langle \mu^{in}, \chi \rangle := \int_{\mathbf{R}^N} \chi(y, U^{in}(y)) \rho^{in}(y) dy\,.$$

In other words

$$\mu^{in} = \mathscr{L}^N_x \otimes \rho^{in}(x) \delta^{in}_{U^{in}(x)}\,.$$

Let $H \in C^2(\mathbf{R}^N \times \mathbf{R}^N)$ satisfy (7), and let Φ_t be the Hamiltonian flow generated by H.

For all $t \in \mathbf{R}$, let $\mu(t) = \Phi_t \# \mu^{in}$ be the push-forward of μ^{in} under Φ_t, defined as follows: for each test function $\chi \in C_b(\mathbf{R}^N \times \mathbf{R}^N)$,

$$\langle \mu(t), \chi \rangle := \langle \mu^{in}, \chi \circ \Phi_t \rangle = \int_{\mathbf{R}^N} \chi(\Phi_t(y, U^{in}(y))) \rho^{in}(y) dy\,. \tag{30}$$

Finally, let $\rho(t)$ be the measure on $\mathbf{R}^N$ defined as

$$\rho(t) := \Pi \# \mu(t) \tag{31}$$

where $\Pi : T^*\mathbf{R}^N \simeq \mathbf{R}^N \times \mathbf{R}^N \ni (x, \xi) \mapsto x \in \mathbf{R}^N$ is the canonical projection. In other words, for each test function $\phi \in C_b(\mathbf{R}^N)$

$$\langle \rho(t), \phi \rangle = \int_{\mathbf{R}^N} \phi(X_t(y, U^{in}(y))) \rho^{in}(y) dy \tag{32}$$

or, equivalently

$$\rho(t) = F_t \# \rho^{in}\,. \tag{33}$$

We shall also use the following definition

$$P_t := \{y \in \mathbf{R}^N \setminus E \,|\, J_t(y) > 0\}\,. \tag{34}$$

Our main result in this section bears on the structure of the measures $\mu(t)$ and its projection $\rho(t)$.

Theorem 5.1. *Under the assumptions above, let $\rho^{in} \in L^1(\mathbf{R}^N)$ be such that $\rho^{in} \geq 0$ a.e. on $\mathbf{R}^N$.*
a) for each $t \in \mathbf{R}$,

$$\rho^{in}\mathbf{1}_{P_t}\mathscr{L}^N \ll J_t\mathscr{L}^N\,, \qquad \textit{and } \rho^{in}\mathbf{1}_{Z_t}\mathscr{L}^N \perp J_t\mathscr{L}^N$$

b) for each $t \in \mathbf{R}$,

$$\mu(t) = \mu_a(t) + \mu_s(t) \qquad \textit{with } \mu_a(t) \perp \mu_s(t)\,,$$

where

$$\begin{cases} \mu_a(t) := \mathscr{L}^N_x \otimes \displaystyle\sum_{y \in F_t^{-1}(\{x\})} \frac{\rho^{in}\mathbf{1}_{P_t}}{J_t}(y)\delta_{\Xi_t(y,U^{in}(y))}\,, \\ \mu_s(t) := \Phi_t\#(\mathscr{L}^N_x \otimes \rho^{in}(x)\mathbf{1}_{Z_t}(x)\delta_{U^{in}(x)})\,. \end{cases}$$

Moreover
c) for each $t \in \mathbf{R}$, one has

$$\operatorname{supp}(\mu(t)) \subset \Lambda_t := \Phi_t(\{(y, U^{in}(y))\,|\, y \in \mathbf{R}^N\})\,;$$

d) for each $t \in \mathbf{R}$, the measure

$$\rho_a(t) := \Pi\#\mu_a(t) \ll \mathscr{L}^N\,;$$

with

$$\frac{d\rho_a(t)}{d\mathscr{L}^N}(x) = \mathbf{1}_{\mathbf{R}^N \setminus C'_t}(x) \sum_{y \in F_t^{-1}(\{x\})} \frac{d(\rho^{in}\mathbf{1}_{P_t}\mathscr{L}^N)}{d(J_t\mathscr{L}^N)}(y)$$

where C'_t is defined in (26);
e) for each $t \in \mathbf{R}$, the measure

$$\rho_s(t) := \Pi_{\#}\mu_s(t) \textit{ is carried by } C_t\,;$$

in particular

$$\rho_a(t) \perp \rho_s(t)\,.$$

A few remarks are in order before we give the proof of Theorem 5.1. In the smooth case — i.e. whenever $U^{in} \in C^1(\mathbf{R}^N; \mathbf{R}^N)$ and satisfies (11), we recall that C_t is closed in $\mathbf{R}^N$ for each $t \in \mathbf{R}$, by statement b) of Proposition 3.3. For any given $t \in \mathbf{R}$, let $\chi \equiv \chi(x, \xi)$ be a test function in $C_c(\mathbf{R}^N \times \mathbf{R}^N)$ such that $\Pi\operatorname{supp}(\chi) \cap C_t = \varnothing$. By (30)

$$\langle \mu(t), \chi \rangle = \int_{\mathbf{R}^N} \chi(\Phi_t(y, U^{in}(y)))\rho^{in}(y)dy\,.$$

Since $\Pi(\operatorname{supp}(\chi))$ is compact and included in the open set $\mathbf{R}^N \setminus C_t$, it intersects at most finitely many connected components of $\mathbf{R}^N \setminus C_t$. Assume without loss of generality that $\Pi(\operatorname{supp}(\chi))$ is connected, so that it intersect exactly one connected component Ω of $\mathbf{R}^N \setminus C_t$; on Ω, the integer-valued function $\mathscr{N}$ is a constant denoted by $\mathscr{N}^\Omega$, by statement c) of Proposition 3.3. With the notation used in that proposition, for each $x \in \Pi(\operatorname{supp}(\chi)) \subset \Omega$

$$F_t^{-1}(\{x\}) = \{y_j(t,x)\,|\, j = 1, \ldots, \mathscr{N}^\Omega\}\,,$$

and

$$y_j(t, \cdot) \in C^1(\Omega) \text{ for all } j = 1, \ldots, \mathscr{N}^\Omega\,.$$

Therefore $y_j(t,\cdot)$ is a C^1-diffeomorphism from Ω on its image O_j, with inverse F_t. Thus

$$F_t^{-1}(\Omega)=\bigcup_{j=1}^{\mathcal{N}^\Omega}O_j\quad\text{ and }O_i\cap O_j=\varnothing\text{ if }i\neq j\,,$$

so that

$$\iint_{\Omega\times\mathbf{R}^N}\chi(t,x)\mu(t,dxd\xi)=\sum_{j=1}^{\mathcal{N}^\Omega}\int_{O_j}\chi(F_t(y),\Xi_t(y,U^{in}(y)))\rho^{in}(y)dy\,.$$

In each of the integrals on the right hand side, F_t is a C^1-diffeomorphism mapping O_j on Ω, so that, changing variables, we see that

$$\begin{aligned}\int_{O_j}&\chi(F_t(y),\Xi_t(y,U^{in}(y)))\rho^{in}(y)dy\\&=\int_\Omega\chi(x,\Xi_t(y_j(t,x),U^{in}(y_j(t,x))))\rho^{in}(y_j(t,x))\,|\det(\nabla_x y_j(t,x))|\,dx\,.\end{aligned}$$

Since

$$|\det(D_xy_j(t,x))|=J_t(y_j(t,x))^{-1}\,,$$

we conclude that the restriction of $\mu(t)$ to $(\mathbf{R}\times\mathbf{R}^N)\setminus C$ is a measure-valued function of (t,x) given by the following formula:

$$\mu(t,x,\cdot):=\sum_{j=1}^{\mathcal{N}(t,x)}\frac{\rho^{in}(y_j(t,x)}{J_t(y_j(t,x))}\delta_{\Xi_t(y_j(t,x),U^{in}(y_j(t,x)))}\tag{35}$$

whenever $(t,x)\notin C$. This formula is strikingly similar to the one giving $\mu_a(t)$ in statement b) of Theorem 5.1. There are however subtle differences, which we shall discuss in more detail in the next section. At this point, it suffices to say that Theorem 5.1 provides a formula for $\mu(t)$ that holds globally on $\mathbf{R}^N\times\mathbf{R}^N$ instead of $(\mathbf{R}^N\setminus C_t)\times\mathbf{R}^N$, and that the argument above requires more regularity on U^{in} than assumed in Theorem 5.1.

Proof of Theorem 5.1. Let $A\subset\mathbf{R}^N$; then the condition

$$\int_A J_t(y)dy=0\text{ implies that }J_t(y)=0\text{ for a.e. }y\in A\,.$$

Therefore $\mathscr{L}^N(P_t\cap A)=0$ so that

$$\int_A(\rho^{in}\mathbf{1}_{P_t})(y)dy=\int_{P_t\cap A}\rho^{in}(y)dy=0\,.$$

Thus $\rho^{in}\mathbf{1}_{P_t}\mathscr{L}^N\ll J_t\mathscr{L}^N$.

On the other hand, for each $t\in\mathbf{R}$

$$\mathbf{R}^N=P_t\cup Z_t\quad\text{ with }P_t\cap Z_t=\varnothing\,.$$

Since

$$J_t(y)=0\text{ for }y\in Z_t\setminus E\quad\text{i.e. }\mathscr{L}^N\text{-a.e. on }Z_t$$

while

$$\rho^{in}(y)\mathbf{1}_{Z_t}(y)=0\quad\text{ for all }y\in P_t\,,$$

we conclude that $\rho^{in}\mathbf{1}_{Z_t}\mathscr{L}^N\perp J_t\mathscr{L}^N$, which proves a).

Define

$$\mu_a^{in} := \mathscr{L}_x^N \otimes (\rho^{in}\mathbf{1}_{P_t})(x)\delta^{in}_{U^{in}(x)}\,,$$
$$\mu_s^{in} := \mathscr{L}_x^N \otimes (\rho^{in}\mathbf{1}_{Z_t})(x)\delta^{in}_{U^{in}(x)}\,,$$

and, for each $t \in \mathbf{R}$

$$\mu_a(t) := \Phi_t\#\mu_a^{in}\,, \quad \mu_s(t) := \Phi_t\#\mu_s^{in}\,,$$

so that one has indeed

$$\mu_a(t) + \mu_s(t) = \Phi_t\#(\mu_a^{in} + \mu_s^{in}) = \Phi_t\#\mu^{in} = \mu(t)\,.$$

Then there exists a unique $b \in L^1(\mathbf{R}^N; J_t\mathscr{L}^N)$ such that

$$\rho^{in}\mathbf{1}_{P_t}\mathscr{L}^N = bJ_t\mathscr{L}^N$$

by the Radon-Nikodym theorem. Thus, for each $\chi \in C_c(\mathbf{R}^N \times \mathbf{R}^N)$, by the area formula (see Theorem 3.4 in [20] and Theorem A in [14])

$$\begin{aligned}\langle \mu_a(t), \chi\rangle &= \int_{\mathbf{R}^N} \chi(F_t(y), \Xi_t(y, U^{in}(y)))b(y)J_t(y)dy\\ &= \int_{\mathbf{R}^N}\left(\sum_{y\in F_t^{-1}(\{x\})} b(y)\chi(x, \Xi_t(y, U^{in}(y)))\right)dx\\ &= \int_{\mathbf{R}^N}\left(\sum_{y\in F_t^{-1}(\{x\})} b(y)\langle\delta_{\Xi_t(y,U^{in}(y))}, \chi(x,\cdot)\rangle\right)dx\,.\end{aligned}$$

In the formula above

$$b := \frac{d(\rho^{in}\mathbf{1}_{P_t}\mathscr{L}^N)}{d(J_t\mathscr{L}^N)}$$

is the Radon-Nikodym derivative of $\rho^{in}\mathbf{1}_{P_t}$ with respect to $J_t\mathscr{L}^N$. Since $J_t > 0$ on the set P_t

$$b = \frac{\rho^{in}\mathbf{1}_{P_t}}{J_t} \text{ a.e. on } \mathbf{R}^N\,, \tag{36}$$

which proves b).

