Wigner Functions versus WKB-Methods in Multivalued Geometrical Optics

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Abstract

We consider the Cauchy problem for a class of scalar linear dispersive equations with rapidly oscillating initial data. The problem of the high-frequency asymptotics of such models is reviewed, in particular we highlight the difficulties in crossing caustics when using (time-dependent) WKB-methods. Using Wigner measures we present an alternative approach to such asymptotic problems. We first discuss the connection of the naive WKB solutions to transport equations of Liouville type (with mono-kinetic solutions) in the prebreaking regime. Further we show how the Wigner measure approach can be used to analyze high-frequency limits in the post-breaking regime, in comparison with the traditional Fourier integral operator method. Finally we present some illustrating examples.

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1 Introduction

In this paper we consider a class of scalar IVP’s for linear dispersive equations with fast temporal and spatial scales subject to highly oscillating initial data. The Cauchy problem of the Schrödinger equation serves as a typical example

\[ i\varepsilon \partial_t \psi^\varepsilon = -\frac{\varepsilon^2}{2} \Delta \psi^\varepsilon + V(x)\psi^\varepsilon = 0, \quad x \in \mathbb{R}^d, t \in \mathbb{R} \quad (1.1) \]

\[ \psi^\varepsilon (x, 0) = A_I(x) e^{i S_I(x)/\varepsilon}, \quad x \in \mathbb{R}^d \quad (1.2) \]

where \( \varepsilon \sim \hbar \) (the scaled Planck’s constant). The small parameter \( \varepsilon \) represents the fast space and time scales introduced in (1.1), as well as the typical wave length of oscillations of the initial data. We are interested in the high frequency limit of these equations, which is usually referred to as ”geometrical-optics”. In the special case of the Schrödinger equation with vanishing Planck’s constant this is precisely the ”(semi-)classical limit”. It is well known that the considered equations propagate oscillations of wave lengths \( \varepsilon \) which inhibit \( \psi^\varepsilon \) from converging strongly in a suitable sense.

Thus the short-wavelength-asymptotics \( \varepsilon \to 0 \) is by no means straightforward, in particular since the physical quantities of interest (observables) are quadratic in \( \psi^\varepsilon \).

The usual way to tackle the problem is the geometrical optics - or WKB-Ansatz (Wentzel-Kramers-Brillouin, see \[ Ke \]), which consists of representing the solution \( \psi^\varepsilon \) in the form

\[ \psi^\varepsilon (x, t) \simeq A^\varepsilon (x, t) \exp \left( \frac{i}{\varepsilon} S(x, t) \right) \quad (1.3) \]

where \( A^\varepsilon \) and \( S \) are realvalued, \( A^\varepsilon \geq 0 \) and in general \( A^\varepsilon \simeq A + \varepsilon A_1 + \varepsilon^2 A_2 + \ldots \).

Then after inserting the above representation into the equation and by considering, as a first approximation, only the lowest order terms, one finds that:

- the phase \( S \) is a solution of a nonlinear first order equation of Hamilton-Jacobi type
- the (zeroth order) amplitude satisfies a linear first order PDE (called transport equation) that can be brought into the form of a conservation law for the energy density \( n = A^2 \).

A severe drawback of this method should be noted. The obtained nonlinear equations do not have global, i.e. for all \( t \in \mathbb{R} \), smooth solutions (except for some special initial data). In other words the system in general develops singularities in some finite time \( t_c \) (”break time”). The formal expansion method clearly can only be justified for smooth, i.e. sufficiently often differentiable, functions \( S \) and \( A^\varepsilon \) and thus the Ansatz (1.3) breaks down at points where the first singularities occur. These singularities are called focal points, or more generally caustics, since, as we will see, the energy of the wave becomes infinite there.
A alternative point of view on this problem is given by considering the so called Quantum Hydrodynamic System, which is obtained by plugging into equation (1.1) the ansatz (1.3), with $S = S^\varepsilon$. Defining $n^\varepsilon := (A^\varepsilon)^2$ and $j^\varepsilon := n^\varepsilon \nabla S^\varepsilon$, one gets (after separating real and imaginary parts)

$$
\partial_t n^\varepsilon + \text{div} \ j^\varepsilon = 0, \quad (1.4)
$$

$$
\partial_t j^\varepsilon + \text{div} \left( \frac{j^\varepsilon \otimes j^\varepsilon}{n^\varepsilon} \right) + n^\varepsilon \nabla_x V = \varepsilon^2 \frac{n^\varepsilon}{2} \nabla \left( \frac{1}{\sqrt{n^\varepsilon}} \Delta \sqrt{n^\varepsilon} \right). \quad (1.5)
$$

This system is exact, i.e. equivalent to the Schrödinger equation (1.1), c.f. [GaMa] and well posed for all $t \in \mathbb{R}$ due to the third order dispersive regularization term. However for $\varepsilon = 0$, where the system simplifies to the zero temperature Euler equations, singularities appear and the equations cannot be used after them to describe the propagation of the energy density $n^\varepsilon$ in the high frequency limit. (This approach is used in particular in one space variable for the non linear Schrödinger equation, i.e. $V^\varepsilon = |\psi^\varepsilon|^2$, see e.g. [LaLe].)

A natural alternative to the standard WKB-method is seeking multivalued phases corresponding to crossing waves. This means that in general for every fixed $(x, t) \in \mathbb{R}^d \times \mathbb{R}$, which is not on the caustic, one tries to construct a (maybe infinite) set of phase functions $\{ S_i(x, t) \}$, $i \in I \subseteq \mathbb{N}$, each of which is a solution of the Hamilton-Jacobi equation in a neighborhood of $(x, t)$. This set is referred to as the multivalued solution of the Hamilton-Jacobi equation and it induces the multivalued solution $\{ n_i(x, t) \}$ of the conservation law for the energy density.

Historically this problem was studied by P. Lax, D. Ludwig, V. Maslov, J. Duistermaat and others (see [Du], [Kr], [La], [Lu], [Mas1]), who showed that Fourier-Integral operators and Lagrangian manifolds in phase space provide a uniform description of the behavior of $\psi^\varepsilon$. (For applications in semi-classical quantum mechanics see the expository article of Robert [Ro].) The qualitative study of the multivalued solution is accomplished using geometrical techniques of singularity theory and contact geometry (see e.g. [Av], [AVG], [Du], [GuSt]).

A considerable amount of work has been done in recent years on constructing numerically the multivalued phase function (see, e.g., [Be1], [Be2], [BKM], [Ra], [JiLi]). We will not cover the arising numerical questions in this paper, instead we refer the interested reader to these references.

In the last decade the use of Wigner functions and Wigner measures has drawn increasing interest, in particular its application to the semi-classical limit of Schrödinger equations ([LiPa], [MaMa], [MMP], [MPP]) and the homogenization of energy densities of dispersive equations (e.g. [BCKP], [GaMa], [Ge], [GMMP]), mostly by groups in Europe. Independently, groups in the US used Wigner functions, too, with some emphasis on waves in random media and applied problems, e.g. [BKPR], [PaRh].

The Wigner transformation provides a phase space description of the equations of the problem, which is extremely useful for the asymptotics since it "unfolds" the caustics (de-projection in phase space). Another advantage is that the high frequency limit, using Wigner functions, needs much lower regularity assumptions on $A_I$ and $S_I$ than the (generalized)
WKB-method. This is not only of purely academic interest since very often in concrete physical models $C^\infty_0$ initial data are simply not available. The price paid for the analytical convenience lies in the doubling of the dimension, i.e. the Wigner function is defined on $\mathbb{R}^{2d}$. This work studies the connection between the WKB-method and the Wigner transformation or, in other words, represents an alternative approach to WKB-asymptotics. It is organized as follows:

- Section 2 is devoted to the setting of the problem. There we also give a short review of the traditional (naive) WKB-method and its generalization using FIO’s.
- In section 3 we present the main theorems on Wigner transforms and show how they can be used to obtain a semi-classical phase-space description.
- This limiting phase-space regime is analyzed in section 4, which is the most important part of this paper.
- Examples are studied in section 5 to illustrate the results of the foregoing section.
- Finally in the Appendix in section 7 we give an example with non-global Hamiltonian flow and comment on the arising fluid type equations, which generalize the zero temperature Euler equations.

2 Setting of the problem and the WKB-method

2.1 The model equation

We consider the following initial value problem (generalized linear dispersive model) for an anti-selfadjoint scalar pseudo-differential operator

$$
\varepsilon \partial_t \psi^\varepsilon + i H_W(x, \varepsilon D)^\psi^\varepsilon = 0, \quad x \in \mathbb{R}^d, t \in \mathbb{R}
$$

subject to the highly oscillatory (WKB) initial data

$$
\psi^\varepsilon(x, 0) = \sqrt{n_I(x)} e^{i S_I(x) / \varepsilon}, \quad x \in \mathbb{R}^d
$$

where $\psi^\varepsilon(t, x)$ is a scalar $L^2$-function on $\mathbb{R}^d$, $D := -i \nabla_x$, $\varepsilon \in (0, \varepsilon_0]$ and $H(x, \varepsilon D)^W$ is the Weyl-operator associated to its symbol $H(x, \varepsilon \xi)$ by Weyl’s quantization rule:

**Definition 2.1.**

$$
H_W(x, \varepsilon D)^\varphi(x) := \frac{1}{(2\pi)^d} \int_{\mathbb{R}^d} \int_{\mathbb{R}^d} H \left( \frac{x + y}{2}, \varepsilon \xi \right) \varphi(y) e^{i(x-y)\xi} d\xi dy
$$

The convenience of the Weyl-calculus lies in the fact that a scalar Weyl-operator is formally selfadjoint iff it has a real-valued symbol.
We have chosen this particular form of pseudo differential-calculus in order to be consistent with the usual framework of the Wigner-functions introduced in [GMMP]. Note that in case $H$ is a sum of separate terms in $x$ and $\xi$, the "Weyl symbol" and the "left symbol" of the classical Fourier multiplier coincide.

**Remarks.**

- The general framework of pseudo-differential operators allows us to include also non-local Hamiltonians, like the one appearing in example (iii) below, in our discussion.
- Further note that the time and spatial scales of (2.1) are "fast", since the small parameter $\varepsilon$ multiplies the time and spatial derivatives.

We shall use in this text the following definition of the Fourier transform $\mathcal{F} : \mathcal{S}(\mathbb{R}^d) \rightarrow \mathcal{S}(\mathbb{R}^d)$:

$$\hat{f}(\xi) := (\mathcal{F}_{x \rightarrow \xi} f)(\xi) := \int_{\mathbb{R}^d} f(x) e^{-ix\xi} dx, \quad (2.4)$$

with the usual extension, by duality, to a mapping from $\mathcal{S}'$ to $\mathcal{S}'$. In (2.2) the amplitude is written in this particular form to match the following definition:

**Definition 2.2.** The energy-density of the solution of (2.1) is defined by

$$n^\varepsilon(x,t) := |\psi^\varepsilon(x,t)|^2. \quad (2.5)$$

We assume on the Weyl operator $H^W$ and on its symbol $H$:

**Assumption (A1)**

(A1)(i) $\exists \sigma \in \mathbb{R} : H \in S^\sigma(\mathbb{R}^d)$ uniformly for $\varepsilon \in (0,\varepsilon_0]$.

(A1)(ii) $\exists$ a unique self adjoint extension of $iH^W(\cdot,\varepsilon D)$ on $L^2(\mathbb{R}^d)$.

By abuse of notation, we denote the unique s.a. extension by $iH^W$ too.

The hypothesis (A1)(i) means (see also [H]) that for all $\alpha, \beta \in \mathbb{N}_0$, there exists $C_{\alpha,\beta} \geq 0$, s.t. for all $l,k \in \{1..m\}$ and for all $\varepsilon \in (0,\varepsilon_0]$ it holds

$$|\frac{\partial^{\alpha+\beta}}{\partial x^\alpha \partial \xi^\beta} H(x,\xi) | \leq C_{\alpha,\beta}(1 + |\xi|)^{\sigma-\beta}, \quad \forall (x,\xi) \in \mathbb{R}^d \times \mathbb{R}^d.$$

In particular this implies that the Sobolev space $H^\sigma(\mathbb{R}^d)$ lies in the domain of the operator $H^W$.

Furthermore this type of hypothesis are made in order to extend the rule of composition from differential operators to pseudo-differential operators modulo lower order terms in $\varepsilon$ (for details see e.g. [H]).

**Remark.** We remark that the regularity assumptions on the symbol $H$ are largely used for convenience and taken from [GMMP] in order to use.
certain results, which were established there. They can be significantly weakened, for example: If $H = |ξ|^2/2 + V(x)$ with $V$ bounded below and $V \in C^{1,1}$ (cf. [LiPa]), all results using Wigner transforms remain valid (see [GaMa]).

