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Multi-phase computations of the semiclassical limit of the Schrödinger equation and related problems: Whitham vs Wigner☆

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Abstract

We present and compare two different techniques to obtain the multi-phase solutions for the Schrödinger equation in the semiclassical limit. The first is Whitham's averaging method, which gives the modulation equations governing the evolution of multi-phase solutions. The second is the Wigner transform, a convenient tool to derive the semiclassical limit equation in the phase space—the Vlasov equation—for the linear Schrödinger equation. Motivated by the linear superposition principle, we derive and prove the multi-phase ansatz for the Wigner function by the stationary phase method, and then use the ansatz to close the moment equations of the Vlasov equation and obtain the multi-phase equations in the physical space. We show that the multi-phase equations so derived agree with those derived by Whitham's averaging method, which can be proved using different arguments. Generic way of obtaining and computing the multi-phase equations by the Wigner function is given, and kinetic schemes are introduced to solve the multi-phase equations. The numerical schemes, based on multiphase closure of the Liouville equation, are purely Eulerian and only operate in the physical space. Several numerical examples are given to explore the validity of this approach. Similar studies are conducted for the linearized Korteweg–de Vries equation and the linear wave equation.

Keywords: Multi-phase computations; Semiclassical limit; Schrödinger equation; Wigner transformation; Kinetic scheme; Liouville equation; Moment system

1. Introduction

We are interested in computing the semiclassical limit of the Schrödinger equation with the high frequency initial data:

$$\mathrm{i}\epsilon\psi_t + \frac{\epsilon^2}{2}\Delta\psi - V(\mathbf{x})\psi = 0, \quad \mathbf{x} \in \mathrm{R}^n, \tag{1}$$

$$\psi(\mathbf{x}, 0) = A_0(\mathbf{x})\, \mathrm{e}^{\mathrm{i}(S_0(\mathbf{x})/\epsilon)}. \tag{2}$$

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In (1) ψ is the wave function, ϵ the re-scaled Planck constant, and $V(\mathbf{x})$ the smooth potential. In the semiclassical regime, where the Planck constant ϵ is small, the wave function $\psi(\mathbf{x}, t)$ and the related physical observables become oscillatory of wave length $O(\epsilon)$. Mathematically, the rapid oscillations will forbid any strong convergence, and the limits have to be defined in the weak sense.

Typically, a direct numerical simulation to (1) and (2) requires mesh sizes and time steps to be $o(\epsilon)$ if a finite difference method is used [30,31], or to be $O(\epsilon)$ when using the time-splitting spectral method [1]. This mesh strategy makes the computation of the semiclassical solution extremely expensive, especially in high space dimension.

A more efficient approach is to solve the asymptotic equation by letting $\epsilon \to 0$. The classical WKB approach gives, to the leading order, the eikonal equation for the phase and transport equation for the amplitude of the wave function [42]. Since the eikonal equation is of the Hamilton–Jacobi type, it may become singular (caustic forms) even if the initial datum is smooth. Beyond the singularity a standard numerical method using shock capturing ideas may select the viscosity solution [11,28], which is not the correct semiclassical limit of the original Schrödinger equation, since this limit is of dispersive type. In fact, the position density $n^\epsilon = |\psi|^2$ and the current density $J^\epsilon = \epsilon \operatorname{Im}(\overline{\psi}\nabla\psi)$ satisfy the so-called quantum hydrodynamic differential equations (QHDE) [24]:

$$n_t^\epsilon + \nabla \cdot J^\epsilon = 0, \qquad J_t^\epsilon + \nabla \cdot \left[\frac{J^\epsilon \otimes J^\epsilon}{n^\epsilon}\right] + n^\epsilon \nabla V = \frac{\epsilon^2}{2} n^\epsilon \nabla \left(\frac{1}{\sqrt{n^\epsilon}} \Delta \sqrt{n^\epsilon}\right). \tag{3}$$

The left-hand side of the QHDE is a (weakly) hyperbolic system, whose solution develops shock and δ-shock [10,36,40]. The term on the right-hand side of the QHDE is a *dispersive* regularization. As ϵ tends to 0, the solution for (3) beyond shocks becomes oscillatory, and the limit is expected to exist only in the weak sense. This limiting behavior is very similar to that of the zero-dispersion limit of the Korteweg–de Vries equation [25], where the limiting behavior is not the viscosity solution, rather it is described by the classical Lax–Levermore theory. The semi-classical limit for the one-dimensional defocusing Schrödinger equation was proved in [22,23]. In particular, the Lax–Levermore theory shows that after the singularity, the solution locally breaks into multi-branches (or multi-phases) whose evolutions are governed by the Whitham's modulation equations [41]. Whitham equations for multi-phase KdV and nonlinear Schrödinger equations were derived in [15,16].