Formula (3) obviously implies that

$$\operatorname{supp}(\mu^{in}) \subset \Lambda_0 := \{(y, U^{in}) \,|\, y \in \mathbf{R}^N\}\,.$$

Since $\mu(t) = \Phi_t\#\mu^{in}$, one has

$$\operatorname{supp}(\mu(t)) \subset \Phi_t(\{(y, U^{in}) \,|\, y \in \mathbf{R}^N\}) = \Lambda_t\,,$$

which is precisely statement c).

In view of the first formula in b) and of the definition $\rho_a(t) = \Pi\#\mu_a(t)$ of the measure $\rho_a(t)$, one has

$$\rho_a(t) = \left(\sum_{y\in F_t^{-1}(\{x\})} b(y)\right)\mathscr{L}^N\,,$$

with b as in (36). The set $F_t^{-1}(\{x\})$ can obviously be infinite, in which case the sum above can be undefined. However, this occurs only if $x \in C_t'$ as defined in (26). Since C_t' is $\mathscr{L}^N$-negligible

$$\rho_a(t) = f_t\mathscr{L}^N$$

with

$$f_t(x) := \mathbf{1}_{\mathbf{R}^N \setminus C'_t}(x) \left(\sum_{y \in F_t^{-1}(\{x\})} b(y) \right).$$

Thus, $\rho_a(t)$ is of the form $\rho_a(t) = f_t \mathscr{L}^N$ with $f_t \geq 0$ measurable on $\mathbf{R}^N$. Besides

$$0 \leq \rho_a(t) \leq \rho(t) \quad \text{and} \quad \int_{\mathbf{R}^N} \rho(t, dx) = \int_{\mathbf{R}^N} \rho^{in}(x) dx) < \infty$$

which implies in particular that $\rho_a(t) \ll \mathscr{L}^N$ with the formula for the Radon-Nikodym derivative as in d).

Consider the measurable set $A := \mathbf{R}^N \setminus C_t$. By (33) applied to $\rho^{in} \mathbf{1}_{Z_t}$ instead of ρ^{in}, one has

$$\rho_s(t)(A) = \int_{F_t^{-1}(A)} \rho^{in}(y) \mathbf{1}_{Z_t}(y) dy = \int_{F_t^{-1}(A) \cap Z_t} \rho^{in}(y) dy = 0 .$$

Indeed, by definition of C_t, one has $F_t^{-1}(A) \cap Z_t = \varnothing$. In other words, $\rho_s(t)$ is carried by C_t.

Finally, since $\rho_a(t) \ll \mathscr{L}^N$ and $\rho_s(t)$ is carried by C_t which is $\mathscr{L}^N$-negligible by (29), we conclude that $\rho_a(t) \perp \rho_s(t)$ which is precisely statement e). $\square$

6. On the caustic and other exceptional sets

In the case of a smooth U^{in} profile — i.e. when $U^{in} \in C^1(\mathbf{R}^N; \mathbf{R}^N)$ satisfies (11), the caustic C is the only exceptional set — C_t being equivalently defined as the image under the projection Π of the set of points in the manifold Λ_t in (12) where the restriction $\Pi\big|_{\Lambda_t}$ is not differentiable.

When U^{in} is not everywhere differentiable, this definition of C_t does not make sense in general since Λ_t is not a differentiable manifold in the first place. In such cases, it is more natural to consider the measures $\mu(t)$ and $\rho(t)$ instead of the sets Λ_t and C_t — all the more so since C_t may not even be closed in $\mathbf{R}^N$. Thus, even though $\rho_s(t)$ is concentrated on C_t, one cannot say that C_t is the support of $\rho_s(t)$ as C_t may not be closed. On the other hand, the inclusion $\operatorname{supp} \rho_s(t) \subset \overline{C_t}$ is of little interest as C_t might be dense in some domain of $\mathbf{R}^N$. Although $\rho_s(t)$ is concentrated on C_t, this obviously does not characterize C_t (if a measure is concentrated on a set, it is also concentrated on the complement in that set of any negligible set for that same measure).

There are analogous difficulties with the absolutely continuous part of the measure $\rho_a(t)$. In formula (35), the restriction of $\mu_a(t)$ to $(\mathbf{R}^N \setminus C_t) \times \mathbf{R}^N$ is viewed as a function of $x \in \mathbf{R}^N \setminus C_t$ with values in the set of Radon measures in the variable $\xi \in \mathbf{R}^N$. This viewpoint is obviously not appropriate if U^{in} is not at least of class C^1 — for instance, if the set C_t is dense in some domain of $\mathbf{R}^N$. In Theorem 5.1, the measure μ is a weakly continuous function of the time variable t with values in the space of Radon measures in the variables (x, ξ), and is therefore globally defined on $\mathbf{R}^N_x \times \mathbf{R}^N_\xi$. Obviously, the ratio $\rho^{in} \mathbf{1}_{P_t} / J_t$ is just one possible choice of the Radon-Nikodym derivative $d(\rho^{in} \mathbf{1}_{P_t} \mathscr{L}^N)/d(J_t \mathscr{L}^N)$ and could be modified arbitrarily on any set of $J_t \mathscr{L}^N$-measure 0 — which could be of positive $\mathscr{L}^N$-measure, as in Examples 3-4 above. The difference induced in the expression

$$\sum_{y\in F_t^{-1}(\{x\})}\frac{d(\rho^{in}\mathbf{1}_{P_t}\mathscr{L}^N)}{d(J_t\mathscr{L}^N)}(y)\delta_{U^{in}(y)} \tag{37}$$

by two different choices of the Radon-Nikodym derivative $d(\rho^{in}\mathbf{1}_{P_t}\mathscr{L}^N)/d(J_t\mathscr{L}^N)$ is of the form

$$\sum_{y\in F_t^{-1}(\{x\})} m(y)\delta_{U^{in}(y)}$$

with $m\geq 0$ being a $J_t\mathscr{L}^N$-measurable function such that $m=0$ a.e. on $\mathbf{R}^N\setminus Z_t$. Therefore

$$\int_{\mathbf{R}^N} m(y)J_t(y)dy = 0 = \int_{\mathbf{R}^N}\left(\sum_{y\in F_t^{-1}(\{x\})}|m(y)|\right)dx$$

so that

$$\sum_{y\in F_t^{-1}(\{x\})} m(y) = 0 \quad \mathscr{L}^N-\text{a.e. on } \mathbf{R}^N$$

and

$$\mathscr{L}^N\otimes\sum_{y\in F_t^{-1}(\{x\})} m(y)\delta_{U^{in}(y)} = 0$$

as a measure on $\mathbf{R}^N\times\mathbf{R}^N$.

On the other hand, even in the smooth case, formula (35) is not enough to define completely $\mu(t)$, as it fails to capture singular parts of the measure carried by $C_t\times\mathbf{R}^N$. For instance, in Example 4, for $t=1$, if one computes the restriction of the measure $\mu(1)$ to $(\mathbf{R}^N\setminus C_1)\times\mathbf{R}^N$ by formula (35), one obtains

$$\begin{aligned}\int_{\mathbf{R}^N\setminus C_1}\left(\int_{\mathbf{R}^N}\mu(t,x,d\xi)\right)dx &= \int_{-\infty}^{-1+\epsilon}\rho^{in}(y)dy+\int_{1-\epsilon}^{+\infty}\rho^{in}(y)dy\\ &\neq\int_{\mathbf{R}^N}\rho^{in}(y)dy=\int_{\mathbf{R}^N}\left(\int_{\mathbf{R}^N}\mu^{in}(x,d\xi)\right)dx\end{aligned}$$

unless $\rho^{in}=0$ on $[-1+\epsilon,1-\epsilon]=J_1^{-1}(\{0\})$. Since this is obviously incompatible with the conservation of the total mass of the measure

$$\iint_{\mathbf{R}^N\times\mathbf{R}^N}\mu(t,dxd\xi)=\iint_{\mathbf{R}^N\times\mathbf{R}^N}\Phi_t\#\mu^{in}(dxd\xi)=\iint_{\mathbf{R}^N\times\mathbf{R}^N}\mu^{in}(dxd\xi)$$

by the transportation under the flow Φ_t, this example confirms that (35) alone is not enough to compute $\mu(t)$.

The expression involved in the formula for μ_a in Theorem 5.1, i.e.

$$\sum_{y\in F_t^{-1}(\{x\})}\frac{\rho^{in}\mathbf{1}_{P_t}}{J_t}(y)\delta_{U^{in}(y)} \tag{38}$$

which is analogous to formula (35) a priori makes sense only if $x\in\mathbf{R}^N\setminus C'_t$. In the rough case, i.e. if U^{in} satisfies only the regularity properties in Theorem 3.4 or Theorem 5.1, it might on principle happen that

$$C'_t\cap(\mathbf{R}^N\setminus C_t)\neq\varnothing\,.$$

Whenever this is the case, the sum in formula (38) above may fail to be defined everywhere on $\mathbf{R}^N\setminus C_t$, as would occur for U^{in} of class C^1, by statement c) in

Proposition 3.3, or (28). Since this may occur at most on a $\mathscr{L}^N$-negligible set, the expression for μ_a in Theorem 5.1 is well defined as a measure on $\mathbf{R}^N \times \mathbf{R}^N$ while the one in (38) may not be defined everywhere on $\mathbf{R}^N \setminus C_t$ as a function of x with values in the space of measures in the variable $\xi \in \mathbf{R}^N$.

Another strategy is to abandon the idea of viewing the caustic C as an exceptional set unambiguously defined by the measure $\rho(t)$, and to investigate those exceptional sets that can be uniquely defined in terms of this measure.

This leads for instance to consider the set

$$C''_t := \{x \in \mathbf{R}^N \mid \mathscr{L}^N(F_t^{-1}(\{x\}) \cap J_t^{-1}(\{0\}) > 0\}\,, \tag{39}$$

which is of particular interest, as shown by the following result.