On the initial data we impose:

**Assumption (A2)**

$$n_I \in L^1(\mathbb{R}^d), \ n_I \geq 0 \text{ a.e. on } \mathbb{R}^d \text{ and } S_I \in W^{1,1}_{\text{loc}}(\mathbb{R}^d).$$

(2.6)

Note that due to the low regularity assumed in (A2) a traditional WKB-expansion method would not be possible here! This is one of the advantages of the Wigner formalism.

**Lemma 2.1.** Let $ψ^\varepsilon_I$ satisfy (A2) and assume (A1), then there exist a unique mild solution $ψ^\varepsilon(t) \in C(\mathbb{R}_t; L^2(\mathbb{R}^d))$ of (2.1), and its energy-density satisfies

$$\|n^\varepsilon(t)\|_1 = \|n^\varepsilon_I\|_1 \ \forall \ t \in \mathbb{R},$$

(2.7)

where $\| \cdot \|_1$ denotes the $L^1$ norm.

**Proof.** Having in mind (A1)(ii) the assertion is a simple consequence of Stone’s famous theorem (see e.g. [ReSi]).

Some particular examples for equation (2.1) are:

**Examples:**

(i) The Schrödinger equation

$$\varepsilon \partial_t ψ^\varepsilon - i\frac{ε^2}{2} \Delta ψ^\varepsilon + iV(x)ψ^\varepsilon = 0,$$

(2.8)

where $ε \sim h$. Here $H(x, ξ) = |ξ|^2/2 + V(x)$.

(ii) The 1-d Airy equation (or linearized KdV equation)

$$\varepsilon \partial_t ψ^\varepsilon - \frac{ε^3}{3} ψ^\varepsilon_{xxx} = 0,$$

(2.9)

where $H(x, ξ) = ξ^3/3$. Here $ε$ denotes the ”physical” dispersion-parameter.

(iii) The spinless Bethe-Salpeter equation (or ”relativistic Schrödinger equation”)

$$\varepsilon \partial_t ψ^\varepsilon - i \left( \sqrt{- \frac{ε^2}{2} \Delta + 1 + V(x)} \right) ψ^\varepsilon = 0.$$

(2.10)
Again $\varepsilon \sim h$ and we have $H(x, \xi) = \sqrt{\xi^2/2 + 1 + V(x)}$. Note that in this example $H^w$ is a "true" pseudo-differential operator (i.e. the Weyl-symbol is not polynomial in $\xi$).

(iv) Another example of a "true" pseudo-differential equation assumes Hamiltonians of the form $H = a(x)|\xi|$, i.e. we have (in Weyl-quantized form)

$$\varepsilon \partial_t \psi^\varepsilon + i\varepsilon |D_y|(a(x + \frac{y}{2})\psi^\varepsilon(y)) \bigg|_{y=x} = 0.$$  

(2.11)

In the constant coefficient case $a(x) \equiv 1$, equations of this type can be traced back to the wave equation $u^\varepsilon_{tt} - \Delta u^\varepsilon = 0$ by noting that, the quantities

$$\psi^\varepsilon_\pm(\xi, t) = \partial_t u^\varepsilon \pm i|D|u^\varepsilon$$

satisfy

$$\partial_t \psi^\varepsilon_\pm \mp i|D|\psi^\varepsilon_\pm = 0.$$  

We are now interested in the high-frequency limit $\varepsilon \to 0$. For the sake of completeness we briefly review the traditional (naive) WKB-method in the next subsection.

2.2 The WKB-method

As stated in the introduction above we make the following ansatz

$$\psi^\varepsilon(x, t) \simeq A^\varepsilon(x, t) \exp\left(\frac{i}{\varepsilon} S(x, t)\right), \quad x \in \mathbb{R}^d, t \in \mathbb{R}$$  

(2.12)

with $A^\varepsilon \geq 0$ assuming (for the moment) that the phase and the amplitude are sufficiently smooth, and we expand the amplitude in powers of $\varepsilon$:

$$A^\varepsilon \simeq A + \varepsilon A_1 + \varepsilon^2 A_2 + \ldots$$

We sketch the (formal) WKB-method for the case of a polynomial Weyl-symbol $H = H(x, \xi)$ with $C^\infty$-coefficients, i.e.

$$H^w(x, \varepsilon D)\varphi(x) = \sum_{|k|=0}^m \varepsilon^{|k|} D_y^k \left(a_k \left(\frac{x + y}{2}\right)\varphi(y)\right) \bigg|_{y=x}. $$  

(2.13)

Substituting the representation (2.12) into (2.1) and collecting terms appropriately gives

$$H^w(x, \varepsilon D)(A^\varepsilon e^{iS/\varepsilon}) = e^{iS/\varepsilon} \sum_{|k|=0}^m (i\varepsilon)^{|k|} R_k[A^\varepsilon],$$  

(2.14)
where $R_k$ acts on $A^\varepsilon$ as a differential operator of order $|k| \leq m$ (with coefficients depending on derivatives of $S,H$). In particular

$$
R_0[A^\varepsilon] = H(x,\nabla_x S)A^\varepsilon,
$$

$$
R_1[A^\varepsilon] = \sum_{j=1}^d \frac{\partial H(x,\nabla_x S)}{\partial \xi_j} \frac{\partial A^\varepsilon}{\partial x_j} + \frac{1}{2} \sum_{j,k=1}^d \frac{\partial^2 S}{\partial x_j \partial x_k} \frac{\partial H(x,\nabla_x S)}{\partial \xi_j \xi_k} A^\varepsilon
$$

$$
+ \frac{1}{2} \sum_{k=1}^d \frac{\partial^2 H(x,\nabla_x S)}{\partial y_k \xi_k} A^\varepsilon,
$$

where here and in the sequel we denote by $\nabla_y$ the gradient w.r.t. the position variable, i.e. we consider $y$ as a placeholder for the position variable $x$: $S = S(y,t)$, $H = H(y,\xi)$ etc.. The last term in the expression $R_1$ is obtained due to the fact that we use Weyl-quantized operators. Note that in the equations above all partial derivatives of the symbol $H$ w.r.t. $\xi$ are evaluated at $\xi = \nabla_x S$. Plugging the above computations into (2.13), separating real and imaginary parts terms we obtain in the lowest orders

$$
\frac{\partial S}{\partial t} + H(x,\nabla_x S) = 0,
$$

$$
\frac{\partial A}{\partial t} + \sum_{j=1}^d \frac{\partial H(x,\nabla_x S)}{\partial \xi_j} \frac{\partial A}{\partial x_j} + \frac{1}{2} \sum_{j,k=1}^d \frac{\partial^2 S}{\partial x_j \partial x_k} \frac{\partial H(x,\nabla_x S)}{\partial \xi_j \xi_k} A
$$

$$
+ \frac{1}{2} \sum_{k=1}^d \frac{\partial^2 H(x,\nabla_x S)}{\partial y_k \xi_k} A = 0.
$$

Note that the second equation is linear in $A$, it is called the transport equation for the amplitude. In terms of $(n,S) \equiv (A^2,S)$ we obtain the following compact form, in the sequel called WKB-system associated to equations of type (2.1)

$$
\partial n + \text{div}(n \nabla_x H(x,\nabla_x S)) = 0, \quad x \in \mathbb{R}^d, t \in \mathbb{R} \tag{2.15}
$$

$$
\partial S + H(x,\nabla_x S) = 0, \tag{2.16}
$$

where the initial data are induced by the initial condition (2.2)

$$
n(x,0) = n_I(x), \quad S(x,0) = S_I(x), \quad x \in \mathbb{R}^d. \tag{2.17}
$$

The first equation (2.15) is a conservation law for the energy-density, the second (2.16) a Hamilton-Jacobi equation for the phase.

To illustrate the method, we derive the (lowest order) WKB-systems for some particular examples of (2.1).

**Examples:**

(i) WKB-system for the Schrödinger equation (2.8):

$$
\partial n + \text{div}(n \nabla_x S) = 0, \quad x \in \mathbb{R}^d, t \in \mathbb{R} \tag{2.18}
$$

$$
\partial S + \frac{\|\nabla_x S\|^2}{2} + V(x) = 0. \tag{2.19}
$$
(ii) WKB-system for the 1-d Airy equation (2.9):
\[
\partial_t n + \partial_x (n(\partial_x S)^2) = 0, \quad x, t \in \mathbb{R}
\]
\[
\partial_t S + \frac{(\partial_x S)^3}{3} = 0.
\]  
(2.20)

(iii) WKB-system for the (spinless) Bethe-Salpeter equation (2.10):
\[
\partial_t n + \text{div} \left( \frac{n\nabla_x S}{\sqrt{|\nabla_x S|^2 + 1}} \right) = 0, \quad x \in \mathbb{R}^d, t \in \mathbb{R}
\]
\[
\partial_t S + \sqrt{|\nabla_x S|^2 + 1} + V(x) = 0.
\]  
(2.22)

(iv) WKB-system for equations of type (2.11):
\[
\partial_t n + \text{div} \left( na \frac{\nabla_x S}{|\nabla_x S|} \right) = 0, \quad x \in \mathbb{R}^d, t \in \mathbb{R}
\]
\[
\partial_t S + a(x) \frac{\sqrt{|\nabla_x S|}}{|\nabla_x S|} = 0.
\]  
(2.24)

The equation (2.23) is the time-dependent eikonal equation of geometrical optics. Note that in one spatial dimension, i.e. $d = 1$, the above system decouples and simplifies to:
\[
\partial_t n + \partial_x (na \text{ sgn}(\partial_x S)) = 0, \quad x, t \in \mathbb{R}
\]
\[
\partial_t S + a(x) \text{ sgn}(\partial_x S) \partial_x S = 0.
\]  
(2.26)

In this case the WKB-approximation is exact if $\partial_x S$ does not change sign, since then no terms $\sim O(\varepsilon^2)$ appear in the expansion when using $A_k = 0$ for $k > 1$.

\[\diamond\]

In general, solving the system (2.15), (2.16) allows an asymptotic description of the solution of (2.1) in the pre-breaking regime, more precisely we have the following proposition, the proof of which is classic, see e.g. [La]:

**Proposition 2.1.** Let $\psi^\varepsilon(t)$ solve (2.1), (2.2), where $H^W$ is of the form (2.13). Assume $\sqrt{nI} \in \mathcal{S}(\mathbb{R}^d)$ and that $S_I$ is bounded, together with all its derivatives up to sufficient order. Let $t_{c_1} < 0 < t_{c_2}$ be such that a smooth solution $(n, S)$ of (2.13), (2.16) exists on $\mathbb{R}^d \times (t_{c_1}, t_{c_2})$ and define
\[
\psi^\varepsilon_{\text{wkb}}(x, t) := \sqrt{n(x, t)} \exp \left( i \varepsilon S(x, t) \right).
\]  
(2.28)

Then, for every finite time-interval $[t_1, t_2] \subset (t_{c_1}, t_{c_2})$ we have
\[
\sup_{t_1 < t < t_2} \| \psi^\varepsilon(t) - \psi^\varepsilon_{\text{wkb}}(t) \|_2 \leq O(\varepsilon),
\]  
(2.29)

where $\| \cdot \|_2$ denotes the $L^2$ norm.
Remark. The proposition can be extended to (systems of) pseudo-differential operators, with somewhat weaker conditions on $n$, $S$ and $H$ (see e.g. [Fed], [Mas1], [Mas2]).

Generally one faces the following problem in this approach:

The solution $S$ of the Hamilton-Jacobi equation (2.16) is obtained, at least locally, by the method of characteristics. This means that, for a fixed $t$, each point $(y, t) \in U$ in a (sufficiently small) neighborhood $U \subset \mathbb{R}^d \times \{t = 0\}$, of the initial manifold $\mathbb{R}^d \times \{t = 0\}$, is reached by a unique integral curve $\hat{x}(t, x)$, called ray, which can be found as described in the following.