One natural approach, based on the linear superposition principle, is to track the multi-phase solutions of the eikonal equations using the ray tracing. This method operates in Lagrangian coordinates and involves solving a set of ODEs along the characteristic curves. A severe drawback of ray tracing is that the numerical resolution will deteriorate in the regions where the rays diverge. Benamou [2,3] adapted and improved this technique. In his method, eikonal equations are solved in separated domains. When caustic forms, a splitting algorithm is used to initialize the branches. Attempt to obtain the multi-valued traveltimes was also made in [11].

Another convenient tool to study the semiclassical limit of the Schrödinger equation (and many other problems) is the Wigner distribution [18,27,34,43], which gives, in the semiclassical limit, the Vlasov (or Liouville) equation in the phase space. Since the Vlasov equation is a linear kinetic equation, it naturally unfolds the caustics and gives the correct multi-phase solutions *globally in time*.

Nevertheless, numerical computation of kinetic equations is impractically expensive due to its high dimensionality. Thus one aims at finding an appropriate 'Maxwellian' that can be used to close the kinetic equation and obtain solutions of physical interest (the physical observables, namely, the moments of the kinetic equation) via the moment equations in the physical space.

To obtain the multi-valued solutions in the semiclassical limit, we start with the linearly superimposed solution for the wave function. In Section 4, by using the Wigner transformation and the stationary phase method, we obtain and prove the ansatz for the Wigner function in the semiclassical limit, which turns out to be the superposition of the Wigner function for each phase. This ansatz can also be attained from the Vlasov equation itself since its solutions can be globally defined through the bicharacteristic curves. If the number of phases is finite and known a

priori, this ansatz yields a system of multi-phase equations in the physical space which will be shown to be weakly hyperbolic. We give a generic way to derive and compute the flux of this weakly hyperbolic system in both one and two space dimensions. The flux is given in such a way that the N phase equations include all possible n phases for $n \leq N$. This allows one to solve one system (assuming a prior knowledge about the total number—should be finite—of phases up to the time of computation) numerically to get all developed phases without artificially tracking the development of the new phases. Namely, starting with the N phase equations (one system of PDEs), we can obtain all multi-valued solutions with phase number no bigger than N.

A Heaviside (and delta) multi-phase ansatz (37) was previously used by Brenier and Corrias [6] to define the multi-valued solution for one-dimensionally scalar conservation laws using a kinetic formulation (see also the recent computations in [19]). Subsequently Engquist and Runborg [12,35] used similar ansatz to obtain the moment equations for the computation of multi-phase solution of geometric optics for the linear wave equation. Recently, independent of our work, it was also proved by Sparber, Markowich and Mauser for the linear Schrödinger equation in [37,38], where the classical WKB was compared with the Wigner distribution approach for general dispersive equations. Some more recent numerical methods for computing geometric optics using the Vlasov (Liouville) equation are introduced in [13,33]. Comparisons between the approach of Brenier–Corrias and the one given here is made, both theoretically and computationally, in our new work [20].

Comparison with the modulation equations by the classical Whitham averaging method, which is discussed in Section 4, shows that both approaches give *exactly* the same multi-phase equations. In Section 5, this is shown to be also true for the linearized Korteweg–de Vries equation and the linear wave equation. However, Whitham's approach yields *local* characterization of the multi-phase solutions, while the Wigner distribution gives a *global* characterization through the Liouville–Vlasov equation defined in the phase space.

Our approach provides a framework to numerically compute the weak limits of physical observables to the initial value problem of the Schrödinger equations (1) and (2), modulus the phase shifts which typically appear after the rays cross the caustic and cannot be detected by the Wigner measure or Whitham averaging method. The computation of the phase shifts can be done by the Fourier integral method [9], which will not be discussed in the most general way here, although in Section 2 we present the analysis based on the Fourier integral method for the Schrödinger equation without potential.