Theorem 6.1. *Assume that $H \in C^2(\mathbf{R}^N \times \mathbf{R}^N)$ satisfies the conditions (7), while $U^{in} \in C(\mathbf{R}^N; \mathbf{R}^N)$ satisfies the sublinearity condition (11) at infinity and the regularity condition (18). Then*

a) $C''_t \subset C_t \cap C'_t$ for each $t \in \mathbf{R}$;
b) for each $t \in \mathbf{R}$ and each $x \in C''_t$, there exists $\rho^{in} \in L^1(\mathbf{R}^N)$ such that $\rho^{in} \geq 0$ a.e. and the projected measure $\rho(t) = \Pi\#\mu(t)$ satisfies

$$\rho(t)(\{x\}) > 0\,;$$

c) C''_t is at most countable for each $t \in \mathbf{R}$;
d) if $\rho^{in} \in L^1(\mathbf{R}^N)$ is such that $\rho^n \geq 0$ a.e. on $\mathbf{R}^N$ and $\rho^{in} = 0$ a.e. on $J_t^{-1}(\mathbf{R}^*_+)$ while $\|\rho^{in}\|_{L^1(\mathbf{R}^N)} > 0$, then

$$\rho(t)(\{x\}) > 0 \quad \text{if and only if } (\rho^{in}\mathscr{L}^N)(F_t^{-1}(\{x\}) \cap J_t^{-1}(\{0\}))) > 0\,.$$

Proof. If $x \in C''_t$, then $\mathscr{L}^N(F_t^{-1}(\{x\}) \cap J_t^{-1}(\{0\}) > 0$ so that in particular the intersection $F_t^{-1}(\{x\}) \cap J_t^{-1}(\{0\}$ is infinite, which implies that $x \in C_t \cap C'_t$, thereby proving a).

Let $R > 0$; since F_t is proper by Proposition 3.1, $F_t^{-1}(\overline{B(0,R)}) = K_R$ is a compact subset of $\mathbf{R}^N$. Pick $\rho^{in} = \mathbf{1}_{K_R}$; obviously $\rho^{in} \in L^1(\mathbf{R}^N)$ and $\rho^{in} \geq 0$ a.e.. Set $\mu^{in} = \mathscr{L}^N \otimes (\mathbf{1}_{K_R}\delta_{U^{in}})$, let $\mu(t) = \Phi\#\mu^{in}$ be the push-forward of μ^{in} under the Hamiltonian flow and let $\rho(t) = \Pi\#\mu(t)$ be the projected measure. As explained above $\rho(t) = F_t\#(\mathbf{1}_{K_R}\mathscr{L}^N)$ so that, whenever $x \in \overline{B(0,R)} \cap C''_t$,

$$\begin{aligned}\rho(t)(\{x\}) = (\mathbf{1}_{K_R}\mathscr{L}^N)(F_t^{-1}(\{x\})) &= \mathscr{L}^N(K_R \cap F_t^{-1}(\{x\})) \\ &= \mathscr{L}^N(F_t^{-1}(\{x\})) \\ &\geq \mathscr{L}^N(F_t^{-1}(\{x\}) \cap J_t^{-1}(\{0\})) > 0\,.\end{aligned}$$

This immediately implies both b) and c). Indeed, b) is satisfied with $\rho^{in} = \mathbf{1}_{K_R}$ for each $R > 0$ such that $x \in C''_t \cap \overline{B(0,R)}$. On the other hand, for each $R > 0$, all the points in $C''_t \cap \overline{B(0,R)}$ are atoms of the same Borel measure $F_t\#(\mathbf{1}_{K_R}\mathscr{L}^N)$ on $\mathbf{R}^N$, which implies c).

As for d), one has again $\rho(t) = F_t\#(\rho^{in}\mathscr{L}^N)$, so that

$$\begin{aligned}\rho(t)(\{x\}) = (\rho^{in}\mathscr{L}^N)(F_t^{-1}(\{x\})) &= (\rho^{in}\mathscr{L}^N)(F_t^{-1}(\{x\}) \cap E) \\ &+ (\rho^{in}\mathscr{L}^N)(F_t^{-1}(\{x\}) \cap J_t^{-1}(\{0\})) \\ &+ (\rho^{in}\mathscr{L}^N)(F_t^{-1}(\{x\}) \cap J_t^{-1}(\mathbf{R}^*_+))\end{aligned}$$

where E is the $\mathscr{L}^N$-negligible set where F_t is not differentiable. The conclusion follows from the fact that $\mathscr{L}^N(E) = 0$ and $\rho^{in} = 0$ a.e. on $J_t^{-1}(\mathbf{R}_+^*)$, so that

$$\rho(t)(\{x\}) = (\rho^{in}\mathscr{L}^N)(F_t^{-1}(\{x\}) \cap J_t^{-1}(\{0\}))$$

□

If $\rho^{in} \in L^1(\mathbf{R}^N)$ satisfies $\rho^{in} \geq 0$ a.e. on $\mathbf{R}^N$ and $\rho^{in} = 0$ a.e. on $J_t^{-1}(\mathbf{R}_+^*)$ while $\|\rho^{in}\|_{L^1(\mathbf{R}^N)} > 0$, one has $(\rho^{in}\mathscr{L}^N) \perp (J_t\mathscr{L}^N)$, so that the projected measure $\rho(t) = \Pi\#\mu(t)$ satisfies $\rho(t) \perp \mathscr{L}^N$ by statement b) in Theorem 5.1. By statement d) in Theorem 6.1, the measure $\rho(t)$ is diffuse if and only if

$$(\rho^{in}\mathscr{L}^N)(F_t^{-1}(\{x\}) \cap J_t^{-1}(\{0\}))) = 0 \text{ for all } x \in C_t\,.$$

This may indeed happen, as shown by the following example.

Example 5. Assume $N = 1$, and set $H(x, \xi) = \frac{1}{2}\xi^2$, which generates the free flow $\Phi_t : (x, \xi) \mapsto (x + t\xi, \xi)$. By regularity of the Lebesgue measure, there exists a compact set $K \subset (0, 1) \setminus \mathbf{Q}$ such that $\frac{1}{2} < \mathscr{L}^1(K) < 1$. Let $\Omega = (0, 1) \setminus K$; since Ω is open in $(0, 1)$ and contains $(0, 1) \cap \mathbf{Q}$, it is a countably infinite union of disjoint nonempty open intervals:

$$\Omega = \bigcup_{n\in\mathbf{N}} I_n\,, \quad \text{so that } \mathscr{L}^1(\Omega) = \sum_{n\in\mathbf{N}} \mathscr{L}^1(I_n)\,.$$

In particular $\lambda := \mathscr{L}^1(\Omega) > 0$ since $\mathscr{L}^1(I_n) > 0$ for each $n \in \mathbf{N}$ (indeed each I_n is an open interval that contains at least one rational). Set $t = 1$ and

$$F_1(y) := \begin{cases} y\,, & \text{if } y \leq 0\,, \\ \displaystyle\int_0^y \mathbf{1}_\Omega(z)dz\,, & \text{if } y \in (0, 1)\,, \\ \lambda + (y - 1)\,, & \text{if } y \geq 1\,. \end{cases}$$

Define

$$U^{in}(y) := F(y) - y\,.$$

The function F_1 is Lipschitz continuous on $\mathbf{R}$, being the indefinite integral of a bounded measurable function. Therefore U^{in} is also Lipschitz continuous on $\mathbf{R}$.

The function F_1 is increasing on $\mathbf{R}$ — this being obvious on $\mathbf{R}_-^*$ and on $(1, \infty)$. Indeed, if $0 < y_1 < y_2 < 1$, the interval (y_1, y_2) contains at least one rational number r, so that

$$F_1(y_2) - F_1(y_1) = \mathscr{L}^1(\Omega \cap (y_1, y_2)) > 0\,,$$

since the open set $\Omega \cap (y_1, y_2)$ contains the intersection of the connected component of r in Ω with (y_1, y_2), which is a nonempty open interval. Since $F_1(y) \to \pm\infty$ as $y \to \pm\infty$, we conclude that $F_1 : \mathbf{R} \to \mathbf{R}$ is one-to-one and onto.

By the Lebesgue differentiation theorem (Theorem 7.11 in [22]), F_1 is differentiable a.e. on $\mathbf{R}$ (in fact it is even of class C^∞ on $\mathbf{R}_-^* \cup (1, \infty)$) and $F_1'(y) = \mathbf{1}_\Omega(y)$ for a.e. $y \in (0, 1)$. Thus, denoting by E the $\mathscr{L}^1$-negligible set on which F_1 is not differentiable, one has $(F_1')^{-1}(\{0\}) \cup E = K$. Since F_1 is one-to-one and onto, $C_1 = F_1(K)$.

Let $\rho^{in}=\mathbf{1}_K$; thus $\|\rho^{in}\|_{L^1}=\mathscr{L}^1(K)>0$, so that $(\rho^{in}\mathscr{L}^1)\perp(|F_1'|\mathscr{L}^1)$. The measure $\rho(t)=\Pi\#\mu(t)$ where $\mu(t)=\Phi\#\mu^{in}$ with $\mu^{in}:=\mathscr{L}^1_x\otimes\rho^{in}(x)\delta_{U^{in}(x)}$ satisfies $\rho(1)\perp\mathscr{L}^N$ by statement b) in Theorem 5.1

$$\rho(1)(\mathbf{R})=\rho(1)(C_1)=\|\rho^{in}\|^2_{L^1}=\mathscr{L}^1(K)>0\,.$$

On the other hand, since F_1 is one-to-one and onto, for each $x\in\mathbf{R}$, one has $\#F_1^{-1}(\{x\})=1$. In particular, for each $x\in C_1=F_1(K)$, one has

$$F_1^{-1}(\{x\})\subset(F_1')^{-1}(\{0\})\quad\text{ so that }\#(F_1^{-1}(\{x\})\cap(F_1')^{-1}(\{0\}))=\#F_1^{-1}(\{x\})=1\,.$$

In particular, for each $x\in C_1$, by statement d) of Theorem 6.1, one has

$$(\rho^{in}\mathscr{L}^1)(F_1^{-1}(\{x\})\cap(F_1')^{-1}(\{0\}))=0\,,$$

so that

$$\rho(1)(\{x\})=0\,.$$

Hence $\rho(1)\perp\mathscr{L}^1$ and is diffuse, while $\rho(1)\neq0$ since $\rho(1)(C_1)>0$.

7. Application to the classical limit of quantum mechanics

In this section, we apply the results obtained above to the classical limit of the Schrödinger equation.

7.1. **The classical scaling.**

Consider the evolution Schrödinger equation

$$i\hbar\partial_t\psi=-\tfrac{1}{2}m\hbar^2\Delta_x\psi+V(x)\psi$$

for the wave function ψ of a point particle of mass m subject to the action of an external potential $V\equiv V(x)\in\mathbf{R}$.