Let us define

$$\hat{\xi}(t, x) := \nabla_y S(\hat{x}(t, x), t). \quad (2.30)$$

It is well known (see for example [Ev]), that the curves $\hat{x}(t, x), \hat{\xi}(t, x)$ solve the IVP

$$\frac{d\hat{x}}{dt} = \nabla \xi H(\hat{x}, \hat{\xi}), \quad \hat{x}(0, x) = x \quad (2.31)$$

$$\frac{d\hat{\xi}}{dt} = -\nabla_y H(\hat{x}, \hat{\xi}), \quad \hat{\xi}(0, x) = \nabla_x S_I(x). \quad (2.32)$$

Having solved this system we obtain the solution of (2.16) by integrating

$$\frac{dS(\hat{x}, t)}{dt} = \nabla \xi H(\hat{x}, \hat{\xi}) \cdot \hat{\xi} - H(\hat{x}, \hat{\xi}), \quad S(\hat{x}(0, x), 0) = S_I(x). \quad (2.33)$$

For details see again [Ev], [Fed]. As it is indicated above this theory is local, since it only gives the unique solution of (2.16) in a neighborhood $U$ of the initial manifold $\mathbb{R}^d \times \{t = 0\}$. In other words, if we consider for every fixed $t \in \mathbb{R}$ the map

$$\hat{x}(t, \cdot) : \mathbb{R}^d \rightarrow \mathbb{R}^d$$

$$x \mapsto \hat{x}(t, x) \quad (2.34)$$

it is, in general, not one-to-one for large times $t \in \mathbb{R}$, see e.g. the examples 1.2, 1.3 in section 5. Further it is known that the phase is discontinuous at caustics, i.e. points of intersection of rays, which in general will happen in finite times $t = t_{c_1}, t = t_{c_2}$, with $t_{c_1} < t < t_{c_2}$, called break-times. It is clear however that the formal WKB-expansion method can only be justified for $t_{c_1} < t < t_{c_2}$ and thus a global, i.e. for all $t \in \mathbb{R}$, asymptotic description can not be obtained from this method.

To overcome this deficiency, several generalizations of the method have been developed in the past decades. Most of them rely on the use of global Fourier-Integral operators (FIO) or the Maslov Canonical operator (MCO), which are now rather standard methods and covered in many books, however for the sake of the reader which may be not familiar with it, we shall now give a flavour of these methods.
2.3 The Fourier Integral Operator (FIO)

Let us again start with an illustrative example: Consider the free Schrödinger equation in $\mathbb{R}^d$, i.e.

$$
\varepsilon \partial_t \psi^\varepsilon - \frac{i \varepsilon^2}{2} \Delta \psi^\varepsilon = 0,
$$

$$
\psi^\varepsilon(t = 0, x) = \sqrt{n_I(x)} e^{i S_I(x)/\varepsilon}.
$$

Straightforward Fourier analysis shows, that its solution is explicitly given by the following oscillatory integral

$$
\psi^\varepsilon(x, t) = (2\pi\varepsilon)^{-d} \int_{\mathbb{R}} \int_{\mathbb{R}} \sqrt{n_I(z)} e^{i S(x,z,\xi,t)/\varepsilon} dz d\xi,
$$

where

$$
S(x, z, \xi, t) := (x - z) \cdot \xi + \frac{t}{2} |\xi|^2 + S_I(z).
$$

Let us recall the theorem of stationary phase ([GuSt], [Mas1, Mas2], [ReSi]):

**Proposition 2.2.** Let $a \in C^\infty_0(\mathbb{R}^d)$, $\Phi \in C^\infty(\mathbb{R}^d)$ and assume that the set $\{ z : \nabla \Phi(z) = 0, z \in \text{supp}(a) \}$ consists of finitely many points $z_i$, with $i = 1 \ldots N$. If the Hessians $D^2 \Phi(z_i)$ are nonsingular, then for $\varepsilon \ll 1$

$$
(2\pi\varepsilon)^{-d} \int_{\mathbb{R}} a(z) e^{i \Phi(z)/\varepsilon} dz = \sum_{i=1}^N \frac{1}{\sqrt{\det D^2 \Phi(z_i)}} \exp \left( \frac{i}{\varepsilon} \Phi(z_i) + \frac{i\pi}{4} m_i \right) (a(z_i) + O(\varepsilon)),
$$

where $z_i = z_i(x, t)$ and $m_i := \text{sgn}(D^2 \Phi(z_i))$ is the so called Maslov index of the $i$-th ray.

This implies that (locally) the main contribution to the solution of the Schrödinger equation stems from stationary points w.r.t. $y$ and $\xi$, i.e. points at which $\nabla_{z,\xi} S = 0$, which gives

$$
\xi = \nabla S_I(z), \quad x = z + t\xi,
$$

i.e. we get a ray-map, c.f. (2.34), defined by the following relation

$$
x = \hat{x}(t, z) = z + t \nabla S_I(z).
$$

For small $t$ the map $z \mapsto \hat{x}(t, z)$ is singlevalued. In general however, there exist (maybe infinitely) many $z_i = z_i(x, t)$, which obey the equation (2.40). Note that the functions $S_I(z_i(x, t))$ are local solutions of the Hamilton Jacobi equation

$$
\partial_t S + \frac{\nabla_x S^2}{2} = 0.
$$
Provided that the Hessians $D^2S(z_i)$ are nonsingular and assuming that there exist only finitely many points $y_i$, the stationary phase theorem then gives us, the following multivalued WKB-approximation of $\psi^\epsilon$

$$\psi^\epsilon(x, t) \simeq \sum_{i=1}^{N} \sqrt{\frac{n_I(z_i(x, t))}{1 + tD^2S_I(z_i(x, t))}} \exp \left( \frac{i}{\epsilon} S_I(z_i(x, t)) + \frac{i\pi}{4} m_i \right) + O(\epsilon).$$

Note that the $m_i$ change sign, each time a ray passes the caustic, which is defined here to be a point at which $D^2S$ is singular.

For equations with variable coefficients, the above concepts have to be generalized, leading to the definition of a FIO acting on the initial datum $\psi^\epsilon_I(x)$ by

$$\psi^\epsilon(x, t) \simeq (2\pi \epsilon)^{-d/2} \int_{\mathbb{R}^d} \int_{\mathbb{R}^d} A(x, z, \xi, t) e^{iS(x, z, \xi, t)/\epsilon} \psi^\epsilon_I(v) dv d\xi.$$

Since for $t = 0$ the FIO has to reduce to the identity operator, we obtain the conditions

$$S(x, z, \xi, t)|_{t=0} = (x - z) \cdot \xi, \quad A(x, z, \xi, t)|_{t=0} = 1. \quad (2.42)$$

At the core of the use of FIOs is the fact that the composition and commutators of two such FIOs is again "locally" a FIO (Hörmander’s Theorem [Ho]) and that the rules to calculate their principal symbols are extensions of the rules of (composition and commutation of) pseudo differential operators.

The leading contribution again stems from the stationary points, which correspond to the asymptotic solutions of the geometrical optics limit $\epsilon \to 0$. For points on the caustic the FIO is an integral which can be brought into a canonical form and evaluated in terms of special integral functions. This is the problem of classification of Lagrangian singularities in contact geometry (see e.g. [Ar], [AVG]). For the detailed implementation of these basic ideas we refer e.g. to [Du], [Fed], [GuSt], [Ho], [Kr], [La], [Lu], [Mas1], [Mas2]), however one should note that these approach generically assumes $S_I, n_I \in C^\infty_0(\mathbb{R}^d)$, which is of course significantly stronger than our assumption (A2).

After reviewing these classical methods of high frequency approximation, we now turn to a new concept, namely the Wigner transformation technique.

### 3 The Wigner function approach

**Definition 3.1.** For given $f, g \in \mathcal{S}'(\mathbb{R}^d)$ and given $\epsilon \in (0, \epsilon_0]$ we define the Wigner-transform on the scale $\epsilon$ by

$$w^\epsilon(f, g)(x, \xi) = \frac{1}{(2\pi)^d} \int_{\mathbb{R}^d} f(x - \frac{\epsilon z}{2}) \overline{g(x + \frac{\epsilon z}{2})} e^{iz\xi} dz. \quad (3.1)$$
For fixed $\varepsilon$ the phase space-valued function $w^\varepsilon$ is a continuous, bilinear mapping:

$$w^\varepsilon : \mathcal{S}'(\mathbb{R}_x^d) \times \mathcal{S}'(\mathbb{R}_\xi^d) \rightarrow \mathcal{S}'(\mathbb{R}_x^d \times \mathbb{R}_\xi^d)$$

In the following we shall use the notation: $w^\varepsilon[f] = w^\varepsilon(f, f)$.

The expression $w^\varepsilon[f]$ is realvalued and for $f \in L^2(\mathbb{R}_x^d)$ we conclude

$$\| w^\varepsilon[f] \|_2 = (4\pi\varepsilon^2)^{-d/2} \| \rho \|_2,$$

where the density "matrix" $\rho$ is defined by $\rho(x,y) := f(x) \overline{f(y)}$.

**Remark.** The Wigner-transform was originally introduced by E. Wigner in 1932 [Wi] in the context of semi-classical Quantum Mechanics. We remark that there are slightly different definitions of the Wigner transform in the literature depending essentially on the definition and normalization of the underlying Fourier transform.

The inverse Wigner transform is given by

$$\rho(x,y) \equiv f(x) \overline{f(y)} = (2\pi)^{-d} \int_{\mathbb{R}_x^d} w^\varepsilon[f] \left( \frac{x + y}{2}, \varepsilon \xi \right) e^{i\xi \cdot (x-y)} d\xi.$$  

(3.3)

Note that this transformation allows to obtain the function $f$ only up to a constant phase factor!

Now a simple calculation shows that formally

$$\int_{\mathbb{R}_x^d} w^\varepsilon[f](x, \xi, t)d\xi = |f(x,t)|^2,$$

which implies, that the energy density, as defined in (2.3), is the zeroth moment of $w^\varepsilon[\psi^\varepsilon]$ w.r.t. the velocity variable $\xi$. This is sometimes called a **microlocal decomposition of the energy** provided by the Wigner transform. A rigorous justification (Note that $w^\varepsilon$ is in general not in $L^1$.) is given by (see [LiPa] for details)

$$n^\varepsilon(x,t) = \lim_{\kappa \rightarrow 0} \int_{\mathbb{R}_x^d} w^\varepsilon[\psi^\varepsilon](x, \xi, t)e^{-\kappa|\xi|^2/2} d\xi,$$

(3.5)

which converges in $L^1$ towards $n^\varepsilon \in L^1_+(\mathbb{R}^d)$. More generally, an important feature of the Wigner transform is that it facilitates a "classical" computation of expectation values (mean values) of physical observables $A^W(x, \varepsilon D)$ in any state $\psi^\varepsilon$, namely

$$\langle \psi^\varepsilon, A^W(x, \varepsilon D)\psi^\varepsilon \rangle_{L^2} = \int_{\mathbb{R}_x^d} \int_{\mathbb{R}_x^d} A(x, \xi) w^\varepsilon[\psi^\varepsilon](x, \xi) dx d\xi.$$  

(3.6)

(Here we assume that the symbol $A(x, \xi)$ is in $\mathcal{S}(\mathbb{R}^{2d})$.) In other words the real-valued function $w^\varepsilon$ acts as an equivalent of the phase-space distribution function, however in contrast to classical phase space distributions...
the Wigner transform is in general *not point-wise positive*! Indeed it has been proved for example in [LiPa], [Hu] that \( w^\varepsilon [f] \geq 0 \) if and only if, either \( f(x) = 0 \), or \( f(x) \) is a Gaussian.

**Remark.** It is well known (see e.g. [LiPa], [MaMa], [Hu]) that averaging the Wigner function over phase space volumes large enough to fulfill the *Heisenberg uncertainty principle* yields a non-negative function. The so-called *Husimi functions* are obtained by convoluting the Wigner function \( w^\varepsilon [f] \) in \( x \) and \( \xi \) with the Gaussian

\[
G^\varepsilon (z) := (\pi \varepsilon)^{-\frac{d}{2}} \exp \left( -\frac{|z|^2}{\varepsilon} \right),
\]

s.t. they become non-negative, i.e. \( w^\varepsilon_H (x, \xi) := w^\varepsilon [f] \ast_x G^\varepsilon \ast_\xi G^\varepsilon \geq 0 \) a.e..