We also adopt a kinetic scheme in Section 6, formulated in [5], for the multi-phase solution and use it to explore the validity of the multi-phase solutions numerically. The Wigner approach gives the globally in time well-defined kinetic Liouville equation, which yields naturally a kinetic scheme especially suitable for numerical computation of such problems than a standard shock capturing methods constructed directly from the moment equations. The kinetic schemes are purely Eulerian and is able to handle solutions near vacuum, which corresponds to diverging rays in the Lagrangian coordinate. In Section 7, comparisons are made with the Lax–Friedrichs scheme, which has been mostly used in [12,19,35] for geometric optics computations. We conclude in Section 8.

2. The semiclassical limits

A classical method to derive the semiclassical limit, characterized locally by the multi-phase equations, is the Whitham's average method. For linear problem, one does not need to take the Whitham average to obtain these multi-phase equations. However, one still needs to use several conservation laws to obtain the equations with the desired number of phases, as in the Whitham's approach. In this section we follow the idea of Fourier integral method [9] to analyze the semiclassical limits of the Schrödinger equation and to derive the multi-phase equations via the Fourier transform and the stationary phase methods. We will relate it to the Whitham averaging method in next section.

We start with the linear Schrödinger equation with zero potential:

$$\mathrm{i}\epsilon\psi_t + \frac{\epsilon^2}{2}\Delta\psi = 0, \qquad \psi(\mathbf{x}, 0) = A_0(\mathbf{x})\,\mathrm{e}^{\mathrm{i}(S_0(\mathbf{x})/\epsilon)}, \quad \mathbf{x} \in \mathrm{R}^n. \tag{4}$$

One first observes that the solution of (4) can be represented by a Fourier integral:

$$\psi(\mathbf{x}, t) = \frac{1}{(\epsilon\sqrt{2\pi})^n}\int_{\mathrm{R}^n} \hat{\psi}\left(\frac{\boldsymbol{\xi}}{\epsilon}, 0\right)\mathrm{e}^{\mathrm{i}(\xi\cdot\mathbf{x}-\omega(\xi)t)/\epsilon}\,\mathrm{d}\xi$$

with

$$\omega(\xi) = \frac{|\xi|^2}{2} \tag{5}$$

being the dispersion relation.

Given $\psi(\mathbf{x}, 0)$, the integral can be well approximated by a wave train solution via the stationary phase method. Since this technique will be used several times in this paper, we quote the theorem below. For its detailed proof and various applications, see [4,14].

Theorem 1. *Let $a(\mathbf{x}) \in C_{\mathrm{c}}^{\infty}(\mathrm{R}^n)$ be an C^{∞} function with a compact support. Suppose that function $\phi(\mathbf{x})$ is smooth, the set*

$$\{\mathbf{y} : D\phi(\mathbf{y}) = 0\} \subset \mathrm{supp}(a)$$

has finitely many points $\{\mathbf{y}_1, \mathbf{y}_2, \ldots, \mathbf{y}_N\}$ and the matrix $D^2\phi(\mathbf{y}_j)$ is nonsingular. Then, for $\epsilon \ll 1$:

$$I_\epsilon = \int_{\mathrm{R}^n} \mathrm{e}^{\mathrm{i}(\phi(\mathbf{y})/\epsilon)}a(\mathbf{y})\,\mathrm{d}\mathbf{y} = (2\pi\epsilon)^{n/2}\sum_{k=1}^{N}\frac{\mathrm{e}^{\mathrm{i}(\phi(\mathbf{y}_k)/\epsilon)}}{\sqrt{|\det D^2\phi(\mathbf{y}_k)|}}\,\mathrm{e}^{\mathrm{i}(\pi/4)\,\mathrm{sgn}(D^2\phi(\mathbf{y}_k))}(a(\mathbf{y}_k) + \mathrm{O}(\epsilon)),$$

where $\mathrm{sgn}(M)$ *denotes the number of positive eigenvalues minus the number of negative eigenvalues of M.*