Choosing "appropriate" units of time T and length L, we recast the Schrödinger equation in terms of dimensionless variables $\hat{t}:=t/T$ and $\hat{x}:=x/L$. We define a rescaled wave function $\hat{\psi}$ and a rescaled, dimensionless potential $\hat{V}$ by the formulas

$$\hat{\psi}(\hat{t},\hat{x}):=\psi(t,x)\quad\text{ and }\hat{V}(\hat{x}):=\frac{T^2}{mL^2}V(x)\,.$$

In these dimensionless variables, the Schrödinger equation takes the form

$$i\partial_{\hat{t}}\hat{\psi}=-\frac{\hbar T}{2mL^2}\Delta_{\hat{x}}\hat{\psi}+\frac{mL^2}{\hbar T}\hat{V}(\hat{x})\hat{\psi}\,.$$

The dimensionless number $2\pi\hbar T/mL^2$ is the ratio of the Planck constant to mL^2/T, that is (twice) the action of a classical particle of mass m moving at speed L/T on a distance L. If the scales of time T and length L have been chosen conveniently, L/T is the typical order of magnitude of the particle speed, and L is the typical length scale on which the particle motion is observed. The classical limit of quantum mechanics is defined by the scaling assumption $2\pi\hbar\ll mL^2/T$ — i.e. the typical action of the particle considered is large compared to $\hbar$. Equivalently, mL/T is the order of magnitude of the particle momentum, so that $2\pi\hbar T/mL$ is its de Broglie wavelength; the scaling assumption $2\pi\hbar T/mL\ll L$ means that the de Broglie wavelength of the particle under consideration is small compared to the observation length scale L.

Introducing the small, dimensionless parameter $\epsilon = \hbar T/mL^2$ and dropping hats in the dimensionless variables as well as on the rescaled wave function and dimensionless potential, we arrive at the following formulation for the Schrödinger equation in dimensionless variables

$$i\epsilon\partial_t\psi = -\tfrac{1}{2}\epsilon^2\Delta_x\psi + V(x)\psi\,. \tag{40}$$

The WKB ansatz postulates that, at time $t = 0$, the wave function is of the form

$$\psi(t,x) = a^{in}(x)e^{iS^{in}(x)/\hbar}\,,\quad x \in \mathbf{R}^N\,.$$

Consistently with the scaling argument above, we set

$$\hat{a}^{in}(\hat{x}) := a^{in}(x) \text{ and } \hat{S}^{in}(\hat{x}) := TS^{in}(x)/mL^2$$

— since S^{in} has the dimension of an action — so that

$$\hat{\psi}(0,\hat{x}) = \hat{a}^{in}(\hat{x})e^{i\hat{S}^{in}(\hat{x})/\epsilon}\,. \tag{41}$$

Dropping hats in the initial data as well as in the Schrödinger equation, one arrives at the following Cauchy problem for the Schrödinger equation in dimensionless variables:

$$\begin{cases} i\epsilon\partial_t\psi_\epsilon = -\tfrac{1}{2}\epsilon^2\Delta_x\psi_\epsilon + V(x)\psi_\epsilon\,, \quad x \in \mathbf{R}^N\,,\ t \in \mathbf{R}\,, \\ \psi_\epsilon(0,x) = a^{in}(x)e^{iS^{in}(x)/\epsilon}\,. \end{cases} \tag{42}$$

The problem of the classical limit of the Schrödinger equation is to describe the wave function ψ_ϵ in the limit as $\epsilon \to 0^+$.

7.2. **The WKB method.** The traditional procedure for describing the classical limit of the Schrödinger equation is the WKB method recalled below. First we recall some mathematical tools and elements of notation used in the presentation of that method.

Assume that $V \in C^\infty(\mathbf{R}^N)$ satisfies

$$\partial^\alpha V \in L^\infty(\mathbf{R}^N) \text{ for each multi-index } \alpha \in \mathbf{N}^N \tag{43}$$

and

$$\frac{V(x)}{|x|} \to 0 \text{ as } |x| \to +\infty\,. \tag{44}$$

Then the Hamiltonian

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

satisfies (7) and therefore generates a global flow

$$\mathbf{R}^N \times \mathbf{R}^N \ni (x,\xi) \mapsto (X_t(x,\xi), \Xi_t(x,\xi)) \in \mathbf{R}^N \times \mathbf{R}^N$$

by Lemma 2.1.

Assume further that

$$\sup_{x\in\mathbf{R}^N}\int_{\mathbf{R}^N}\Gamma_\eta(x-y)V^-(y)dy \to 0 \text{ as } \eta \to 0 \quad \text{if } N \geq 2 \tag{45}$$

with

$$\Gamma_\eta(z) = \begin{cases} \mathbf{1}_{[0,\eta]}(|z|)|z|^{2-N} & \text{if } N \geq 3\,, \\ \mathbf{1}_{[0,\eta]}(|z|)\ln(1/|z|) & \text{if } N = 2\,, \end{cases}$$

while

$$\sup_{x\in\mathbf{R}^N}\int_{x-1}^{x+1} V^-(y)dy < \infty \quad \text{if } N = 1\,. \tag{46}$$

Under assumptions (45)-(46), the operator $-\frac{1}{2}\epsilon^2\Delta_x + V$ has a self-adjoint extension on $L^2(\mathbf{R}^N)$ that is bounded from below.

Under assumption (43), there exists a FIO that is a parametrix for the operator

$$G_\epsilon(t) := e^{i\frac{t}{\epsilon}\left(\frac{1}{2}\epsilon^2\Delta_x - V\right)}$$

see for instance Theorem 2.1 in [17], whose main features are recalled below.

Consider the action

$$S(t,x,\xi) := \int_0^t \left(\tfrac{1}{2}|\Xi_s(x,\xi)|^2 - V(X_s(x,\xi))\right) ds \tag{47}$$

Given $T > 0$, we shall have to deal with the class of phase functions

$$\varphi \equiv \varphi(t,x,y,\eta) \in C \text{ of class } C^\infty \text{ on } [0,T)\times\mathbf{R}^N\times\mathbf{R}^N\times\mathbf{R}^N)$$

satisfying the conditions

$$\begin{cases} \varphi(t,X_t(y,\eta),y,\eta) = S(t,y,\eta)\,, \\ D_x\varphi(t,X_t(y,\eta),y,\eta) = \Xi_t(y,\eta)\,, \\ iD_x^2\varphi(t,x,y,\eta) \leq 0 \text{ is independent of } x\,, \\ \det(D_{x\eta}\varphi(t,X_t(y,\eta),y,\eta)) \neq 0 \text{ for each } (t,y,\eta)\in[0,T)\times\mathbf{R}^N\times\mathbf{R}^N\,. \end{cases} \tag{48}$$

Pick $\chi \in C_c^\infty(\mathbf{R}^N\times\mathbf{R}^N)$ and $T > 0$. Then, for any phase function φ satisfying (48) and any $n \geq 0$, there exists $A_n \equiv A_n(t,y,\eta,\epsilon) \in C_c^\infty([0,T]\times\mathbf{R}^N\times\mathbf{R}^N)[\epsilon]$ such that the FIO $G_n(t)$ with Schwartz kernel

$$G_{\epsilon,n}(t,x,y) = \int A_n(t,y,\eta,\epsilon)e^{i\varphi(t,x,y,\eta)/\epsilon}\frac{d\eta}{(2\pi\epsilon)^N}$$

satisfies

$$\sup_{0\leq t\leq T}\|(G_\epsilon(t) - G_{\epsilon,n}(t))\chi(x,-i\epsilon\partial_x)\|_{\mathcal{L}(L^2(\mathbf{R}^N))} \leq C[V,T,\chi]\epsilon^{n-2N}\,.$$

In this inequality the notation $\chi(x,-i\epsilon\partial_x)$ designates the pseudo-differential operator defined by the formula

$$\chi(x,-i\epsilon\partial_x)\phi(x) := \iint_{\mathbf{R}^N\times\mathbf{R}^N} e^{i(x-y)\cdot\eta/\epsilon}\chi(x,\eta)\phi(y)\frac{dyd\eta}{(2\pi\epsilon)^N}$$

Taking Theorem 2.1 in [17] for granted, one arrives at the following description of the classical limit of (42). It is stated without proof in Appendix 11 of [6] or as Theorem 5.1 in [4].

Let $U^{in} = \nabla S^{in}$ and let C be defined as in (15); let $\mathcal{N}(t,x)$ and $y_j(t,x)$ be defined as in Proposition 3.3 for each $(t,x)\in\mathbf{R}\times\mathbf{R}^N\setminus C$. Let $J_t(y)$ be defined as in (14).

Proposition 7.1. *Let $a^{in} \in C_c^m(\mathbf{R}^N)$ and $S^{in} \in C^{m+1}(\mathbf{R}^N)$ with $m > 6N+4$. For all $\epsilon > 0$ and all $(t,x)\in\mathbf{R}_+\times\mathbf{R}^N\setminus C$, set*

$$\Psi_\epsilon(t,x) = \sum_{j=1}^{\mathcal{N}(t,x)} \frac{a^{in}(y_j(t,x))}{J_t(y_j(t,x))^{1/2}} e^{iS_j(t,x)/\epsilon}e^{i\pi\nu_j(t,x)/2}\,, \tag{49}$$

where

$$S_j(t,x) := S^{in}(y_j(t,x)) + S(t, y_j(t,x), \nabla S^{in}(y_j(t,x))) , \quad j = 1, \ldots, \mathcal{N}(t,x)$$

$S(t,y,\xi)$ *is given by* (47) *and* $\nu_j(t,x) \in \mathbf{Z}$ *for all* $(t,x) \in \mathbf{R}_+ \times \mathbf{R}^N \setminus C$ *is constant on each connected component of* $\mathbf{R} \times \mathbf{R}^N$ *where* $j \leq \mathcal{N}$.

Then the solution ψ_ϵ *of the Cauchy problem (42) satisfies*

$$\psi_\epsilon(t,x) = \Psi_\epsilon(t,x) + R^1_\epsilon(t,x) + R^2_\epsilon(t,x) \tag{50}$$

for all $T > 0$, *where*

$$\sup_{0 \leq t \leq T} \|R^1_\epsilon\|_{L^2(B(0,R))} = O(\epsilon) \textit{ for all } R > 0$$

and

$$\sup_{(t,x) \in K} |R^2_\epsilon(t,x)| = O(\epsilon) \textit{ for each compact } K \subset \mathbf{R}_+ \times \mathbf{R}^N \setminus C$$

as $\epsilon \to 0^+$.

A self-contained proof of Proposition 7.1 based on the parametrix construction of [17] is given in Appendix A .

The integer $\nu_j(t,x)$ in (49) is defined precisely in the proof (see formula 66 below). How this integer is related to the Morse index of the path

$$[0,t] \ni s \mapsto X_s(y_j(t,x), \nabla S^{in}(y_j(t,x))),$$

is not needed in the sequel and will not be discussed here. We refer to [4] for more details concerning this point.

7.3. **The Wigner transform.** Alternately, the asymptotic limit of ψ_ϵ can also be investigated with the help of Wigner's transform [26, 18].