For the sake of illustration we present some particular examples of the "Wignerized" evolution equation (2.1):

**Examples:**

(i) The "Wignerized" Schrödinger equation (2.8) or *Wigner equation* (for details on this equation see e.g. [GaMa], [MaMa])

\[
\partial_t w^\varepsilon + \xi \cdot \nabla_x w^\varepsilon - \theta^\varepsilon [V] w^\varepsilon = 0, \quad x, \xi \in \mathbb{R}^d, t \in \mathbb{R}
\]

where \( \theta^\varepsilon [V] \) is the (non-local) pseudo-differential operator

\[
\theta^\varepsilon [V] w^\varepsilon (x, \xi, t) := \frac{i}{(2\pi)^d \varepsilon} \int_{\mathbb{R}^d} \int_{\mathbb{R}^d} [V(x + \varepsilon \frac{z}{2}) - V(x - \varepsilon \frac{z}{2})] \cdot w^\varepsilon (x, \xi, t) e^{i \varepsilon (\xi - \xi')} dz d\xi',
\]

and \( w^\varepsilon (t) := w^\varepsilon [\psi^\varepsilon (t)] \), where \( \psi^\varepsilon \) solves (2.1), (2.2). Note that in the free motion case, i.e. \( V(x) \equiv 0 \), the Wigner equation becomes the free transport equation of classical statistical mechanics

\[
\partial_t w^\varepsilon + \xi \cdot \nabla_x w^\varepsilon = 0, \quad x, \xi \in \mathbb{R}^d; t \in \mathbb{R}.
\]

Further note that in the case of potentials \( V \) which are quadratic in \( x \) the operator \( \theta^\varepsilon [V] \) simplifies to the classical force term \( \nabla_x V \) for all positive \( \varepsilon \). The harmonic oscillator, \( V(x) = \frac{|x|^2}{2} \), is a typical example

\[
\partial_t w^\varepsilon + \xi \cdot \nabla_x w^\varepsilon - x \cdot \nabla_\xi w^\varepsilon = 0, \quad x, \xi \in \mathbb{R}^d, t \in \mathbb{R}.
\]

(ii) The "Wignerized" 1-d Airy equation (2.9)

\[
\partial_t w^\varepsilon + \xi^2 \partial_x w^\varepsilon - \frac{\varepsilon^2}{12} w^\varepsilon_{xxx} = 0, \quad x, \xi, t \in \mathbb{R}.
\]

This equation is obtained after a straightforward, but lengthy calculation. ♦

We shall now perform the \( \varepsilon \to 0 \) limit associated to the dispersive equation (2.1) with initial data (2.2), assuming (A1), (A2).
3.1 The WKB-limit using Wigner transforms

One of the crucial properties (for a proof see [GMMP]) of the Wigner transform is

**Proposition 3.1.** [GMMP] If \( f \) and \( g \) lie in a bounded subset \( B \) of \( L^2(\mathbb{R}^d) \), then \( w^\varepsilon(f, g) \) is bounded uniformly in \( \mathcal{S}'(\mathbb{R}^d_x \times \mathbb{R}^d_\xi) \) as \( \varepsilon \to 0 \). More precisely we have

\[
(F_{\xi \to z}w^\varepsilon(f, g))(x, z) \in C_0(\mathbb{R}_x^d; L^1(\mathbb{R}_\xi^d))
\] (3.10)

uniformly for \( f, g \in B \) as \( \varepsilon \to 0 \).

Thus, by compactness, there exists a sub-sequence \( \varepsilon_k \) and a distribution \( w^0 \in \mathcal{S}'(\mathbb{R}_x^d \times \mathbb{R}_\xi^d) \) such that

\[
w^{\varepsilon_k}[f^{\varepsilon_k}] \xrightarrow{k \to \infty} w^0 \text{ in } \mathcal{S}'(\mathbb{R}_x^d \times \mathbb{R}_\xi^d).
\] (3.11)

It has been shown (for example in [LiPa], [MaMa]) that the limiting points of the Husimi function \( w^\varepsilon_H \) are also the limiting points of the Wigner function. Since \( w^\varepsilon_H \) is non-negative, this implies that also \( w^0 \) is non-negative. More precisely it is a positive Borel-measure, i.e. \( w^0 \in M^+ \), (the cone of bounded positive Borel measures) and therefore can be interpreted indeed as a classical phase-space measure, called the *Wigner measure* of \( f^{\varepsilon_k} \) (See [Ge], [GMMP] for a proof of the positivity of \( w^0 \)).

**Remark.** The Wigner measures are a particular version of \( L^2 \) defect measures, related to the \( H \) measures of L. Tartar [Ta] and P. Gérard [Ge]. For more details see the expository article of N. Burq [Bu].

For simplicity we now restrict the scale \( \varepsilon \) to a sub-sequence, such that the Wigner measure \( w^0 \) is unique, i.e. independent of the choice of the subsequence, and in the following we denote it by \( w = w^0 \).

We further introduce the \( d \)-dimensional Poisson-bracket of two functions \( f, g \), i.e.

\[
\{f, g\} := \nabla_x f \cdot \nabla_\xi g - \nabla_\xi f \cdot \nabla_x g.
\] (3.12)

In proposition 3.2 below we state the well known fact that the Wigner transform translates the action of an Weyl-operator asymptotically in zeroth order into a multiplication and in first order into a Poisson bracket. (A proof can be found in the appendix of [GMMP].)

**Proposition 3.2.** [GMMP] Let \( P \in S^{\sigma} \) for some \( \sigma \geq 0 \). Then if \( f, g \) lie in a bounded subset \( B \) of \( L^2(\mathbb{R}^d) \), the expansion

\[
w^\varepsilon(P^W(x, \varepsilon D)f, g) = Pw^\varepsilon(f, g) + \frac{\varepsilon}{2i}\{P, w^\varepsilon(f, g)\} + O(\varepsilon^2)
\] (3.13)

holds in \( \mathcal{S}'(\mathbb{R}_x^d \times \mathbb{R}_\xi^d) \) uniformly for \( f, g \in B \).
Now let $\psi^\varepsilon$ satisfy the IVP (2.1), (2.2). In view of (2.7) and proposition 3.1 one obtains the uniform boundness of $w^\varepsilon[\psi^\varepsilon](t)$ in $L^\infty(\mathbb{R}; \mathcal{S}^d(\mathbb{R}_x \times \mathbb{R}_\xi))$ and thus the existence of $w \in L^\infty(\mathbb{R}; \mathcal{M}^+(\mathbb{R}_x \times \mathbb{R}_\xi))$ such that
\[
\lim_{\varepsilon \to 0} w(dx,d\xi,t) \in L^\infty(\mathbb{R}; \mathcal{M}^+(\mathbb{R}_x \times \mathbb{R}_\xi)) \text{ weak-}. (3.14)
\]

Remark. It has been shown in [Ge], [GMMP], [LiPa] that the limiting process is actually locally uniform in $t$, i.e.
\[
w \in C^b(\mathbb{R}; \mathcal{M}^+(\mathbb{R}_x \times \mathbb{R}_\xi))^\star).
\]

To derive an evolution equation for the limiting phase space distribution $w$ we differentiate
\[
\partial_t w^\varepsilon = w^\varepsilon(\psi^\varepsilon_t, \psi^\varepsilon) + w^\varepsilon(\psi^\varepsilon, \psi^\varepsilon_t) = 2 \text{ Re } w^\varepsilon(\psi^\varepsilon_t, \psi^\varepsilon).
\]

Now using equation (2.1) and proposition 3.2, having in mind that $w^\varepsilon$ and $H(x,\xi)$ are real-valued, we obtain the following essential equation
\[
\partial_t w - \{H, w\} + O(\varepsilon), (3.15)
\]
which is a linear PDE in $w^\varepsilon$. Passing to the limit $\varepsilon \to 0$ yields, in the sense of distributions, the classical Liouville equation
\[
\partial_t w + \{H, w\} = 0, \quad x \in \mathbb{R}^d, t \in \mathbb{R}. (3.16)
\]

We calculate the corresponding initial data $w_I$ which is the limit of the Wigner transform of the WKB-initial data $\psi^\varepsilon_I := \sqrt{n_I} e^{iS_I/\varepsilon}$
\[
w^\varepsilon[\psi^\varepsilon_I](x,\xi) = \frac{1}{(2\pi)^d} \int_{\mathbb{R}^d} \sqrt{n_I(x - \frac{\varepsilon z}{2})n_I(x + \frac{\varepsilon z}{2})} \exp \left[ \frac{i}{\varepsilon} \left( S_I(x - \frac{\varepsilon z}{2}) - S_I(x + \frac{\varepsilon z}{2}) \right) + iz\xi \right] dz. (3.17)
\]

Lemma 3.1. Let $w^\varepsilon[\psi^\varepsilon_I]$ be given by (3.17), then
\[
w^\varepsilon[\psi^\varepsilon_I] \xrightarrow{\varepsilon \to 0} w_I := n_I(x)\delta(\xi - \nabla_x S_I(x))dx. (3.18)
\]

Proof. The proof is a straightforward computation having in mind that the amplitude $n_I(x)$ and the phase $S_I(x)$ are by assumption $\varepsilon$-independent. \qed

Remarks.

- This special type of initial phase space distributions (3.18) are called mono-kinetic initial data, i.e. for every $x \in \mathbb{R}^d$ there is exactly one (characteristic) speed $v_I(x) := \nabla S_I(x)$. Note that we have chosen the scale of oscillations in the initial data to be equal to the small parameter $\varepsilon$ in the equation (2.1).

We further remark that in case $S_I(x) \in C^\infty$ the set $\{(x, \nabla_x S_I(x))\}$ is a Lagrangian submanifold of phase-space $\mathbb{R}^{2d}$, i.e. a manifold on which the symplectic form $\omega := dx \wedge d\xi$ vanishes (for details see e.g. [Fe], [Ho]).
• The Wigner measure approach works for much more general initial data (cf [GMP], in this work we restrict to WKB data for the sake of comparison.

Further we have:

**Lemma 3.2. [GMP]** Let \( w^\varepsilon[\psi(t)] \) be the Wigner transform of the solution of (2.1) (2.2) (calculated from (3.16), (3.18)) and assume (A1), (A2), then the associated density \( n^\varepsilon(x,t) \) given by (3.4) satisfies

\[
n^\varepsilon(x,t) \xrightarrow{\varepsilon \to 0} n(x,t) := \int_{\mathbb{R}^d} w(x,d\xi,t) \in \mathcal{C}_b(\mathbb{R}^d; \mathcal{M}^+(\mathbb{R}^d)) \quad (3.19)
\]

where the convergence is locally uniform in \( t \).

**Proof.** A proof can be found for example in [GaMa], [GMP], [LiPa]. Note that the technical assumptions of "\( \varepsilon \)-oscillatory" and "compact at infinity" initial data, which are introduced in [Ge], [GMP], are fulfilled if one imposes (A2).

**Remark.** One can show that the \( \varepsilon \to 0 \) limit of other observables \( A^W \), or more general expressions which are quadratic in \( \psi^\varepsilon \) with a specific growth in \( \xi \), can be computed essentially in the same way, i.e. the limit is given by the right hand side of (3.6) with \( w^\varepsilon \) replaced by \( w \). For details see again [GaMa], [GMP], [LiPa].

Thus by using the Wigner transform we obtained a (semi-) classical phase-space description, which we shall analyse in the next section.

### 4 Analysis of the Wigner measure

This is the main part of the work, in which we will try to establish the precise relation between WKB-asymptotic solutions of (2.1) and the Wigner measure that has been obtained in the last section. We start with the following definition:

**Definition 4.1.** The Hamiltonian flow \( F_t \) associated to the Liouville equation (3.16) is given by

\[
F_t(x,\xi) = (\tilde{x}(t,x,\xi),\tilde{\xi}(t,x,\xi))
\]

where \((\tilde{x}, \tilde{\xi})\) solve the initial value problem

\[
\frac{d\tilde{x}}{dt} = \nabla_\xi H(\tilde{x}, \tilde{\xi}), \quad \tilde{x}(0,x,\xi) = x \quad (4.2)
\]

\[
\frac{d\tilde{\xi}}{dt} = -\nabla_y H(\tilde{x}, \tilde{\xi}), \quad \tilde{\xi}(0,x,\xi) = \xi. \quad (4.3)
\]

**Remark.** The above ODE's are usually referred to as Hamilton's equations and the curves \((\tilde{x}, \tilde{\xi})\) are often called bicharacteristics.
For the sake of simplicity we shall assume in the sequel:

**Assumption (A3)**

The Hamiltonian flow $F_t$ is a continuously differentiable globally defined map for every $t \in \mathbb{R}$.

**Remark.** The global existence of $F_t$ is a priori not guaranteed for general $H \in S^\sigma$, except for $\sigma \leq 1$. (For more details see for example [Ar], [ReSi].) We further remark that well known situations for which (A3) is valid, like the case of $\alpha$-elliptic Hamiltonians $H \geq C_1|\xi|^\alpha - C_2$ with $C_1, C_2, \alpha > 0$ are covered by our theory.

An illustrative example where the Hamiltonian flow is not global in time is given in Appendix 1.