In light of the initial condition (4), we have

$$\hat{\psi}\left(\frac{\xi}{\epsilon}, 0\right) = \frac{1}{(\sqrt{2\pi})^n}\int A_0(\mathbf{y})\,\mathrm{e}^{-\mathrm{i}(\xi\cdot\mathbf{y}/\epsilon)}\,\mathrm{e}^{\mathrm{i}(S_0(\mathbf{y})/\epsilon)}\,\mathrm{d}\mathbf{y}$$

and thus

$$\psi(\mathbf{x}, t) = \frac{1}{(2\pi\epsilon)^n}\iint A_0(\mathbf{y})\,\mathrm{e}^{\mathrm{i}(\xi\cdot\mathbf{x}-\xi\cdot\mathbf{y}-(1/2)|\xi|^2t+S_0(\mathbf{y}))/\epsilon}\,\mathrm{d}\xi\,\mathrm{d}\mathbf{y}.$$

Now define the phase

$$\theta(\xi, \mathbf{y}) = \xi\cdot\mathbf{x} - \xi\cdot\mathbf{y} - \tfrac{1}{2}|\xi|^2t + S_0(\mathbf{y}).$$

By the stationary phase method (note that we have an integral over R^{2n}), we have

$$\psi(\mathbf{x}, t) = \sum_{k=1}^{N}\frac{A_0(\mathbf{y}_k)}{\sqrt{|\det(1 + tD^2S(\mathbf{y}_k))|}}\,\mathrm{e}^{\mathrm{i}(\pi/4)\,\mathrm{sgn}(D^2\theta(\xi_k,\mathbf{y}_k))}\,\mathrm{e}^{\mathrm{i}(\theta(\xi_k,\mathbf{y}_k)/\epsilon)} + \mathrm{O}(\epsilon),$$

where $(\xi_k(\mathbf{x}, t), \mathbf{y}_k(\mathbf{x}, t))$'s are the stationary points of $\theta(\xi, \mathbf{y})$:

$$\xi_k(\mathbf{x}, t) = \xi_0(\mathbf{y}), \qquad \mathbf{y} - \mathbf{x} + t\xi_0(\mathbf{y}) = 0 \tag{6}$$

with $\xi_0 = \nabla S_0$. This asymptotic form is valid almost everywhere except for the caustic points, where $\det(1 + tD^2S(\mathbf{y}_k)) = 0$.

This striking fact tells us that an initial WKB data will split into several branches (A_k's are allowed to be complex):

$$\psi(\mathbf{x}, t) = \sum_k A_k(\mathbf{x}, t)\, \mathrm{e}^{\mathrm{i}(S_k(\mathbf{x},t)/\epsilon)} + \mathrm{O}(\epsilon), \tag{7}$$

after the single phase solution ceases to be valid. Since (6) is the Lagrangian representation of Burgers' equation, each phase has to solve the Burgers' equation and they superimpose when they meet.

Let $S_k(\mathbf{x}, t) = \theta(\xi_k(\mathbf{x}, t), \mathbf{y}_k(\mathbf{x}, t))$, then one has $\xi = \nabla S_k$ and S_k solves the eikonal equation:

$$S_t + \tfrac{1}{2}|\nabla S|^2 = 0, \tag{8}$$

which can be derived as the leading order approximation from the linear Schrödinger equation (4) using the classical WKB analysis [42].

For the sake of simplicity we first consider the linear Schrödinger equation (4) in one-dimensional with zero potential and define

$$\begin{aligned} &m_0^\epsilon(x, t) = |\psi|^2, \qquad m_1^\epsilon(x, t) = \epsilon\, \mathrm{Im}(\overline{\psi}\psi_x), \qquad m_2^\epsilon(x, t) = -\frac{\epsilon^2}{2}\mathrm{Re}(\overline{\psi}\psi_{xx}) + \frac{\epsilon^2}{2}|\psi_x|^2, \\ &m_3^\epsilon(x, t) = \epsilon^3\, \mathrm{Im}(\tfrac{3}{4}\overline{\psi}_x\psi_{xx} - \tfrac{1}{4}\overline{\psi}\psi_{xxx}), \qquad m_4^\epsilon(x, t) = \epsilon^4\tfrac{3}{8}|\psi_{xx}|^2 - \epsilon^4\,\mathrm{Re}(\tfrac{1}{2}\overline{\psi}_x\psi_{xxx} - \tfrac{1}{8}\overline{\psi}\psi_{xxxx}), \end{aligned} \tag{9}$$

where m_0^ϵ is the position density, m_1^ϵ the current density, and m_2^ϵ the energy density, etc., and they satisfy the following conservation equations:

$$\partial_t m_0^\epsilon + \partial_x m_1^\epsilon = 0, \qquad \partial_t m_1^\epsilon + \partial_x m_2^\epsilon = 0, \qquad \partial_t m_2^\epsilon + \partial_x m_3^\epsilon = 0, \qquad \partial_t m_3^\epsilon + \partial_x m_4^\epsilon = 0. \tag{10}$$