For each $\Psi \in L^2(\mathbf{R}^N)$, one defines the Wigner transform of Ψ at scale ϵ by the formula

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

Let us define the ϵ-Fourier transform $\mathcal{F}_\epsilon$ as follows:

$$\mathcal{F}_\epsilon \Psi(\xi) := \frac{1}{(2\pi\epsilon)^{N/2}} \int_{L^2(\mathbf{R}^N)} \Psi(x) e^{i\frac{x\xi}{\epsilon}} dx.$$

Given $b \equiv b(x,\xi)$ in the Schwartz space $\mathcal{S}(\mathbf{R}^N \times \mathbf{R}^N)$, we recall that the ϵ-pseudodifferential operator B_ϵ with Weyl symbol b is the integral operator with integral kernel

$$(x,y) \mapsto \int_{\mathbf{R}^N} b\left(\frac{x+y}{2}, \xi\right) e^{i\xi\cdot(x-y)/\epsilon} \frac{d\xi}{(2\pi\epsilon)^N}$$

Straightforward computations lead to the following identities: for each $\Psi \in \mathcal{S}(\mathbf{R}^N)$

$$\int_{\mathbf{R}^N} W_\epsilon[\Psi](x,\xi) d\xi = |\Psi(x)|^2 , \quad \int_{\mathbf{R}^N} W_\epsilon[\Psi](x,\xi) dx = |\mathcal{F}_\epsilon \Psi(\xi)|^2 . \tag{51}$$

Likewise, for each $\Psi \in L^2(\mathbf{R}^N)$ and each ϵ-pseudodifferential B_ϵ operator with Weyl symbol $b(x,\xi)$ in the Schwarts space $\mathcal{S}(\mathbf{R}^N \times \mathbf{R}^N)$, one has

$$\int_{\mathbf{R}^N} W_\epsilon[\Psi](x,\xi) b(x,\xi) dx d\xi = \langle \Psi, B_\epsilon \Psi \rangle_{L^2(\mathbf{R}^N)} . \tag{52}$$

Lemma 7.2. *Let $a^{in} \in L^2(\mathbf{R}^N)$ and $S^{in} \in W^{1,1}_{loc}(\mathbf{R}^N)$. Then*

$$W_\epsilon[a^{in} e^{iS^{in}/\epsilon}](x,\xi) \to (a^{in})^2(x)\delta(\xi - \nabla S^{in}(x)) \text{ in } \mathcal{S}'(\mathbf{R}^N \times \mathbf{R}^N)$$

as $\epsilon \to 0$.

See Example III.5 in [18].

Proposition 7.3 ([18]). *Assume that $V \in C^{1,1}(\mathbf{R}^N)$ satisfies (45)-(46)-(43)-(44). Let*

$$\mu_\epsilon(t,x,\xi) := W_\epsilon[\psi_\epsilon(t,\cdot)](x,\xi)$$

for each $\epsilon > 0$ and each $t \in \mathbf{R}$, and for a.e. $(x,\xi) \in \mathbf{R}^N \times \mathbf{R}^N$.

Then the family $\mu_\epsilon(t)$ converges in $\mathcal{S}'(\mathbf{R}^N \times \mathbf{R}^N)$ uniformly in $|t| \le T$ for each $T \ge 0$ as $\epsilon \to 0$ to the unique solution of the Liouville equation

$$\left\{\begin{array}{l} \partial_t \mu + \xi \cdot \nabla_x \mu - \nabla_x V(x) \cdot \nabla_\xi \mu = 0\,, \quad x,\xi \in \mathbf{R}^N\,,\ t \in \mathbf{R}\,, \\ \mu(0,x,\xi) := a^{in}(x)^2 \delta_{\nabla S^{in}(x)}(\xi)\,. \end{array}\right. \tag{53}$$

In particular, $\mu \in C_b(\mathbf{R}, w - \mathcal{M}(\mathbf{R}^N \times \mathbf{R}^N))$ and $\mu(t)$ is a positive Radon measure for all $t \in \mathbf{R}$ satisfying

$$\iint_{\mathbf{R}^N \times \mathbf{R}^N} \mu(t, dxd\xi) = 1$$

for each $t \in \mathbf{R}$.

This proposition is stated as Theorem IV.1 in [18], to which we refer for a complete proof.

Therefore, the structure of the measure $\mu(t)$ is given by Theorem 5.1 with

$$\rho^{in} = (a^{in})^2 \quad \text{and} \quad U^{in} = \nabla S^{in}\,.$$

Likewise, Theorem 6.1 provides a precise description of the exceptional sets associated to $\mu(t)$.

7.4. **WKB vs. monokinetic measures: the case of rough phases.** The WKB asymptotic solution (49) obviously contains more information than the regular part $\mu_a(t)$ of the Wigner measure $\mu(t)$ that is the solution of the Liouville equation (53) — for the definition of $\mu_a(t)$ and its structure, see Theorem 5.1.

For instance, the (finitely many) phase functions $S_j(t,x)$ appearing in (49) define velocity fields $U_j(t,x) := \nabla_x S_j(t,x)$ as in the formula giving $\mu_a(t)$ in Theorem 5.1. On the contrary, the Morse indices $\nu_j(t,x)$ do not appear in the formula for $\mu_a(t)$.

One can go a little further, and compute the Wigner measure associated to the WKB asymptotic solution (49), under the assumptions used in Proposition 7.1.

Let $t \in \mathbf{R}$; for each $x \in \mathbf{R}^N \setminus C_t$ and $j \in \{1, \ldots, \mathcal{N}(t,x)\}$, one has

$$\begin{aligned} \nabla_x S_j(t,x) &= DS^{in}(y_j(t,x))D_x y_j(t,x) + D_y S(t, y_j(t,x), DS^{in}(y_j(t,x)))D_x y_j(t,x) \\ &\quad + D_\eta S(t, y_j(t,x), DS^{in}(y_j(t,x)))D^2 S^{in}(y_j(t,x)D_x y_j(t,x) \\ &= \Xi_t(y_j(t,x), DS^{in}(y_j(t,x))) \cdot (D_y X_t(y_j(t,x), DS^{in}(y_j(t,x)))D_x y_j(t,x) \\ &\quad + D_\eta X_t(y_j(t,x), DS^{in}(y_j(t,x)))D^2 S^{in}(y_j(t,x))D_x y_j(t,x))\,, \end{aligned}$$

in view of formulas (3.1-2) in [17] recalled above (see (61)). By definition

$$X_t(y_j(t,x), DS^{in}(y_j(t,x))) = x\,, \quad j = 1, \ldots, \mathcal{N}(t,x)\,, \tag{54}$$

so that

$$\begin{aligned}D_y X_t(y_j(t,x), DS^{in}(y_j(t,x)))D_x y_j(t,x)\\+D_\eta X_t(y_j(t,x), DS^{in}(y_j(t,x)))D^2 S^{in}(y_j(t,x))D_x y_j(t,x) = I\end{aligned}$$

which implies in turn that

$$\nabla_x S_j(t,x) = \Xi_t(y_j(t,x), DS^{in}(y_j(t,x)))\,, \quad j=1,\ldots,\mathcal{N}(t,x)\,. \tag{55}$$

Because of (54) and of the condition

$$y_j(t,x) \neq y_k(t,x) \quad \text{if } 1 \leq j < k \leq \mathcal{N}(t,x)\,,$$

one has

$$\begin{aligned}\nabla_x S_j(t,x) &= \Xi_t(y_j(t,x), DS^{in}(y_j(t,x)))\\&\neq \Xi_t(y_k(t,x), DS^{in}(y_k(t,x))) = \nabla_x S_k(t,x) \quad \text{if } 1 \leq j < k \leq \mathcal{N}(t,x)\,,\end{aligned}$$

by uniqueness of the solution of the Cauchy problem for Hamilton's equations.

Applying Proposition 1.5 in [10] implies that

$$W_\epsilon[\Psi_\epsilon(t,\cdot)] \to \mu(t) \quad \text{in } \mathcal{D}'((\mathbf{R}^N \setminus C_t) \times \mathbf{R}^N)$$

as $\epsilon \to 0$, where

$$\mu(t,x,d\xi) := \sum_{j=1}^{\mathcal{N}(t,x)} \frac{|a^{in}(y_j(t,x))|^2}{J_t(y_j(t,x))} \delta_{\nabla_x S_j(t,x)}\,.$$

The expression in the right hand side of the equality above coincides with the regular part $\mu_a(t)$ of the Wigner measure $\mu(t)$ in Theorem 5.1.

Obviously Theorem 5.1 (bearing on Wigner measures) holds under assumptions on the phase of the WKB type initial condition much weaker than in Proposition 7.1 (bearing on solutions of the Schrödinger equation). How much information on solutions of the Schrödinger equation can be extracted from Theorem 5.1 is therefore a natural question. Since the Wigner measure is the limit of the Wigner transform as $\epsilon \to 0$ and the Wigner transform is quadratic in the wave function, it is natural to expect that Theorem 5.1 carries information on the vanishing ϵ limit of appropriate quadratic expressions in the solution of the Schrödinger equation (42) with rough initial data.

Using (51) and (52), we arrive at the following statement.

Proposition 7.4. *Let ψ_ϵ the solution of the Schrödinger equation* (42) *where $a^{in} \in L^2(\mathbf{R}^N)$ satisfies $\|a^{in}\|_{L^2(\mathbf{R}^N)} = 1$ and while $S^{in} \in C^1(\mathbf{R}^N)$ is such that $U^{in} := \nabla S^{in}$ satisfies (11) and the regularity condition (18). Assume that the potential $V \in C^{1,1}(\mathbf{R}^N)$ satisfies (45)-(46)-(43)-(44). Then*

a) for each ϵ-pseudodifferential operator B_ϵ of Weyl symbol $b \equiv b(x,\xi)$ in the Schwartz class $\mathcal{S}(\mathbf{R}^N \times \mathbf{R}^N)$ and for each $t \in \mathbf{R}$, one has

$$\lim_{\epsilon\to 0} \langle \psi_\epsilon, B_\epsilon \psi_\epsilon \rangle_{L^2(\mathbf{R}^N)} = \int_{\mathbf{R}^N \times \mathbf{R}^N} b(x,\xi)\mu(t,dxd\xi)$$

where $\mu(t)$ is the Wigner measure described in Theorem 5.1;

b) for each $t \in \mathbf{R}$ and each $\chi \in C_b(\mathbf{R}^N)$ satisfying

$$\chi(x) = 0 \quad \text{for all } x \in C_t\,,$$

one has

$$\int_{\mathbf{R}^N} \chi(x)|\psi_\epsilon(t,x)|^2 dx \to \int_{\mathbf{R}^N} \chi(x) \sum_{y\in F_t^{-1}(\{x\})} \frac{|a^{in}|^2 \mathbf{1}_{P_t}}{J_t}(y) dx$$

as $\epsilon \to 0$*;*

c) for each $t \in \mathbf{R}$ *and each* $\chi \in C_b(\mathbf{R}^N)$ *satisfying*

$$\chi(\Xi_t(y, \nabla S^{in}(y)) = 0 \quad \text{for all } y \in F_t^{-1}(C_t)\,,$$

one has

$$\int_{\mathbf{R}^N} \chi(\xi)|\mathcal{F}_\epsilon\psi_\epsilon(t,\xi)|^2 d\xi \to \int_{\mathbf{R}^N} \sum_{y\in F_t^{-1}(\{x\})} \chi(\Xi_t(y, \nabla S^{in}(y))) \frac{|a^{in}|^2 \mathbf{1}_{P_t}}{J_t}(y) dx$$

as $\epsilon \to 0$*. (Recall that* C_t *is defined in (27) — see also (22) and (19) — while* P_t*,* J_t*,* Ξ_t *and* F_t *are as in Theorem 5.1.)*

Proof. Statement a) follows from formula (52) and Proposition 7.3.