A straightforward calculation shows that the Hamiltonian function $H(x, \xi)$ is constant along the flow $F_t$, i.e.

$$H(\tilde{x}(t, x, \xi), \tilde{\xi}(t, x, \xi)) = H(x, \xi), \quad \forall \ t \in \mathbb{R}, x, \xi \in \mathbb{R}^d. \quad (4.4)$$

Also, by the classical Theorem of Liouville (see e.g. [Ar]), we have that $F_t$ is volume preserving; i.e. its Jacobian satisfies

$$\det \left( \frac{\partial (\tilde{x}(t, x, \xi), \tilde{\xi}(t, x, \xi))}{\partial (x, \xi)} \right) = 1, \quad \forall \ t \in \mathbb{R}, x, \xi \in \mathbb{R}^d. \quad (4.5)$$

With the above definitions the method of characteristics guarantees that the unique (weak) solution of the Liouville equation (3.16) subject to the initial condition $w(t = 0) = w_I \in \mathcal{M}^+(\mathbb{R}_x^d \times \mathbb{R}_\xi^d)$ satisfies

$$\int_{\mathbb{R}^d} \int_{\mathbb{R}^d} \varphi(x, \xi) w(dx, d\xi, t) = \int_{\mathbb{R}^d} \int_{\mathbb{R}^d} \varphi(F_t(x, \xi)) w_I(dx, d\xi) \quad (4.6)$$

for all test functions $\varphi \in C_b(\mathbb{R}_x^d \times \mathbb{R}_\xi^d)$. In other words the solution $w$ of (3.16) remains constant along all bicharacteristic curves $(\tilde{x}, \tilde{\xi})$. Since (3.16) is a linear equation and (A3) is assumed we know that the above solution $w$ exists for all $t \in \mathbb{R}$. In contrast to the case of a nonlinear first order PDE we have global solutions for equation (3.16); i.e. no caustics appear in phase space! This is sometimes referred to as "unfolding" of caustics.

In the next subsection we connect the WKB-system (2.15), (2.16) with a special class of solutions to the Liouville-equation, which we shall link to the traditional WKB method in the pre-caustic regime.

### 4.1 On mono-kinetic phase space distributions

Taking into account the monokinetic form of the initial data, we observe that, with the use of equation (3.18), identity (4.6) reads

$$\int_{\mathbb{R}^d} \int_{\mathbb{R}^d} \varphi(x, \xi) w(dx, d\xi, t) = \int_{\mathbb{R}^d} n_I(x) \varphi(\hat{x}(t, x), \hat{\xi}(t, x)) \ dx, \quad (4.7)$$
for all $\varphi \in C_b(\mathbb{R}^d_x \times \mathbb{R}^d_\xi)$ where the curves $(\hat{x}(t, x), \hat{\xi}(t, x))$ solve the IVP (2.31), (2.32). Note that, since the initial data are given by $\xi = \nabla_x S_I(x)$, the curves $\hat{x}(t, x)$ are the rays associated to the Hamilton-Jacobi equation

$$\partial_t S + H(x, \nabla_x S) = 0, \quad S(x, 0) = S_I(x).$$

The above reflects the fact that the $(\tilde{x}, \tilde{\xi})(t, x, \xi)$ bicharacteristics in phase space are projected down to rays $\hat{x}(t, x)$ in position space plus an additional curve $\hat{\xi}(t, x)$, which is the gradient of the phase $S$ along the rays. More precisely, we have

$$(\hat{x}, \hat{\xi})(t, x) = (\tilde{x}, \tilde{\xi})(t, x, \nabla_x S_I(x)).$$

The function $S$ is often called the generating function of the flow $F_t$.

We shall use the following lemma for the proof of theorem 4.1.

**Lemma 4.1.** Assume (A1)-(A3) and let $w(t)$ be a (weak) solution of (3.16) with mono-kinetic initial data $w_I$ (3.18). Then $\forall t \in \mathbb{R}$

$$\int_{\mathbb{R}^d_x} \int_{\mathbb{R}^d_\xi} \phi(H(x, \xi)) w(dx, d\xi, t) = \int_{\mathbb{R}^d_x} \phi(H(x, v_I(x))) n_I(dx)$$

for every real valued continuous and bounded from below function $\phi$ for which the right hand side of (4.1) is finite.

**Proof.** At first take $\phi \in C(\mathbb{R})$ bounded. Setting $\varphi(x, \xi) = \phi(H(x, \xi))$ in (4.7) combined with the fact that $H(\tilde{x}, \tilde{\xi})$ is conserved proves the claim. For unbounded $\phi$ a density argument gives the result. \qed

**Remark.** If the Hamiltonian is bounded from below and gauged such that $H(x, \xi) \geq 0$ the above lemma states the energy conservation property of the Liouville equation, when setting $\phi(\cdot) = \text{id}$ on $\mathbb{R}^+$. 

**Definition 4.2.** We define the following set of functions:

$$\Lambda := \{ \lambda \in C(\mathbb{R}; \mathbb{R}^+) : \int_{\mathbb{R}^d_x} \int_{\mathbb{R}^d_\xi} \lambda(H(x, \xi)) w_I(dx, d\xi) < \infty \}. \quad (4.10)$$

Now the following theorem holds:

**Theorem 4.1.** Assume (A1)-(A3) and let $-\infty < t_{c_1} < 0 < t_{c_2} \leq \infty$.

(i) The unique (weak) solution of (3.16)

$$\partial_t w + \{H, w\} = 0 \quad \text{in } D'(\mathbb{R}^d_x \times \mathbb{R}^d_\xi \times (t_{c_1}, t_{c_2}))$$

is given by

$$w(x, \xi, t) = n(x, t) \delta(\xi - v(x, t)), \quad (4.11)$$
if and only if the pair \((n, v)(x, t),\) where \(n \in C_0((t_{c_1}, t_{c_2}); \mathcal{M}^+(\mathbb{R}^d))\) and \(v \in L^\infty((t_{c_1}, t_{c_2}); L^1(\mathbb{R}^d; dn(t))^d)\) is a solution of
\[
\partial_t(n \sigma(v)) + \text{div}(n \sigma(v) \nabla \xi H(x, v)) + n \nabla \xi \sigma(v) \nabla y H(x, v) = 0 \quad (4.12)
\]
in \(\mathcal{D}'(\mathbb{R}^d \times (t_{c_1}, t_{c_2}))\), for every \(\sigma \in C^1(\mathbb{R}^d)\) for which there exists a \(\lambda \in \Lambda\) such that:
\[
\frac{|\sigma|}{1 + \lambda(H)} \in L^\infty(\mathbb{R}^d), \quad \frac{|\sigma| \nabla \xi H}{1 + \lambda(H)} \in L^\infty(\mathbb{R}^d), \quad \frac{|\nabla \xi \sigma| \nabla y H}{1 + \lambda(H)} \in L^\infty(\mathbb{R}^d).
\]
(4.13)
(ii) Moreover if \(H\) is such that \(\sigma \equiv 1\) and \(\sigma \equiv v_i, i = 1 \ldots d\) satisfy (4.13), then the monokinetic solution \((4.11)\) is uniquely determined by the following system of fluid-type equations
\[
\begin{align*}
\partial_t n + \text{div}(n \nabla \xi H(x, v)) &= 0, \quad (4.14) \\
\partial_t (n v) + \text{div}(\nabla \xi H(x, v) \otimes n v) + n \nabla y H(x, v) &= 0 \quad (4.15)
\end{align*}
\]
in \(\mathcal{D}'(\mathbb{R}^d \times (t_{c_1}, t_{c_2}))\) with initial data
\[
n(x, 0) = n_I(x), \quad v(x, 0) = v_I(x). \quad (4.16)
\]
The equation (4.12) is called a generalized formulation of the system (4.14), (4.15). It reflects the fact, that different moments of the monokinetic Wigner measure can be chosen, which is sometimes useful for numerical purposes.

**Proof.** Choose a test function \(\varphi = \gamma(x, t) \sigma(\xi) \in \mathcal{D}(\mathbb{R}^d_x \times \mathbb{R}_\xi \times (t_{c_1}, t_{c_2}))\), then the weak formulation of (4.16) reads:
\[
\int_{t_{c_1}}^{t_{c_2}} \int_{\mathbb{R}^d} \int_{\mathbb{R}_\xi} [(\sigma(\xi) \partial_t + \sigma(\xi) \nabla \xi H(x, \xi) \cdot \nabla x) \gamma(x, t) \\
- \nabla y H(x, \xi) \cdot \nabla \xi \sigma(\xi) \gamma(x, t)] \ w(dx, d\xi, dt) = 0
\]
by inserting \(w\) given by (4.11) we obtain:
\[
\int_{t_{c_1}}^{t_{c_2}} \int_{\mathbb{R}^d} \int_{\mathbb{R}_\xi} [(\sigma(v(x, t)) \partial_t + \sigma(v(x, t)) \nabla \xi H(x, v(x, t)) \cdot \nabla x) \gamma(x, t) \\
- \nabla y H(x, v(x, t)) \cdot \nabla \xi \sigma(v(x, t)) \gamma(x, t)] \ n(dx, dt) = 0
\]
which is exactly the weak formulation of (4.12). Now let \(\sigma_l \in \mathcal{D}(\mathbb{R}_\xi^d)\) be a sequence of test functions satisfying the conditions stated in the theorem and converging a.e. to \(\sigma \in C^1(\mathbb{R}_\xi^d)\) as \(l \to \infty\). Because the test functions \(\sigma_l\) satisfy the conditions above (4.13), the dominated convergence theorem (with the use of lemma 4.1. and definition 4.2. implies the assertion (ii). Now we can choose successively \(\sigma \equiv 1\) and \(\sigma \equiv v_i, i = 1, \ldots, d\) in equation (4.12) to obtain the system (4.14), (4.15).
\[\square\]
Remark. Note that in case $H$ is given by
\[ H(x, \xi) = \frac{|\xi|^2}{2} + V(x), \quad x, \xi \in \mathbb{R}^d, \] (4.17)
where $V$ is bounded from below we can choose $\lambda(\cdot) = \text{id}$ and the above system of fluid-type equations (4.14), (4.15) simplifies to the well known zero-temperature Euler-equations of rarefied gas dynamics
\[ \partial_t n + \text{div}(nv) = 0, \quad x \in \mathbb{R}^d, t \in (t_{c_1}, t_{c_2}) \] (4.18)
\[ \partial_t (nv) + \text{div}(nv \otimes v) + n \nabla_x V = 0, \] (4.19)
\[ n(x, 0) = n_I, \quad v(x, 0) = v_I, \] (4.20)
which is, for $t_{c_1} < t < t_{c_2}$, the $\varepsilon \to 0$ limit of the QHD system (1.4), (1.5) that has been mentioned in the introduction.

We now establish the precise connection between the WKB-system (2.15), (2.16) and the above theorem in the following corollary.

Corollary 4.1. Let $(t_{c_1}, t_{c_2})$ be as above;
(i) Further let $S \in C^2(\mathbb{R}^d \times (t_{c_1}, t_{c_2}))$ be a smooth solution of the Hamilton-Jacobi equation (2.16)
\[ \partial_t S + H(x, \nabla_x S) = 0, \quad S(x, 0) = S_I(x). \]
Define $v(x, t) := \nabla_x S(x, t)$, and let $n$ be the unique solution of (4.15), then $(n, v)$ satisfies (4.14), (4.15) and is a generalized solution in the sense defined above.
(ii) Let $(n, v) \in C^1(\mathbb{R}^d \times (t_{c_1}, t_{c_2}))$ be a smooth solution of (4.14), (4.15). If the initial velocity is given by $v_I(x) = \nabla_x S_I(x) \in C^1(\mathbb{R}^d)$, then there exists a phase function $S(x, t)$, unique up to a constant, which is a solution of (2.14) on the same time interval. In particular the velocity $v$ is a gradient field and the solution of (3.16) can be written in the form
\[ w(x, \xi, t) = n(x, t)\delta(\xi - \nabla_x S(x, t)) \in C_b((t_{c_1}, t_{c_2}); M^+(\mathbb{R}^d \times \mathbb{R}^d_\xi)). \]

Proof. Differentiating (2.16) w.r.t. $x_i$ and using the chain rule (which is rigorous because we are in the regime of classical solutions) yields
\[ \partial_{x_i}^2 S + \frac{\partial}{\partial y_i} H(x, \nabla_x S) + \nabla_\xi H(x, \nabla_x S) \cdot \frac{\partial}{\partial x_i} \nabla_x S = 0 \]
and, with $v_i := \frac{\partial}{\partial x_i} S$ we get
\[ \partial_t v + (\nabla_\xi H(x, v) \cdot \nabla_x) v + \nabla_y H(x, v) = 0. \] (4.21)
We multiply by $\nabla_v \sigma(v)$ to obtain
\[ \sigma v_t + (\nabla_\xi H(x, v) \cdot \nabla_x) \sigma(v) + \nabla_v \sigma(v) \nabla_y H(x, v) = 0. \]
Again multiplying this equation by a regular solution $n$ of the continuity equation (1.14) yields (1.13). Hence choosing appropriate test functions
we have proved that \((n, v)\) is a generalized solution on \((t_{c_1}, t_{c_2})\). We prove claim (ii), by first eliminating \(n\) from equation (4.12). Using (4.11) we obtain on \((t_{c_1}, t_{c_2})\) the equation (4.21) above subject to \(v(x, 0) = \nabla_x S_I(x)\). One checks that the characteristic ODE system for this PDE is given by (2.31), (2.32). Thus we can identify \(v(\hat{x}(t, x), t) = \hat{\xi}(x, t)\) and conclude the existence of a unique (up to a constant) function \(S(x, t)\) s.t. \(v = \nabla_x S\). The rest of the proof is identical to the one of (i) read from bottom up.