In the single phase case:

$$\psi(x, t) = A(x, t)\, \mathrm{e}^{\mathrm{i}(S(x,t)/\epsilon)},$$

m_j^ϵ's do not exhibit oscillations. Let $\rho = |A|^2$, $\xi = \partial_x S$. At any point one has

$$m_0^\epsilon = \rho, \qquad m_1^\epsilon = \rho\xi, \qquad m_2^\epsilon = \rho\xi^2 + \mathrm{O}(\epsilon^2), \qquad m_3^\epsilon = \rho\xi^3 + \mathrm{O}(\epsilon^2), \qquad m_4^\epsilon = \rho\xi^4 + \mathrm{O}(\epsilon^2).$$

Thus, after letting $\epsilon \to 0$, one yields $m_j^\epsilon \to m_j = \rho\xi^j$ and

$$\partial_t m_j + \partial_x m_{j+1} = 0, \quad j = 0, 1, 2, 3.$$

Certainly, one can find as many conservation laws as needed. In the simplest case, every two of them are independent and the first two equations can be closed as

$$\partial_t m_0 + \partial_x m_1 = 0, \qquad \partial_t m_1 + \partial_x m_2 = 0 \tag{11}$$

by using

$$m_2 = \frac{m_1^2}{m_0}. \tag{12}$$

The corresponding system is often referred to as the pressureless gas equations or sticky particle system if one replaces the variable in (11) by $\rho = m_0$ and $m_1/m_0 = u$ where u is the velocity.

This system is valid as long as its solution remains regular (no shock formation). After shock formation the linear superposition principle implies that solutions from different phases superimpose.

To proceed with the our procedure, we assume that ρ_i's are positive and $\xi_i = \partial_x S_j$'s are distinct to make the ansatz nondegenerate and to distinguish different phases. This is in fact a result from the stationary phase analysis of the Schrödinger equation [9].

For easier explanation, we take $N = 2$. Clearly we only need to analyze the crossing term which contains oscillatory term:

$$\mathrm{e}^{\mathrm{i}(S_1-S_2)/\epsilon}.$$

Since $\xi_1 \neq \xi_2$, there is no stationary point. Therefore, after integrating with a test function ϕ, we have

$$\int m_k^\epsilon \phi \,\mathrm{d}x = \int (\rho_1 \xi_1^k + \rho_2 \xi_2^k)\phi \,\mathrm{d}x + \mathrm{O}(\epsilon^{3/2}), \quad k = 0, 1, 2, 3, 4.$$

Hence $m_j^\epsilon \to m_j = \rho_1 \xi_1^j + \rho_2 \xi_2^j$ weakly (can be understood in L^p_{loc} or distributional sense) and

$$\partial_t m_j + \partial_x m_{j+1} = 0, \quad j = 0, 1, 2, 3, \tag{13}$$

again by integrating with test functions. In fact because of possible concentration effects, the solutions of these equations may only be understood in the weak sense, namely, for any function $\eta(x, t)$ which is smooth and has compact support in $\mathrm{R} \times [0, +\infty)$, one has

$$\int_{\mathrm{R}^+} \int_{\mathrm{R}} m_j \partial_t \eta + m_{j+1} \partial_x \eta \,\mathrm{d}x \,\mathrm{d}t + \int_{\mathrm{R}} m_j(x, 0)\eta(x, 0) \,\mathrm{d}x = 0.$$

Since this identity also holds for m_j^ϵ and m_{j+1}^ϵ, it certainly holds as one passes the weak limits. Clearly one can express m_4 as

$$m_4 = \frac{m_3^2 m_0 - 2m_1 m_2 m_3 + m_2^3}{m_0 m_2 - m_1^2}, \tag{14}$$

which yields a closed system of four equations for m_0, m_1, m_2, m_3.