Now for statements b) and c). Denote

$$g_\epsilon(x) := \frac{1}{(\pi\epsilon)^{N/2}} e^{-|x|^2/\epsilon}\,, \quad G_\epsilon(x,\xi) := g_\epsilon(x) g_\epsilon(\xi)\,.$$

Defining

$$\Psi_\epsilon^{x_0,\xi_0}(x) = (\pi\epsilon)^{-N/4} e^{-|x-x_0|^2/2\epsilon} e^{i\xi_0\cdot x/\epsilon}\,,$$

one has

$$W_\epsilon[\Psi_\epsilon^{x_0,\xi_0}] = G_\epsilon\,.$$

Along with the Wigner transform $W_\epsilon[\psi_\epsilon(t,\cdot)]$, we consider the Husimi transform

$$\widetilde{W_\epsilon}[\psi_\epsilon(t,\cdot)] = W_\epsilon[\psi_\epsilon(t,\cdot)] \star_{x,\xi} G_\epsilon\,.$$

Applying (52) with $b = G_\epsilon$ and $\Psi = \psi_\epsilon(t,\cdot)$, one finds that

$$B_\epsilon = \frac{1}{(2\pi\epsilon)^N} |\Psi_\epsilon^{x_0,\xi_0}\rangle\langle\Psi_\epsilon^{x_0,\xi_0}|$$

so that, for each $x_0, \xi_0 \in \mathbf{R}^N$ and each $\epsilon > 0$

$$\widetilde{W_\epsilon}[\psi_\epsilon(t,\cdot)](x_0,\xi_0) = \frac{1}{(2\pi\epsilon)^N} |\langle\Psi_\epsilon^{x_0,\xi_0}|\psi_\epsilon(t,\cdot)\rangle|^2 \ge 0\,.$$

Elementary computations based on this formula show that

$$\begin{aligned} \int_{\mathbf{R}^N} \widetilde{W_\epsilon}[\psi_\epsilon(t,\cdot)](x_0,\xi_0) d\xi_0 &= (g_\epsilon \star |\psi_\epsilon(t,\cdot)|^2)(x_0) \\ \int_{\mathbf{R}^N} \widetilde{W_\epsilon}[\psi_\epsilon(t,\cdot)](x_0,\xi_0) dx &= (g_\epsilon \star |\mathcal{F}_\epsilon\psi_\epsilon(t,\cdot)|^2)(\xi_0) \end{aligned} \tag{56}$$

so that

$$\begin{aligned} \iint_{\mathbf{R}^N\times\mathbf{R}^N} \widetilde{W_\epsilon}[\psi_\epsilon(t,\cdot)](x_0,\xi_0) &= \iint_{\mathbf{R}^N\mathbf{R}^N} g_\epsilon(x-x_0)|\psi_\epsilon(t,x)|^2 dx dx_0 \\ &= \|\psi_\epsilon(t,\cdot)\|_{L^2(\mathbf{R}^N)} = \|\psi_\epsilon^{in}\|_{L^2(\mathbf{R}^N)} = \|a^{in}\|_{L^2(\mathbf{R}^N)} = 1\,. \end{aligned}$$

On the other hand

$$\iint_{\mathbf{R}^N\times\mathbf{R}^N} \mu(t, dx d\xi) = \iint_{\mathbf{R}^N\times\mathbf{R}^N} \mu(0, dx d\xi) = \|a^{in}\|_{L^2(\mathbf{R}^N)} = 1$$

since $\mu(t)$ is the push-forward of the probability measure $\mu(0)$ under the Hamiltonian flow of $\frac{1}{2}|\xi|^2 + V(x)$.

Since $\widetilde{W}_\epsilon[\psi_\epsilon(t,\cdot)] \geq 0$ and

$$\iint_{\mathbf{R}^N\times\mathbf{R}^N} \widetilde{W}_\epsilon[\psi_\epsilon(t,\cdot)](x,\xi)\chi(x,\xi)dxd\xi \to \iint_{\mathbf{R}^N\times\mathbf{R}^N} \chi(x,\xi)\mu(t,dxd\xi) \tag{57}$$

for each $\chi \in C_c(\mathbf{R}^N \times \mathbf{R}^N)$ while

$$\iint_{\mathbf{R}^N\times\mathbf{R}^N} \widetilde{W}_\epsilon[\psi_\epsilon(t,\cdot)](x,\xi)dxd\xi = 1 = \iint_{\mathbf{R}^N\times\mathbf{R}^N} \mu(t,dxd\xi)\,,$$

we conclude that (57) holds for each $\chi \in C_b(\mathbf{R}^N \times \mathbf{R}^N)$ (see for instance Theorem 6.8 in chapter II of [19]).

On the other hand, for each $\chi \in C_b^1(\mathbf{R}^N)$

$$\begin{aligned}\left|\int_{\mathbf{R}^N} \chi(x)(|\psi_\epsilon(t,x)|^2 - |\psi_\epsilon(t,\cdot)|^2 \star g_\epsilon(x))dx\right| \\ \leq \int_{\mathbf{R}^N} |\chi(x) - \chi \star_x g_\epsilon(x)||\psi_\epsilon(t,x)|^2dx \\ \leq \sqrt{\epsilon}\|\nabla\chi\|_{L^\infty}\int_{\mathbf{R}^N}|y|g_1(y)dy \to 0\end{aligned}$$

and likewise

$$\left|\int_{\mathbf{R}^N} \chi(\xi)(|\mathcal{F}_\epsilon\psi_\epsilon(t,\xi)|^2 - |\mathcal{F}_\epsilon\psi_\epsilon(t,\cdot)|^2 \star g_\epsilon(\xi))d\xi\right| \to 0\,.$$

We conclude that, for each $\chi \in C_b^1(\mathbf{R}^N)$

$$\begin{aligned}\int_{\mathbf{R}^N} \chi(x)|\psi_\epsilon(t,x)|^2dx \to \iint_{\mathbf{R}^N\times\mathbf{R}^N} \chi(x)\mu(t,dxd\xi)\\ \int_{\mathbf{R}^N} \chi(\xi)|\mathcal{F}_\epsilon\psi_\epsilon(t,\xi)|^2d\xi \to \iint_{\mathbf{R}^N\times\mathbf{R}^N} \chi(\xi)\mu(t,dxd\xi)\end{aligned} \tag{58}$$

as $\epsilon \to 0$. On the other hand,

$$1 = \int_{\mathbf{R}^N} |\psi_\epsilon(t,x)|^2dx = \int_{\mathbf{R}^N} |\mathcal{F}_\epsilon\psi_\epsilon(t,\xi)|^2d\xi = \int_{\mathbf{R}^N\times\mathbf{R}^N} \mu(t,dxd\xi)$$

so that (58) holds for each $\chi \in C_b(\mathbf{R}^N)$ by a standard density argument.

Statement b) follows from the first convergence statement in (58): by Theorem 5.1 e),

$$\iint_{\mathbf{R}^N\times\mathbf{R}^N} \chi(x)\mu(t,dxd\xi) = \int_{\mathbf{R}^N} \chi(x)\rho(t,dx) = \int_{\mathbf{R}^N} \chi(x)\rho_a(t,dx)$$

if the test function χ vanishes on C_t. One concludes with the formula for ρ_a in Theorem 5.1 d) with $\rho^{in} = |a^{in}|^2$, the restriction to $\mathbf{R}^N \setminus C'_t$ being unessential since $\mathscr{L}^N(C'_t) = 0$.

On the other hand, if $\chi(\Xi_t(y, \nabla S^{in}(y))) = 0$ for all $y \in F_t^{-1}(C_t)$, then

$$\int_{\mathbf{R}^N\times\mathbf{R}^N} \chi(\xi)\mu(t,dxd\xi) = \int_{\mathbf{R}^N\times\mathbf{R}^N} \chi(\xi)\mathbf{1}_{\mathbf{R}^N\setminus C_t}(x)\mu(t,dxd\xi)$$

by Theorem 5.1 c). By Theorem 5.1 b) and e), since $\mu(t)$ is a positive measure, its singular part $\mu_s(t)$ is carried by $C_t \times \mathbf{R}^N$, and therefore

$$\int_{\mathbf{R}^N\times\mathbf{R}^N} \chi(\xi)\mathbf{1}_{\mathbf{R}^N\setminus C_t}(x)\mu(t,dxd\xi) = \int_{\mathbf{R}^N\times\mathbf{R}^N} \chi(\xi)\mathbf{1}_{\mathbf{R}^N\setminus C_t}(x)\mu_a(t,dxd\xi)$$
$$= \int_{\mathbf{R}^N} \sum_{y\in F_t^{-1}(x)} \chi(\Xi_t(y,\nabla S^{in}(y)))\frac{|a^{in}|^2\mathbf{1}_{P_t}}{J_t}(y)dx\,.$$

This proves statement c). □

7.5. **Conclusions and perspectives.** Although Proposition 7.1 can be improved by adding extra assumptions on a^{in} and S^{in}, *in full generality* the approximation stated there holds in $\mathbf{R}\times\mathbf{R}^N\setminus C$, and only after localization in compact subsets of $\mathbf{R}\times\mathbf{R}^N\setminus C$. In particular, the approximation of the wave function ψ_ϵ by the WKB ansatz Ψ_ϵ is *not uniform* as (t,x) approaches C. (For more on this well known fact in a different, yet related context, we refer the reader to the last paragraph in §55 and on the problem in §59 in [15].)

On the contrary, the result obtained in Theorem 5.1 is *global*, holds in the sense of measures and does not involve the caustic C as explained in the previous sections.

Even in the case of rough phase functions, statements b) and c) of Proposition 7.4 show that our approach provides information on the solution ψ_ϵ of the Schrödinger equation(specifically, on $|\psi_\epsilon|$ and $|\mathcal{F}_\epsilon\psi_\epsilon|$) consistent with a WKB ansatz, in a situation where the approximation (50) by a WKB asymptotic solution of the form (49) is not justified at the time of this writing.