Note that the system (4.14), (4.15) is defined \(n(t)\)-a.e. and thus remains valid as long as the density is single-valued! In particular this holds in the examples 1.2, 2 in section 5 below.

4.2 Multiple phases

We will now show, under some more stringent assumptions, that away from the caustic we can locally extend \(w(t)\) beyond \(t_{c_1,2}\) as a sum over mono-kinetic distributions, which will lead to a generalization of the asymptotic expression of the solution \(\psi^\varepsilon(t)\) of (2.1).

Since the Wigner measure remains constant along the flow \(F_t\), we can write for \(\varphi \in C_b(\mathbb{R}_x^d \times \mathbb{R}_\xi^d)\)

\[
\langle w(t), \varphi \rangle = \langle w_I(F_{-t}), \varphi \rangle = \langle n_I(\hat{x}(-t, x, \xi)) \delta(f_{x,t}(\xi)), \varphi \rangle \tag{4.22}
\]

where \(\langle \cdot, \cdot \rangle\) denotes the duality bracket in the sense of measures and further we have used the following definition:

**Definition 4.3.** The mapping \(f_{x,t}(\cdot) \in C^1 : \mathbb{R}^d \rightarrow \mathbb{R}^d\) is defined by

\[
f_{x,t}(\xi) := \hat{\xi}(-t, x, \xi) - \nabla_x S_I(\hat{x}(-t, x, \xi)). \tag{4.23}
\]

Above \((x, t)\) are parameters as the notation indicates.

**Definition 4.4.** We denote the nullset of \(f_{x,t}(\cdot)\) by

\[
\mathcal{K}(x, t) := \{ \xi \in \mathbb{R}^d : f_{x,t}(\xi) = 0 \} \tag{4.24}
\]

and the corresponding functional determinant by

\[
Df_{x,t}(\xi) := \det \left( \frac{\partial f_{x,t}(\xi)}{\partial \xi} \right). \tag{4.25}
\]

In general we cannot hope for \(f_{x,t}(\cdot)\) to be a diffeomorphism in the whole propagation domain, at least we can get local results if we impose:

**Assumption (A4)**

Let \(U \subseteq \mathbb{R}_x^d \times \mathbb{R}_t^d\) be such an open set and \(N \in \mathbb{N}\) be such an integer that the nullset (4.24) can be written as

\[
\mathcal{K}(x, t) = \bigcup_{i=1}^N \{ v_i(x, t) \} \quad \text{for all } (x, t) \in U. \tag{4.26}
\]
This means that we only allow situations with a finite number $N$ of (gradients of) phases at each point of the propagation domain. Of course $w$ is well defined even if (A4) does not hold, however in general no upper bound $N$ can be found, $N = \infty$ is possible!

**Remark.** Indeed very little is known about this problem in general situations, so far the only well studied example is the one dimensional free motion case, i.e. $H = H(\xi), \xi \in \mathbb{R}$. Under the additional assumption that $H(\xi)$ is strictly convex, i.e. there exists $c > 0$ such that $H''(\xi) \geq c$, Tadmor and Tassa have shown in [TaTa], that if $H'(S'_i(x))$ has a finite number of inflection points, then the number number of "original" shocks, i.e. shocks that do not result from the interaction of other shocks, in the entropy solution to the corresponding conservation law is finite, which implies (A4). An example of an initial condition $\nabla S_I$ which evolves, in the particular case of $H = \xi^2/2$, into an a.e. $C^\infty$ function with countably many original shocks can be found in [Sch].

**Theorem 4.2.** Assume (A1)-(A4) and denote by $v_i(x,t), i = 1 \ldots N$, the elements of the nullset $\mathcal{K}(x,t)$.

If the point $(x,t) \in \mathcal{U}$ is such, that $Df_{x,t}(v_i) \neq 0$ for all $i = 1 \ldots N$, then the measure-valued solution of the Liouville equation (4.14) can be written as

$$w(x,\xi,t) = \sum_{i=1}^{N} \frac{n_I (\tilde{\tau}(-t,x,\nabla_x S_i(x,t)))}{|Df_{x,t}(\nabla_x S_i(x,t))|} \delta(\xi - \nabla_x S_i(x,t))$$

(4.27)

where $S_i \in C^2_\text{loc}(\mathcal{U})$ such that $\nabla_x S_i = v_i \in \mathcal{K}(x,t)$ for all $i \in \{1 \ldots N\}$.

**Proof.** Choose tests functions $\varphi(x,\xi,t) = \gamma(x,t)\sigma(\xi) \in C^0_b(\mathbb{R}^d; C^b_b(\mathbb{R}^d))$.

As above we write

$$\langle w(t), \varphi \rangle = \langle n_I (\tilde{\tau}(-t,x,\xi))\delta(f_{x,t}(\xi)), \varphi \rangle.$$  

(4.28)

By the coarea formula (see [Ev], [Fe]) we have

$$\langle \delta(f_{x,t}(\xi)), \sigma(\xi) \rangle = \langle \delta(\zeta), \bar{\sigma}_{x,t}(\zeta) \rangle$$

with

$$\bar{\sigma}_{x,t}(\zeta) := \int_{\{f_{x,t}^{-1}(\zeta)\}} \sigma(\xi) \frac{d\xi}{|Df_{x,t}(\xi)|},$$

(4.29)

which is well defined as long as $Df_{x,t}(\xi) \neq 0$, even if $f_{x,t}(\xi)$ is not an isomorphism for all points $\xi \in \mathbb{R}^d$! By the definition of the delta distribution the above is equal to

$$\langle \delta(\zeta), \bar{\sigma}(\zeta) \rangle \equiv \bar{\sigma}(0) = \int_{\mathcal{K}(x,t)} \sigma(\xi) \frac{d\xi}{|Df_{x,t}(\xi)|},$$

since $\{f_{x,t}^{-1}(0)\} = \{\xi \in \mathbb{R}^d : f_{x,t}(\xi) = 0\} =: \mathcal{K}(x,t)$. By assumption (A4) we have that $\mathcal{K}(x,t)$ is a finite union of points $v_i(x,t)$, thus we can
evaluate the integral in terms of
\[
\int_{\mathcal{K}(x,t)} \sigma(\xi) \frac{d\xi}{|Df_{x,t}(\xi)|} = \sum_{i=1}^{N} \frac{\sigma(v_i(x,t))}{|Df_{x,t}(v_i(x,t))|},
\]
which in the sense of measures can be written in the form
\[
\sum_{i=1}^{N} \frac{\langle \delta(\xi - v_i(x,t)), \sigma(\xi) \rangle}{|Df_{x,t}(v_i(x,t))|}.
\] (4.30)

The local differentiability of \(v_i, i = 1 \ldots N\), is a direct consequence of the implicit function theorem. The existence of phase functions \(S_i(x,t)\) such that \(v_i = \nabla_x S_i\) can be concluded essentially in the same way as in Corollary 4.1, using
\[
f_{x,0}(\xi) = \xi - \nabla_x S_I(x)
\] (4.31)
and thus
\[
f_{x,0}(v_i(x,0)) = v_i(x,0) - \nabla_x S_I(x) = 0
\] (4.32)
since by construction \(v_i(x,t) \in \mathcal{K}(x,t)\). Thus we obtain (4.27) by inserting (4.30) into (4.28).

In view of the above theorem we can now define the **caustic set** \(\mathcal{C} \subset \mathbb{R}^d_x \times \mathbb{R}_t\) by

**Definition 4.5.**
\[
\mathcal{C} := \{(x,t) : Df_{x,t}(\xi) = 0 \text{ for at least one } \xi \in \mathcal{K}(x,t)\}
\] (4.33)

This definition becomes more clear by the following lemma.

**Lemma 4.2.** Denote by \(\hat{x}^{-1}(t,x) \subseteq \mathbb{R}^d\) the pre-image of the point \((x,t)\) under the flow \(\hat{x}(t,\cdot)\) (i.e. the set of all points \(z\) with \(\hat{x}(t,z) = x\)) and by \(\hat{x}(t,\cdot)\) the (locally defined) inverse map of \(\hat{x}(t,\cdot)\). Let \(\mathcal{V} \subseteq \mathbb{R}^d_x \times \mathbb{R}_t\) be such that there exists only one \(v = \nabla_x S \in \mathcal{K}(x,t)\), then we have
\[
|Df_{x,t}(\nabla_x S)| \equiv J(\hat{x}(t,x),t), \quad \forall (x,t) \in \mathcal{V}
\] (4.34)
where
\[
J(z,t) := |\det \left( \frac{\partial \hat{x}(t,z)}{\partial z} \right)|.
\] (4.35)

Thus the Jacobian \(J\) of the rays \(\hat{x}(t,x)\) becomes zero at the caustics, c.f. theorem 4.3. This property is usually used to define caustics in the WKB-framework (see e.g. [BKM], [Fed]).

**Proof.** The claim follows directly from identity (4.6), having in mind that if there exist only one \(v \in \mathcal{K}(x,t)\) then \(\hat{x}(t,\cdot)\) is locally one-to-one and
thus we can apply the transformation law of integrals (see \[4.4\]) on the right hand side of (4.6), to obtain
\[
n(x, t) = n_f(\hat{x}(t, x)) \left| \det \left( \frac{\partial \hat{x}(t, x)}{\partial x} \right) \right|.
\]
Since \(\hat{x}(t, \cdot)\) in this case is, by assumption, invertible the basic calculus for determinants implies
\[
n(x, t) = n_f(\hat{x}(t, x)) \frac{1}{J(\hat{x}(t, x), t)}.
\]
Finally note that \(\hat{x}(t, x) = \tilde{x}(t - x, v(x, t))\) with \(v = \nabla_S(t, x)\) as long as \(\hat{x}(t, \cdot)\) is one-to-one. Thus the claim is proven. \(\square\)

Note that (4.36) is the solution of the conservation law (2.15) before the caustic onset, i.e. for \(t \leq t_{c_1}, t \geq t_{c_2}\).

We have obtained a multivalued description of the solution of the WKB-system for all \(t \in \mathbb{R}\), locally away from caustics \(C\), by representing the limiting phase space density \(w(t)\) as a sum over mono-kinetic terms, each of which can be associated to a single branch of the multivalued solution of the Hamilton-Jacobi equation (2.16). Note however that, since \(\nabla_x S_i = \nabla_x S_i\) with \(S_i(x, t) = S_i(x, t) + C_i, C_i \in \mathbb{R}\), it is clear that for each \(v_i \in K\) we obtain the corresponding phase \(S_i\) only up to a constant.

**Remark.** Physically the multivaluedness can be interpreted as interference of the wave with itself, or in terms of classical mechanics, that faster particles overtake slower ones for times \(t \leq t_{c_1}, t \geq t_{c_2}\).

To close the argument, the following corollary shows, that the Wigner measure given by (4.27) is indeed the limiting measure of a superposition of (WKB) waves.