We refer to the system as the double phase equations. Similar procedures will also give multi-phase equations for $N \geq 3$. See Section 5 for the precise definition of these systems.

In the case of nonzero potential $V(x) \neq 0$, assumed to be smooth, the mathematical analysis for the semiclassical limit is technically much involved. The best known methods that are able to generalize the WKB result beyond caustics use the Maslov Canonical Operators [32] or the Fourier Integral Operators [9]. We will just summarize the final formula using the Maslov approach. For a point not at the caustic, based on the method of stationary phase for nearby points, one obtains

$$\psi(\mathbf{x}, t) = \sum_k A_k(\mathbf{x}, t)\, \mathrm{e}^{\mathrm{i}(S_k(\mathbf{x},t)/\epsilon) - \mathrm{i}(\pi/2)\mu_k} + \mathrm{O}(\epsilon), \tag{15}$$

where μ_k is the Maslov index of the kth ray. By including the phase shift terms in A_k's, one gets the same multi-phase ansatz (7), with S_k solving the eikonal equation:

$$S_t + \tfrac{1}{2}|\nabla S|^2 + V(\mathbf{x}) = 0.$$

In the Fourier Integral Operator approach, one approximates ψ as an "oscillatory integral" operator acting on the initial datum, namely, ψ is represented as a continuous superposition of WKB solution. The main contribution again comes from stationary points.

For nonzero potential, the single phase equations then become

$$\partial_t m_0 + \partial_x m_1 = 0, \qquad \partial_t m_1 + \partial_x m_2 = -m_0 V'(x) \tag{16}$$

with

$$m_2 = \frac{m_1^2}{m_0}. \tag{17}$$

The double phase equations are

$$\partial_t m_0 + \partial_x m_1 = 0, \qquad \partial_t m_1 + \partial_x m_2 = -m_0 V'(x), \qquad \partial_t m_2 + \partial_x m_3 = -2m_1 V'(x),$$
$$\partial_t m_3 + \partial_x m_4 = -3m_2 V'(x) \tag{18}$$

with

$$m_4 = \frac{m_3^2 m_0 - 2m_1 m_2 m_3 + m_2^3}{m_0 m_2 - m_1^2}. \tag{19}$$

3. Multi-phase modulation equations by the Whitham averaging method

In this section, we will study the Whitham's averaging method which generates the multi-phase modulation equations. Although these equations have been derived in the previous section, the motivation for the study of Whitham's averaging method has its very important applications to nonlinear, completely integrable systems such as the KdV and the nonlinear Schrödinger equations, see [15,16,41].

The main observation made by Whitham was that the rapid oscillations can be efficiently eliminated by an averaging procedure. The Whitham average is defined as an average over one period of the averaged quantity, namely

$$\overline{P^\epsilon}(x) = \frac{1}{\lambda(x)} \int_0^{\lambda(x)} P^\epsilon(x + \epsilon y)\, \mathrm{d}y,$$

where $\lambda(x)$ is the *local period* (to be defined below) of the function $P^\epsilon(x)$, related to the wave number $\xi(x)$ and period T via $\lambda(x) = T/\xi(x)$.

To derive Whitham's equations for multi-phase solutions, one usually starts by seeking periodic solutions with the amplitude and wave number as slowly varying parameters. Then physical quantities can be represented by the amplitude and the wave number after the averaging. This averaging is taken over a balance equation (there are infinitely many such conservation laws in integrable systems):

$$P_t^\epsilon + Q_x^\epsilon = 0.$$

Since the conservation equation is invariant under the averaging process:

$$\overline{P^\epsilon}_t + \overline{Q^\epsilon}_x = 0$$

and as we will show, the averaged quantity $\overline{P^\epsilon}(x, t)$ will converge (strongly) to the weak limit of $P^\epsilon(x, t)$ as $\epsilon \to 0$, thus this procedure will produce the balance equations for the amplitude and the wave number, which is known as the Whitham equations. Depending on the number of phases one has to pick up the corresponding number of conservation laws to average [15,41,42]. For the linear Schrödinger equation with the zero potential case, the averages of the quantities defined in (9) satisfy exactly the balance equations for single phase (11) and (12), double

phases (13) and (14), etc. Even in the case when the potential gradient is not zero, since the potential is independent of ϵ, one can Taylor expand $V(x+\epsilon y)$ and get

$$\overline{m_k^\epsilon V(x)} = V(x)\overline{m_k^\epsilon} + \mathrm{O}(\epsilon),$$

which yields the systems (11)–(14).