Appendix A. Proof of Proposition 7.1

Let $\chi(x,\xi)=\chi_1(x)\chi_2(\xi)$ with $\chi_1,\chi_2\in C_c^\infty(\mathbf{R}^N)$, satisfying

$$\mathbf{1}_{B(0,R)}(x)\le\chi_1(x)\le\mathbf{1}_{B(0,R+1)} \text{ and } \mathbf{1}_{B(0,Q)}(\xi)\le\chi_2(\xi)\le\mathbf{1}_{B(0,Q+1)}$$

for all $x,\xi\in\mathbf{R}^N$, where $R>0$ and Q is to be chosen later. Pick $n>2N$; then

$$\psi_\epsilon(t,\cdot)-G_{\epsilon,n}(t)\chi(x,-i\epsilon\partial_x)\psi_\epsilon^{in} = G_\epsilon(t)(1-\chi(x,-i\epsilon\partial_x))\psi_\epsilon^{in}$$
$$+ (G_\epsilon(t)-G_{\epsilon,n}(t))\chi(x,-i\epsilon\partial_x)\psi_\epsilon^{in}\,.$$

Since $G_\epsilon(t)$ is a unitary group on $L^2(\mathbf{R}^N)$

$$\begin{aligned}\|\psi_\epsilon(t,\cdot)-G_{\epsilon,n}(t)\chi(x,-i\epsilon\partial_x)\psi_\epsilon^{in}\|_{L^2(\mathbf{R}^N)} &\le \|(1-\chi(x,-i\epsilon\partial_x))\psi_\epsilon^{in}\|_{L^2(\mathbf{R}^N)}\\ &\quad+\|(G_\epsilon(t)-G_{\epsilon,n}(t))\chi(x,-i\epsilon\partial_x)\psi_\epsilon^{in}\|_{L^2(\mathbf{R}^N)}\\ &\le \|(1-\chi(x,-i\epsilon\partial_x))\psi_\epsilon^{in}\|_{L^2(\mathbf{R}^N)}\\ &\quad+C_{T,Q}\epsilon^{n-2N}\|a^{in}\|_{L^2(\mathbf{R}^N)}\end{aligned}$$

for all $t\in[0,T]$, where $C_{Q,T}=C[V,T,\chi]$.

Now, $\chi(x,-i\epsilon\partial_x)\psi_\epsilon^{in}=\chi_1(x)\chi_2((-i\epsilon\partial_x)\psi_\epsilon^{in}$ and since $\operatorname{supp}(a^{in})\subset B(0,R)$

$$\begin{aligned}\|(1-\chi(x,-i\epsilon\partial_x))\psi_\epsilon^{in}\|_{L^2(\mathbf{R}^N)} &= \|\chi_1(1-\chi_2(-i\epsilon\partial_x))\psi_\epsilon^{in}\|_{L^2(\mathbf{R}^N)}\\ &\le \|(1-\chi_2(-i\epsilon\partial_x))\psi_\epsilon^{in}\|_{L^2(\mathbf{R}^N)}\\ &= (2\pi)^{-N}\|(1-\chi_2(\epsilon\xi))\widehat{\psi_\epsilon^{in}}\|_{L^2(\mathbf{R}^N)}\\ &\le (2\pi)^{-N}\|\mathbf{1}_{[Q/\epsilon,\infty)}(|\xi|)\widehat{\psi_\epsilon^{in}}\|_{L^2(\mathbf{R}^N)}\end{aligned}$$

Since

$$\widehat{\psi_\epsilon^{in}}(\zeta/\epsilon) = \int_{\mathbf{R}^N} e^{-i(\zeta\cdot x - S^{in}(x))/\epsilon} a^{in}(x)dx$$

we conclude from estimate (7.7.1') in [12] that

$$|\widehat{\psi_\epsilon^{in}}(\zeta/\epsilon)| \le \frac{C\|a^{in}\|_{W^{m,\infty}(\mathbf{R}^N)}}{(|\zeta| - \|\nabla S^{in}\|_{L^\infty(B(0,R))})^m}\epsilon^m$$

provided that $\mathrm{supp}(a^{in}) \subset B(0,R)$ and $|\zeta| > 1 + \|\nabla S^{in}\|_{L^\infty(B(0,R))}$. Therefore

$$\begin{aligned}\|\psi_\epsilon(t,\cdot) - G_{\epsilon,n}(t)\chi(x,-i\epsilon\partial_x)\psi_\epsilon^{in}\|_{L^2(\mathbf{R}^N)} &\le C_{T,Q}\|a^{in}\|_{L^2(\mathbf{R}^N)}\epsilon^{n-2N} \\ &+C\|(1+|\zeta|)^{-m}\|_{L^2(\mathbf{R}^N)}\|a^{in}\|_{W^{m,\infty}(\mathbf{R}^N)}\epsilon^m\end{aligned} \tag{59}$$

for all $m > N/2$.

Next we analyze the term

$$\begin{aligned}&G_{\epsilon,n}(t)\chi(x,-i\epsilon\partial_x)\psi_\epsilon^{in}(x) \\ &\quad= \iiiint A_n(t,y,\eta,\epsilon)a^{in}(z)\chi_2(\zeta)e^{i(\varphi(t,x,y,\eta)+\zeta\cdot(y-z)+S^{in}(z))/\epsilon}\frac{dzd\zeta dyd\eta}{(2\pi\epsilon)^{2N}}\end{aligned} \tag{60}$$

with the stationary phase method.

Choose φ of the form

$$\varphi(t,x,y,\eta) = S(t,y,\eta) + (x - X_t(y,\eta))\cdot\Xi_t(y,\eta) + iB : (x - X_t(y,\eta))^{\otimes 2}$$

where the matrix $B = B^T > 0$ is constant (see formula (2.7) [17] and the following Remark 2.1). Critical points of the phase in the oscillating integral (60) are defined by the system of equations

$$\begin{cases} -\zeta + DS^{in}(z) = 0\,, \\ y - z = 0\,, \\ \partial_y S(t,x,y) - \Xi_t(y,\eta)\cdot D_yX_t(y,\eta) + (x - X_t(y,\eta))\cdot D_y\Xi_t(y,\eta) \\ -iB : (x - X_t(y,\eta))\otimes D_yX_t(y,\eta) + \zeta = 0\,, \\ \partial_\eta S(t,x,y) - \Xi_t(y,\eta)\cdot D_\eta X_t(y,\eta) + (x - X_t(y,\eta))\cdot D_\eta\Xi_t(y,\eta) \\ -iB : (x - X_t(y,\eta))\otimes D_\eta X_t(y,\eta) + \zeta = 0\,. \end{cases}$$

At this point, we recall formulas (3.1-2) from [17]

$$\begin{aligned}\partial_y S(t,x,y) &= \Xi_t(y,\eta)\cdot D_yX_t(y,\eta) - \eta\,, \\ \partial_\eta S(t,x,y) &= \Xi_t(y,\eta)\cdot D_\eta X_t(y,\eta)\,,\end{aligned} \tag{61}$$

together with the following definitions

$$\begin{aligned}Y(t,y,\eta) &:= D_y\Xi_t(y,\eta) - iBD_yX_t(y,\eta)\,, \\ Z(t,y,\eta) &:= D_\eta\Xi_t(y,\eta) - iBD_\eta X_t(y,\eta)\,.\end{aligned}$$

Thus the critical points of the phase in (60) are given by

$$\begin{cases} \zeta = DS^{in}(z)\,, \\ y = z\,, \\ (x - X_t(y,\eta))^TY(t,y,\eta) + \zeta = \eta\,, \\ (x - X_t(y,\eta))^TZ(t,y,\eta) = 0\,. \end{cases}$$

Since the matrix Z is invertible by Lemma 4.1 of [17], we conclude that the system of equations above is equivalent to

$$\begin{cases} \zeta = DS^{in}(z)\,, \\ y = z\,, \\ \zeta = \eta\,, \\ x = X_t(y,\eta)\,. \end{cases}$$

In other words,

$$F_t(z) = x\,, \quad y = z\,, \quad \zeta = \eta = DS^{in}(z)\,.$$

Assuming that $(t,x) \notin C$, we apply Proposition 3.3 and conclude that the set of critical points of the phase in (60) is of the form

$$\begin{cases} y = z = y_j(t,x)\,, \\ \zeta = \eta = DS^{in}(y_j(t,x))\,, \end{cases} \qquad j = 1,\ldots,\mathcal{N}(t,x)\,.$$

At this point, we apply the stationary phase method (Theorem 7.7.5 in [12]). First we need to compute the Hessian of the phase in (60) at its critical points. One finds

$$H_j(t,x) := \begin{pmatrix} D^2S^{in} & -I & 0 & 0 \\ -I & 0 & +I & 0 \\ 0 & +I & -YD_yX_t & -YD_\eta X_t - I \\ 0 & 0 & -ZD_yX_t & -ZD_\eta X_t \end{pmatrix}\Bigg|_{\substack{y=y_j(t,x)\\ \eta=DS^{in}(y_j(t,x))}}$$

and it remains to compute $\det(H_j(t,x))$. Adding the first row of $H_j(t,x)$ to the third row, one finds that

$$\begin{aligned} \det H_j(t,x) &= \begin{vmatrix} D^2S^{in} & -I & 0 & 0 \\ -I & 0 & +I & 0 \\ D^2S^{in} & 0 & -YD_yX_t & -YD_\eta X_t - I \\ 0 & 0 & -ZD_yX_t & -ZD_\eta X_t \end{vmatrix}_{\substack{y=y_j(t,x)\\ \eta=DS^{in}(y_j(t,x))}} \\ &= (-1)^N \begin{vmatrix} -I & +I & 0 \\ D^2S^{in} & -YD_yX_t & -YD_\eta X_t - I \\ 0 & -ZD_yX_t & -ZD_\eta X_t \end{vmatrix}_{\substack{y=y_j(t,x)\\ \eta=DS^{in}(y_j(t,x))}} \\ &= (-1)^N \begin{vmatrix} -I & 0 & 0 \\ D^2S^{in} & -YD_yX_t + D^2S^{in} & -YD_\eta X_t - I \\ 0 & -ZD_yX_t & -ZD_\eta X_t \end{vmatrix}_{\substack{y=y_j(t,x)\\ \eta=DS^{in}(y_j(t,x))}} \end{aligned}$$

where the last equality follows from adding the first column in the right hand side of the second equality to the second column. Eventually, one finds that

$$\det H_j(t,x) = \begin{vmatrix} -YD_yX_t + D^2S^{in} & -YD_\eta X_t - I \\ -ZD_yX_t & -ZD_\eta X_t \end{vmatrix}_{\substack{y=y_j(t,x)\\ \eta=DS^{in}(y_j(t,x))}}$$

which is computed as follows. First

$$\begin{vmatrix} I & -YZ^{-1} \\ 0 & I \end{vmatrix} \begin{vmatrix} -YD_yX_t + D^2S^{in} & -YD_\eta X_t - I \\ -ZD_yX_t & -ZD_\eta X_t \end{vmatrix} = \begin{vmatrix} D^2S^{in} & -I \\ -ZD_yX_t & -ZD_\eta X_t \end{vmatrix}$$

so that

$$\det H_j(t,x) = \begin{vmatrix} D^2S^{in} & -I \\ -ZD_yX_t & -ZD_\eta X_t \end{vmatrix}_{\substack{y=y_j(t,x) \\ \eta=DS^{in}(y_j(t,x))}}$$

On the other hand

$$\begin{aligned}\begin{vmatrix} D^2S^{in} & -I \\ -ZD_yX_t & -ZD_\eta X_t \end{vmatrix} &= \det(ZD_yX_t + ZD_\eta X_t D^2S^{in}) \\ &= \det(Z)\det(D_yX_t + D_\eta X_t D^2S^{in})\end{aligned}$$

by the following elementary lemma (that is a variant of the Schur complement formula in a special case: see for instance Proposition 3.9 on pp. 40-41 in [23]).