**Corollary 4.2.** Assume (A1)-(A4). and let \(U \cap C = \emptyset\), with \(C\) defined in (4.33). Define for all \((x, t) \in U\) a generalized WKB-asymptotic solution
\[
\psi_{\text{wkb}}^\varepsilon(x, t) := \sum_{k=1}^N \sqrt{n_i(x, t)} \exp \left( \frac{i}{\varepsilon} S_i(x, t) \right), \quad (x, t) \in U
\]
where \(\nabla_x S_i \in K, \forall i = 1 \ldots N\) and each branch of the energy density reads
\[
n_i(x, t) := \frac{n_f(\hat{x}(-t, x, \nabla_x S_i(x, t)))}{|Df_{x,t}(\nabla_x S_i(x, t))|}.
\]
For a localization let \(\phi \in C_0^\infty(\mathbb{R}_d \times \mathbb{R}_t)\) with \(\text{supp} \phi \subseteq U\). Then the unique (semi-)classical Wigner measure \(w_\phi\) of \(\phi \psi_{\text{wkb}}^\varepsilon\) is given by (4.27) multiplied by \(\phi^2\).
Proof. Having in mind lemma 3.1, the proof follows directly from the fact (see [Ge]) that if \( f^\varepsilon, g^\varepsilon \) have Wigner measures \( w_f, w_g \), which are mutually singular, i.e. there exist two disjoint Borel-sets \( A, B \) with \( w_f(A^c) = 0, w_g(B^c) = 0 \), then
\[
w^\varepsilon \left[ f^\varepsilon + g^\varepsilon \right] \xrightarrow{\varepsilon \to 0} w_f + w_g \text{ in } S'(\mathbb{R}^d_x \times \mathbb{R}_\xi^d).
\]
(4.39)

Clearly this is true in our case, since each term in the expression (4.27) is a measure which is supported on \( \{ (x, \nabla_x S_i(x,t)) \} \). By construction, we have \( \nabla_x S_i \neq \nabla_x S_j \) for \( i \neq j \), which implies the assertion.

Observe that \( \psi_w \text{ does not explicitly contain the so called } \text{"Maslov-phase shifts"} \) (c.f. section 2.3) due to the fact that each branch of the multivalued phase \( S_i \), obtained by our kinetic approach, is uniquely determined only up to a constant, which is not explicitly specified by the approach. In each region \( \mathcal{U} \) the Maslov indices are such constants. More precisely, we connect the notation used in our Wigner measure approach with the one used in section 2.3 (FIO’s) by stressing that
\[
z_i(x,t) = \tilde{x}(-t,x,\nabla_x S_i(x,t)),
S_i(x,t) = S_I(z_i(x,t)) + \varepsilon\frac{\pi}{4} m_i.
\]

On the other hand it is clear, see section 2.3 and e.g. [GuSt], for more details, that once the the Lagrangian manifold generated by \( \nabla_x S_i(t,x) \) is given, the Maslov phase shift can be calculated from it from purely geometrical considerations. Thus although it does not appear explicitly, the Wigner measure (in the representation (4.27)) contains all information needed to obtain the phase shift, which then allows the construction of the correct multivalued WKB-expansion after the caustic.

Remark. Although the Wigner measure gives the correct multivalued description after the first caustic its computation in general is quite labourintensive, in particular since it involves \( 2d + 1 \) variables. From a numerical point of view one would like to work in physical space \( \mathbb{R}^d_x \times \mathbb{R}_t \). This requires the approximation of \( w \) by a system of \( 2N \) equations for the \( 2N \) unknowns \( (n_i, v_i) \), \( 1 \leq i \leq N \). This system for the \( 2N \) moments of \( w \) in general is not closed. However, in geometrical optics, the multivalued form of the Wigner measure (for a fixed \( N \)) gives a closing condition which allows (in principle) the correct description of multivalued situations until the next caustic forms. For details on this problem (in \( d = 1 \)) see [JiLi] and for some alternative approaches we refer to [Be1], [Be2], [Ru].

4.3 Concentration effects

We now describe the behavior of the density at focal points, which typically arise as the onset of caustics. We will be able to distinguish between two specific cases of energy concentrations.
Theorem 4.3. Fix $t \neq 0, y \in \mathbb{R}^d$ and let $\mathcal{V} \subseteq \mathbb{R}_x^d \times \mathbb{R}_t$ be a region (closed set), with $(y,t) \in \mathcal{V}$, such that there exists only one $v \in K(x,t)$ for all $(x,t) \in \mathcal{V}$. Further assume that there exists $r > 0$ such that $\{(x,t) : |y - x| < r\} \subseteq \mathcal{V}$. Then we have

$$n(x,t) = \frac{n_I(\tilde{x}(t,x,v))}{|Df_{x,t}(v(x,t))|} \chi_{\{x \neq y\}} + \mu \delta(x-y), \quad |y - x| < r \quad (4.40)$$

where $\chi$ denotes the characteristic function and

$$\mu := \int_{\{\tilde{x}^{-1}(y,t)\}} n_I(z)dz. \quad (4.41)$$

Proof. Applying identity (4.6) to the monokinetic form of the initial data with $\varphi(x,\xi) = \gamma(x)$ we obtain

$$\int_{\mathbb{R}^d} \gamma(x)n(dx,t) = \int_{\mathbb{R}^d} n_I(x)\gamma(\dot{x}(t,x))dx$$

Thus we can write

$$\int_{\mathbb{R}^d} \gamma(x)n(dx,t) = \int_{\mathbb{R}^d} n_I(x)\gamma(\dot{x}(t,x))\chi_{\{x \neq \tilde{x}^{-1}(y,t)\}}dx + \int_{\mathbb{R}^d} n_I(x)\gamma(\dot{x}(t,x))\chi_{\{x \in \tilde{x}^{-1}(y,t)\}}dx. \quad (4.42)$$

Now let $\gamma(\dot{x}(t,\cdot))$ be supported in $\{x \in \mathbb{R}^d : |y - x| < r\}$. In the last term of the right hand side we obtain

$$\gamma(y)\int_{\{\tilde{x}^{-1}(y,t)\}} n_I(z)dz \equiv \langle \mu \delta(x-y), \gamma(x) \rangle$$

where $\langle \cdot, \cdot \rangle$ denotes the duality bracket. In the first term on the right hand side the transformation law of integrals can be applied thus using lemma 4.2 we obtain the expression (4.40) which proves the claim.

If there is a nonzero amount of initial mass $\mu$ carried by rays into the point $(y,t)$ the energy density $n$ "concentrates" as the last term of (4.40) shows. This is also an explanation of the word "caustic", since its Greek origin means "which burns". We shall refer to these caustic points as "hot".

We deduce from the theorem above the following easy consequences:

Corollary 4.3. If $w_I(\{\tilde{x}^{-1}(t,y)\} \times \mathbb{R}_x^d) = 0$, then locally around $y$

$$n(x,t) = \frac{n_I(\tilde{x}(t,x))}{J(\tilde{x}(t,x))} \chi_{\{x \neq y\}}, \quad (x,t) \in \mathcal{V}. \quad (4.43)$$

In particular the density remains in $L^1_{loc}(\mathbb{R}^d)$ in this case. Clearly if $\tilde{x}(t,\cdot)$ is a diffeomorphism in $\mathcal{V}$ the expression (4.43) is valid for all $(x,t) \in \mathcal{V}$.
Proof. The claim follows from \( n_I(A) = 0 \) iff \( w_I(A \times \mathbb{R}^d) = 0 \), where \( A \) is an arbitrary Borel set.

It is important to note, that although the amplitude blows up at the caustic \( C \), the density \( n \), still makes sense as a measure. For this reason the amplitude is sometimes called \( \text{half-density} \). In other words: Although some rays \( \hat{x}(t, \cdot) \) may cross, the density, as the corollary shows, may still be in \( L^{1}_{\text{loc}}(\mathbb{R}^d) \). This will be referred to as a "cool" caustic point, in contrast to a hot caustic where we obtain a concentration of the density. A particular case of such a cool caustic is given in example 1.3. in section 5 below. (See also [MPP] for a numerical study.) Another cool caustic is given by example 1 in [GaMa].

Remark. Clearly the above theorem and corollary can be extended to regions in which finitely many (gradients of) phases appear. This is in particular true for points on the one dimensional cusp-caustic (see example 1.3), where within the caustic region we have 3 zeros \( v_i(x, t) \) and outside there is only one. Thus we obtain cool focus points on each branch of the caustic, whereas the caustic-onset point, or focus point, is hot.

5 Case studies

We now illustrate the above analysis with examples.

1. Free motion

One should note that the following calculations are generalizations of the formulas given in the example of the free Schrödinger equation in section 2.3.

Although the generalized free motion case, i.e.

\[
H = H(\xi),
\]

is the most simple one, it nevertheless features a remarkable variety of interesting phenomena. The associated Hamiltonian flow is given by

\[
F_t(x, \xi) = (x + t\nabla_\xi H(\xi), \xi).
\]

The velocity remains constant \( \tilde{\xi}(t, x, \xi) = \xi \), \( \forall t \in \mathbb{R}, x, \xi \in \mathbb{R}^d \) and thus the rays are straight lines, with slope \( \nabla_\xi H(\nabla_x S_I(x)) \), i.e. we have \( \hat{x}(t, x) = x + t\nabla_\xi H(\nabla_x S_I(x)) \). In this particular case definition 4.2 reads

\[
f_{x, t}(\xi) := \xi - \nabla_x S_I(x - t\nabla_\xi H(\xi))
\]

and its zeros \( v_i(x, t) \in \mathcal{K}(x, t) \) satisfy the implicit relation

\[
v_i(x, t) = \nabla_x S_I(x - t\nabla_\xi H(v_i(x, t)))
\]
This is the well known (multivalued) implicit solution formula of the conservation law
\[
\begin{align*}
\partial_t v + \nabla_x H(v) &= 0, \quad x \in \mathbb{R}^d, t \in \mathbb{R} \\
v_I(x, 0) &= \nabla_x S_I(x),
\end{align*}
\]
which holds as long as the determinant of the Jacobian is nonzero
\[
Df_{x,t}(v_i) = \operatorname{det}(I + tD^2S_I(x - t\nabla_\xi H(v_i))D^2H(v_i)) \neq 0
\]
(Here \(D^2f\) denotes the Hessian of \(f\).) The multivalued phase \(S_I(x, t)\) is obtained, locally in each region \(U\) in which \(N\) is constant, by using standard Hamilton-Jacobi theory, i.e. by integrating (2.33)
\[
\frac{dS_i(\hat{x}, t)}{dt} = H'(\hat{\xi}) \cdot \hat{\xi} - H(\hat{\xi}), \quad S_i(x, 0) = S_I(x)
\]
after inserting \(\hat{\xi}(t, x) = v_i(\hat{x}(t, x), t)\) and using \(v_i(x, 0) = \nabla_x S_I(x, 0)\) to determine the initial condition. Finally, it follows from (4.27), that for all \((x, t)\) \(\in U\), \((x, t) \notin C\), the density is given by
\[
n(x, t) = \sum_{i=1}^{N} \frac{n_I(x - t\nabla_\xi H(v_i))}{|\operatorname{det}(1 + tD^2S_I(x - t\nabla_\xi H(v_i))D^2H(v_i))|}.
\]
In the examples 1.1.-1.3. below we restrict ourselves, for simplicity to the case of one spatial dimension, i.e. \(d = 1\). We further assume that \(H(\xi)\) is equal to the classical kinetic energy
\[
H(\xi) = \frac{\xi^2}{2}, \quad \xi \in \mathbb{R},
\]
which corresponds to case of the free Schrödinger equation. Then we analyse for \(t \geq 0\) the behavior of the WKB-system subject to different types of initial phases \(S_I\).

**Example 1.1. "No caustic"**
\[
S_I(x) := \frac{x^2}{2}, \quad x \in \mathbb{R}
\]
Here the rays \(\hat{x}(t, x)\) never cross, instead they spread out, forming a so called rarefaction wave (see fig. 1). The only element \(v(x, t) \in K(x, t)\) is given by
\[
v(x, t) = \frac{x}{t + 1}.
\]
The solution of the Hamilton-Jacobi equation, which is single valued and smooth for all times \(t \geq 0\), reads
\[
S(x, t) = \frac{x^2}{2(t + 1)}
\]
and the limiting density (5.8) simplifies to

\[ n(x,t) = \frac{1}{|t+1|} n_I \left( \frac{x}{t+1} \right). \] (5.13)

**Example 1.2. "Focusing at a point"**

By simply changing the sign of the initial phase we obtain

\[ S_I(x) := -\frac{x^2}{2}, \quad x \in \mathbb{R}, \] (5.14)

which leads to the single focus case. All rays intersect at the hot focus point \((x,t_c) = (0,1)\) and spread afterwards (see fig. 2), i.e. there is a.e. only one phase

\[ S(x,t) = \frac{x^2}{2(t-1)}, \quad t \neq 1. \] (5.15)

The above theory does not tell us anything about the precise description of the phase \(S(x,t)\) at \(t = 1\). With the use of the theorem 4.2 and equation (5.8) the density is given by

\[ n(x,t) = \frac{1}{|t-1|} n_I \left( \frac{x}{t-1} \right), \quad t \neq 1, \] (5.16)

\[ n(x,1) = \int_{\mathbb{R}} n_I(x) dx \delta(x). \] (5.17)

In this example there exists a generalized solution \((n,\sigma(v))\) of (4.12) \(n(t)\)-a.e..