Lemma A.1. *Let $A, B, C, D \in M_N(\mathbf{C})$. If $AB = BA$, one has*

$$\begin{vmatrix} A & B \\ C & D \end{vmatrix} = \det(DA - CB)\,.$$

Therefore

$$\begin{aligned}\det H_j(t,x) &= \det(Z)\det(D_yX_t + D_\eta X_t D^2S^{in})\Big|_{y=y_j(t,x),\,\eta=DS^{in}(y_j(t,x))} \\ &= \det(Z(y_j(t,x), DS^{in}(y_j(t,x)))\det(DF_t(y_j(t,x)))\end{aligned} \tag{62}$$

where F_t is defined in (13) with $U^{in} = DS^{in}$.

Pick a nonempty closed ball $B \subset \mathbf{R}\times\mathbf{R}^N \setminus C$, let $\mathcal{N}_B = \mathcal{N}(t,x)$ for all $(t,x) \in B$, and let

$$K_j = \{(y_j(t,x), \nabla S^{in}(y_j(t,x)))\,|\,(t,x) \in B\}\,, \qquad j = 1,\ldots,\mathcal{N}_B\,.$$

Assuming that B is of small enough radius, $K_j \cap K_k = \varnothing$ for $j \neq k \in \{1,\ldots,\mathcal{N}_B\}$. Let $\kappa_j \in C_c^\infty(\mathbf{R}^{2N})$ for all $j = 1,\ldots,\mathcal{N}_B$, such that

$$\begin{cases} \kappa_j \geq 0 \text{ and } \kappa_j\big|_{K_j} = 1\,, \quad j = 1,\ldots,\mathcal{N}_B\,, \\ \text{while } \kappa_j\kappa_k = 0 \text{ for } j \neq k \in \{1,\ldots,\mathcal{N}_B\}\,, \end{cases}$$

Applying Theorem 7.7.1 in [12] shows that

$$\begin{aligned}\sup_{(t,x)\in B}\Bigg|\iiiint A_n(t,y,\eta,\epsilon)a^{in}(z)\chi_2(\zeta)e^{i(\varphi(t,x,y,\eta)+\zeta\cdot(y-z)+S^{in}(z))/\epsilon}\frac{dzd\zeta dyd\eta}{(2\pi\epsilon)^{2N}} \\ -\sum_{j=1}^{\mathcal{N}_B}\iiiint A_n(t,y,\eta,\epsilon)a^{in}(z)\chi_2(\zeta)\kappa_j(y,\eta)\kappa_j(z,\zeta) \\ e^{i(\varphi(t,x,y,\eta)+\zeta\cdot(y-z)+S^{in}(z))/\epsilon}\frac{dzd\zeta dyd\eta}{(2\pi\epsilon)^{2N}}\Bigg| = O(\epsilon)\end{aligned} \tag{63}$$

as $\epsilon \to 0$.

Next we set

$$\begin{aligned}I_j(t,x,\epsilon) := \iiiint & A_n(t,y,\eta,\epsilon)a^{in}(z)\chi_2(\zeta)\kappa_j(y,\eta)\kappa_j(z,\zeta) \\ & \times e^{i(\varphi(t,x,y,\eta)+\zeta\cdot(y-z)+S^{in}(z))/\epsilon}\frac{dzd\zeta dyd\eta}{(2\pi\epsilon)^{2N}}\end{aligned}$$

for $j = 1, \ldots, \mathcal{N}_B$. By Theorem 7.7.5 in [12], we conclude that

$$\sup_{(t,x)\in B} |I_j(t,x,\epsilon) - A_0(t, y_j(t,x), \nabla S^{in}(y_j(t,x)), 0) a^{in}(y_j(t,x))\chi_2(\nabla S^{in}(y_j(t,x))) \times e^{i(\varphi(t,x,y_j(t,x),\nabla S^{in}(y_j(t,x)))+S^{in}(y_j(t,x)))/\epsilon} (\det H_j(t,x))^{-1/2}| = O(\epsilon) \tag{64}$$

as $\epsilon \to 0$. Our choice of χ_2 and φ implies that $\chi_2(\nabla S^{in}(y_j(t,x))) = 1$ and

$$\varphi(t,x,y_j(t,x),\nabla S^{in}(y_j(t,x))) = S(t, y_j(t,x), \nabla S^{in}(y_j(t,x)))$$

so that

$$(\varphi(t,x,y_j(t,x),\nabla S^{in}(y_j(t,x))) + S^{in}(y_j(t,x))) = S_j(t,x)\,.$$

By formula (2.13) in [17]

$$A_0(t, y_j(t,x), \nabla S^{in}(y_j(t,x)), 0) = \sqrt[cont]{Det(Z(y_j(t,x), DS^{in}(y_j(t,x)))}\,, \tag{65}$$

where the notation $\sqrt[cont]{z}$ designates the analytic continuation of the square-root along the path $t \mapsto Det(Z(y_j(t,x), DS^{in}(y_j(t,x))$. This analytic continuation is uniqueley defined since $Det(Z(y_j(t,x), DS^{in}(y_j(t,x))) \neq 0$ for all t: see for instance section 1.3 in chapter 8 of [1]. According to (65), (62), Lemma 5.1 and formula (5.15) in [17], we have

$$\begin{aligned} &A_0(t, y_j(t,x), \nabla S^{in}(y_j(t,x)), 0)(\det H_j(t,x))^{-1/2} \\ &= |\det(DF_t(y_j(t,x)))|^{-1/2} e^{i\pi\nu_j(t,x)/2} = J(y_j(t,x))^{-1/2} e^{i\pi\nu_j(t,x)/2}\,, \end{aligned} \tag{66}$$

where $\nu_j(t,x)$ is an integer.

Putting together (59)-(63)-(64)-(66) concludes the proof of Proposition 7.1.

Proof of Lemma A.1. If A is nonsingular and $AB = BA$, one has

$$\begin{aligned} \begin{vmatrix} A & B \\ C & D \end{vmatrix} = (-1)^N \begin{vmatrix} A & B \\ C & D \end{vmatrix} \begin{vmatrix} A^{-1} & B \\ 0 & -A \end{vmatrix} &= (-1)^N \begin{vmatrix} I & 0 \\ CA^{-1} & CB - DA \end{vmatrix} \\ &= (-1)^N \det(CB - DA) = \det(DA - CB)\,. \end{aligned}$$

Since both sides of the identity above are continuous functions of A and the set of nonsingular matrices $GL_N(\mathbf{C})$ is dense in $M_N(\mathbf{C})$, this identity holds for all $A \in M_n(\mathbf{C})$ such that $AB = BA$. □

References

[1] L.V. Ahlfors: "Complex Analysis", McGraw Hill, 2nd edition, New York 1966.

[2] L. Ambrosio, A. Figalli, G. Friesecke, J. Giannoulis, T. Paul: *Semiclassical limit of quantum dynamics with rough potentials and well posedness of transport equations with measure initial data*, Comm. Pure Appl. Math. **64** (2011), 1199–1242.

[3] L. Ambrosio, N. Fusco, D. Pallara: "Functions of Bounded Variations and Free Discontinuity Problems", Oxford University Press, Oxford 2000.

[4] V.I. Arnold: *Characteristic class entering in quantization condition*, Func. Anal. Appl. **1** (1967), 1–14.

[5] V.I. Arnold: "Geometrical methods of the theory of ordinary differential equations", Springer-Verlag, New York 1997.

[6] V.I. Arnold: "Mathematical Methods of Classical Mechanics", Springer-Verlag, New York 1989.

[7] Y. Brenier, U. Frisch, M. Hnon, G. Loeper, S. Matarrese, R. Moyhayaee, A. Sobolevskii: *Reconstruction of the early Universe as a convex optimization problem*, Mon. Not. Royal. Astron. Soc.

[8] Y. Brenier, E. Grenier: *Sticky particles and scalar conservation laws*, SIAM J. Numer. Anal. **35** (1998), 2317–2328.
[9] W. E, Y. Rykov, Ya. Sinai: *Generalized variational principles, global weak solutions and behavior with random initial data for systems of conservation laws arising in adhesion particle dynamics*, Comm. Math. Phys., **177** (1996), 349–380.
[10] P. Gérard, P. Markowich, N. Mauser, F. Poupaud: *Homogenization limit and Wigner Transforms*, Comm. on Pure and App. Math. **50** (1997), 323–379.
[11] V. Guillemin, S. Sternberg: "Geometric Asymptotics", Amer. Math. Soc., Providence 1977.
[12] L. Hörmander: "The analysis of linear partial differential operators I", Springer-Verlag, Berlin, Heidelberg 1983, 1990.
[13] L. Hörmander: "The analysis of linear partial differential operators II", Springer-Verlag, Berlin, Heidelberg 1983, 1990.
[14] J. Kauhannen, P. Koskela, J. Malý: *On functions with derivatives in a Lorentz space*, Manuscripta Math. **100** (1999), 87–101.
[15] L. Landau, E. Lifshitz: "The Classical Theory of Fields", Butterworth-Heinemann, Oxford, 1976.
[16] L. Landau, E. Lifshitz: "Quantum Mechanics Nonrelativistic Theory", Butterworth-Heinemann, Oxford, 1977.
[17] A. Laptev, I. Sigal: *Global Fourier Integral Operators and Semiclassical Asymptotics*, Review of Math. Phys. **12** (2000), 749–766.
[18] P.-L. Lions, T. Paul: *Sur les mesures de Wigner*, Rev. Mat. Iberoamericana **9** (1993), 553–618.
[19] P. Malliavin, H. Airault, G. Letac, L. Kay: "Integration and Probability", Springer-Verlag, New York 1995.
[20] J. Malý: *Absolutely Continuous Functions of Several Variables*, J. Math. Anal. Appl. **231** (1999), 492–508.
[21] J. Malý, D. Swanson, W. Ziemer: *The Co-Area Formula for Sobolev Mappings*, Trans. Amer. Math. Soc. **355** (2002), 477–492.
[22] W. Rudin: "Real and Complex Analysis", McGraw Hill, Singapore, 1986.
[23] D. Serre: "Matrices", Springer-Verlag, 2nd edition, New York 2010.
[24] J. Smoller: Shock Waves and Reaction-Diffusion Equations"; Springer-Verlag, New York, 1983.
[25] C. Sparber, P. A. Markowich, N. Mauser: *Wigner Functions versus WKB-Methods in Multivalued Geometrical Optics*, Asymptot. Anal., **33** (2003), 153–187.
[26] E. Wigner: *On the Quantum Correction For Thermodynamic Equilibrium*, Phys. Rev. **40** (1932), 749–759.
[27] Ya. Zeldovich: *Gravitational instability: An approximate theory for large density perturbations*, Astron. Astrophys. **5** (1970), 84–89.

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