**Example 1.3. "Caustic"**

We choose

\[ S_I(x) := -\ln(\cosh(x)), \quad x \in \mathbb{R} \] (5.18)

such that the initial data for the ODE-system of rays is "compressing":

\[ S'_I(x) := -\tanh(x). \] (5.19)

The equation which characterizes the kernel \(K(x,t)\) cannot be solved explicitly, however a precise numerical study is given in [MP]. We want to stress again that in this case no "hot" focus appears, i.e. the limiting density \(n \in L^1_{loc}(\mathbb{R})\) for all \(t \in \mathbb{R}\).

An explicitly solvable example (see also [GaMa]) which has a similar qualitative behavior (except that the focus is hot) is given by

\[ S_I(x) := x\chi_{\{x<0\}} + (x - \frac{x^2}{2})\chi_{\{0 \leq x \leq 1\}}, \quad x \in \mathbb{R} \] (5.20)
where $\chi$ denotes the characteristic function. Note that the initial condition is only Lipschitz continuous, i.e. differentiable almost everywhere.

Up to the time $t = 1$ the rays do not intersect, at $t = 1$ a focus point occurs at $(x, t_c) = (1, 1)$ from which two caustics emanate, forming a *cusp* (see fig. 3). By applying theorem 4.2, in a neighborhood of the focus, we obtain for the density

$$n(x, 1) = n_I(x)\Theta(x - 1) + n_I(x - 1)\Theta(1 - x) + \mu\delta(x - 1).$$

Here the amount of mass that gets concentrated at the point $(1, 1)$ is given by

$$\mu := \int_0^1 n_I(x)dx$$

and the Heaviside function $\Theta(x)$ denotes the Heaviside function.

For $t > 1$ the solution of the Hamilton-Jacobi equation is triple-valued (as it is generic for the singularities in one dimension) within the region $1 < x \leq t$, since $f_{x,t}(\cdot)$ has three zeros there

$$v_1(x, t) = 1, \quad v_2(x, t) = \frac{1 - x}{1 - t}, \quad v_3(x, t) = 0$$

and thus we get for the density within the caustics

$$n(x, t)\chi_{(1 < x \leq t)} = n_I(x - t) + \frac{1}{|t - 1|}n_I\left(\frac{x - t}{1 - t}\right) + n_I(x).$$

The corresponding phases are obtained by a simple integration using (2.33), for example the phase function, that gets transported into the caustic region from the left, is given by

$$S_1(x, t) = x - \frac{t}{2}.$$  

We now turn to an explicitly solvable case with $x$-dependent Hamiltonian $H(x, \xi)$.

**2. Harmonic Oscillator**

Consider in the example of the harmonic oscillator (see also [GaMa])

$$H(x, \xi) = \frac{1}{2}|\xi|^2 + \frac{1}{2}|x|^2 \quad x, \xi \in \mathbb{R}^d$$

In this case the Hamiltonian flow $F_t$ is given by

$$\dot{x}(t, x, \xi) = x \cos t + \xi \sin t$$

$$\dot{\xi}(t, x, \xi) = -x \sin t + \xi \cos t.$$  

If we choose in particular

$$S_I(x) := kx, \quad k > 0, x \in \mathbb{R}$$

we obtain a constant initial velocity $v_I(x) = k > 0$, such that all rays intersect at hot focal points (see fig. 4) given by

$$(x, t_c) = ((-1)^{m+1}k, (2m + 1)\pi/2) \quad m \in \mathbb{Z}.$$  

We obtain a.e. only one zero $\xi = v(x,t) \in \mathcal{K}(x,t)$ of $f_{x,t}(\xi)$, given by

$$v(x,t) = \frac{k - x \sin t}{\cos t}, \quad t \neq (2m + 1)\frac{\pi}{2}$$

and thus the solution of the Hamilton Jacobi equation is unique $n(t)$-a.e.

$$S(x,t) = -\frac{1}{2}(x^2 + k^2) \tan t + \frac{kx}{\cos t}, \quad t \neq (2m + 1)\frac{\pi}{2}. \quad (5.28)$$

The density is given by

$$n(x,t) = \frac{1}{|\cos t|^d} n_I \left( \frac{x - k \sin t}{\cos t} \right), \quad t \neq (2m + 1)\frac{\pi}{2}, \quad (5.29)$$

In this case again there exists a generalized solution $(n,\sigma(v))$ of (5.12) $n(t)$-a.e.

6 Conclusion

In this paper we compare two important approaches within the theory of geometrical optics for linear dispersive operators (acting on $\psi_{\varepsilon}$), namely the Wigner transform and time-dependent WKB-asymptotics. Whereas the latter faces the problem of caustics the limiting Wigner measure is insensitive for such obstacles, due to the fact that it lives in a 2d-dimensional phase space in which the appearing singularities become unfolded. This feature makes the Wigner transform the method of choice if one is particularly interested in the high frequency behavior of energy densities, which are obtained as moments (w.r.t. the velocity variable $\xi$) of the Wigner measure.

Maybe the most important conclusion from this paper is the fact that for WKB-initial data the limiting Wigner measure $w$ can be (locally away from caustics) decomposed into a sum of monokinetic terms (4.27). Each term carries all the information needed, namely $(n_i, S_i), i = 1 \ldots N$, to obtain a (local) approximation $\psi_{\varepsilon, \text{wkb}}$ of the solution $\psi_{\varepsilon}$ to the dispersive equation at the order $O(\varepsilon)$, despite the fact that the measure $w$ does not explicitly contain the phase shifts obtained by the stationary phase method used in the FIO approaches. However since it is well known that, given $S_i$, these phase shifts can be obtained by a purely geometrical computation, we conclude that these important feature of geometrical optics is actually hidden in $w$.

In other words the Wigner measure which is a description for $\varepsilon = 0$ does indeed allow to obtain a approximation of $\psi_{\varepsilon}$ for finite $\varepsilon$ and can thus be seen as a necessary (but of course not sufficient) condition for the validity of the multivalued WKB approximation. Higher order correction can be also obtained from the Wigner transform (using the expansion (3.13)), although we neglected them in this work for the sake of simplicity.
We further stress the fact that although the amplitude of the WKB approach becomes infinite at the caustic, the energy density \( n \) ("square of the amplitude") remains well defined in the sense of measures, as theorem 4.3 shows. What can not be obtained from the Wigner measure is information on the phase at caustic points, which is clearly in agreement with the fact that the multivalued WKB approximation breaks down there too and the fact that the only correct description at caustics is given by FIO’s.

It remains to say that the Wigner transform can be used in situations with much less regularity of the initial data than the WKB approach or its generalizations, since all our computations remain valid for \( n_I \in L^1 \) and \( S_I \in C^1 \) with Lipshitz continuous derivative.

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7 Appendix

As an appendix to the main results of this paper we first present a (rather exotic) example where key assumptions of the presented theory are violated. Then we briefly comment on the physical interpretation of the fluid type equations, which arise in our work.

7.1 Appendix 1 : A counterexample to global Hamiltonian flow

As a "caveat" that the assumption of essential self adjointness (A1) (ii) and global Hamiltonian flow (A3) are not trivial we consider a variable coefficient Airy-type equation (2.9) in one space dimension

\[
H(x,\xi) = -x\xi^3, \quad x, \xi \in \mathbb{R}.
\]  

(7.1)

A lengthy calculation shows that the Weyl-quantized Hamiltonian operator corresponding to this symbol does not have a self adjoint extension.

Moreover the Hamiltonian flow \( F_t \) associated to (7.1) is only locally defined as an explicit calculation shows:

\[
\tilde{x}(t,x,\xi) = x(1 - 2\xi^2 t)^{3/2},
\]

(7.2)

\[
\tilde{\xi}(t,x,\xi) = \frac{\xi}{\sqrt{1 - 2\xi^2 t}}, \quad t < \frac{1}{2\xi^2}.
\]

(7.3)

We remark that to our knowledge it is an open question if essential self
adjointness of $H^W(.,\varepsilon D)$ is a sufficient condition for global Hamiltonian flow defined by $H(x,\xi)$.

If we again choose

$$S_I(x) := kx, \quad k > 0, \quad x \in \mathbb{R},$$

(7.4)

all rays $\hat{x}(t,x)$ focus at the point $(x,t_c) = (0, 1/2k^2)$, i.e. we again obtain a single focus case as in example 1.3. above. The corresponding phase-function is given by

$$S(x,t) = \frac{kx}{\sqrt{1 - 2k^2 t}}, \quad t < \frac{1}{2k^2}.$$  

(7.5)

It is not possible to extend the solution beyond the break time since $F^I_t(x,\xi = k)$ is only defined for $t < t_c$.

In this example neither the WKB nor the Wigner approach give an asymptotic description of solutions of (2.1), (2.2) after breaktimes.

We further remark that changing the sign in the Hamiltonian function gives rise to an expansive flow of rarefaction-wave type.

### 7.2 Appendix 2: On the arising fluid-type equations

As indicated above the fluid-type system (4.14), (4.15) admits a physical interpretation if the Hamiltonian function is given by $H = |\xi|^2/2 + V(x)$ (see the remark below theorem 4.1). In general this is not the case. However we state in the lemma below that one can find indeed an equivalent system which is of the same form as the Euler-equation of gas dynamics, and which can be defined for general Hamiltonian functions.

We define the generalized velocity $u$ and the (time dependent) modified force term $f$ by

$$u(x,t) := \nabla_\xi H(x,v(x,t)), \quad (7.6)$$

$$f(x,t) := \{\nabla_\xi H, H\}|_{(x,v(x,t))}, \quad (7.7)$$

where $v(x,t)$ is a $d$-dimensional vector field. With these definitions we obtain the following result:

**Lemma 7.1.** Let $(n,v)$ be a smooth solution of (4.14), (4.15) and let $u,f$ be defined as above on the same time interval $(t_{c_1}, t_{c_2})$, then $(n,u)$ satisfies

$$\partial_t n + \text{div} (nu) = 0, \quad n(x,0) = n_I(x)$$

(7.8)

$$\partial_t (nu) + \text{div} (nu \otimes u) + nf = 0, \quad u(x,0) = u_I(x)$$

(7.9)

with $u_I(x) := \nabla_\xi H(x,v_I(x))$.

**Proof.** By definition (7.6), it is clear that the conservation law (7.8) is equivalent to (4.14). Further note, that after eliminating $n(x,t)$ from (7.9) using (7.8) one obtains for $u(x,t)$ the *Burgers equation* with source term

$$\partial_t u + (u \cdot \nabla_x) u + f = 0.$$  

(7.10)
Thus it remains to show that if $u(x,t)$ solves (7.10), then $v(x,t)$ is a solution of
\begin{equation}
\partial_t v + (\nabla_\xi H(x,v) \cdot \nabla_x) v + \nabla_x H(x,v) = 0,
\end{equation}
which is again obtained from (4.15) by elimination of $n(x,t)$. Calculating inner derivatives we obtain for the $i$-th component of (7.10)
\begin{equation}
\sum_{k=1}^d \left[ \partial_{\xi_k} (\partial_{\xi_i} H) \right] \partial_t v_k + \sum_{l=1}^d \partial_{\xi_i} H \partial_{x_l} v_k + \sum_{l=1}^d \partial_{\xi_l} H \partial_{y_l} \left( \partial_{\xi_i} H \right) + f_i = 0.
\end{equation}
In order to have a classical solution $v(x,t)$ of (7.11) this implies that each component $f_i$, $i = 1 \ldots d$, of the modified force term must satisfy the relation
\begin{equation}
f_i(x,t) = \sum_{k=1}^d \left( \partial_{\xi_k}^2 \omega \right) \partial_{y_k} H - \sum_{l=1}^d \left( \partial_{\xi_l} H \right) \partial_{y_l} \left( \partial_{\xi_i} H \right)
\end{equation}
which is exactly definition (7.7) above and the claim is proved. \square
Clearly the fluid-type system formulated in $(n,v)$ and the Euler system in $(n,u)$ are equivalent (for smooth solutions) if the relation (7.6) can be uniquely solved for $v$ in terms of $u$. In case
\begin{equation}
H = \omega(\xi) + V(x),
\end{equation}
where $\omega$ is a general dispersion relation, we obtain $u = \nabla_\xi \omega(v)$ and $f = D^2 \omega(v) \nabla_x V$ (where again $D^2 \omega$ denotes the Hessian matrix of $\omega$) and thus
\begin{align}
\partial_t n + \text{div}(nu) &= 0, \quad n(x,0) = n_I \quad (7.13) \\
\partial_t (nu) + \text{div}(nu \otimes u) + nD^2 \omega(v) \nabla_x V &= 0, \quad u(x,0) = u_I. \quad (7.14)
\end{align}
Further note that by definition $u$ in general is not the gradient of a phase function $S$.

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