The next theorem can be used to mathematically justify the Whitham average.

Theorem 2. *Let $G(x) \in L^\infty(\mathrm{R})$ be a periodic function with period T, and let*

$$\tilde{G} = \frac{1}{T}\int_0^T G(x)\,\mathrm{d}x.$$

Suppose that a function $g_\epsilon(x) \in L^\infty(\mathrm{R})$ is locally periodic in the sense that at any point x, g_ϵ has the following expansion:

$$g_\epsilon(x+\epsilon y) = C(x) + A(x)G(\eta(x)y) + \mathrm{O}(\epsilon),$$

where $\eta(x) \in C_\mathrm{b}(\mathrm{R})$ and is bounded away from 0, and $A \in L^\infty$. Then, we have

$$g_\epsilon(x) \to C(x) + A(x)\tilde{G}$$

in the weak sense.

To prove the theorem, one can make a partition $\{x_j, 0 \le j \le J+1\}$ and $x_{J+1} = b$ on any given interval $[a, b]$. For instance, one may take

$$x_0 = a, \quad x_{j+1} = x_j + \frac{\epsilon T}{\eta(x_j)}$$

and let $J = \max\{j : x_j < b\}$. Note that the length of last interval is of order ϵ. Hence as one integrates on the interval $[a, b]$, one yields

$$\begin{aligned}\int_a^b g_\epsilon(x)\,\mathrm{d}x &= \sum_{0\le j<J}\int_{x_j}^{x_{j+1}} g_\epsilon(x)\,\mathrm{d}x = \sum_{0\le j<J}\int_0^{\epsilon T/\eta(x_j)} g_\epsilon(x_j+x)\,\mathrm{d}x \\ &= \epsilon\sum_{0\le j<J}\int_0^{T/\eta(x_j)} g_\epsilon(x_j+\epsilon y)\,\mathrm{d}y = \sum_{0\le j<J}(C(x_j)+A(x_j)\tilde{G})\frac{\epsilon T}{\eta(x_j)} + \mathrm{O}(\epsilon).\end{aligned}$$

Notice that the above sum is a Riemann sum because the wave number is bounded above. Therefore, one gets

$$\frac{1}{b-a}\int_a^b g_\epsilon(x)\,\mathrm{d}x \to \frac{1}{b-a}\int_a^b C(x) + A(x)\tilde{G}\,\mathrm{d}x, \quad \text{as } \epsilon \to 0.$$

Since the weak convergence in L^p is equivalent to convergence in averages, The statement of the theorem is proven.

In fact, it is not the theorem, rather its proof, that can be used to mathematically justify the weak limit of the Whitham average for problems where the solution is locally periodic (for example, KdV equation [39]). To illustrate the idea, we first show that locally the asymptotic solution of the linear Schrödinger equation:

$$\psi \approx \sum_{j=1}^N A_j(x)\,\mathrm{e}^{\mathrm{i}(S_j(x)/\epsilon)}$$

is in fact branch-wise periodic. For instance, one can change the space and time variable to $(x+\epsilon y, t)$, and expand the phase variable near a fixed point (x, t):

$$S_j(x+\epsilon y, t) = S_j(x,t) + \epsilon \partial_x S_j(x,t) y + \mathrm{O}(\epsilon^2).$$

Let $\xi_j = \partial_x S_j$, one has

$$S_j(x+\epsilon y, t) = S_j(x,t) + \epsilon \xi_j y + \mathrm{O}(\epsilon^2).$$

Hence locally the solution can be written as

$$\psi(x+\epsilon y, t) = \sum_{j=1}^{N} A_j(x,t)\, \mathrm{e}^{\mathrm{i}S_j(x,t)/\epsilon}\, \mathrm{e}^{\mathrm{i}\xi_j y} + \mathrm{O}(\epsilon),$$

which shows that each branch is locally periodic.

We now can compute the physical quantities around the point (x, t). For example, m_0^ϵ defined in (9) gives

$$m_0^\epsilon(x+\epsilon y) = \sum_{k=1}^{N} \rho_k(x,t) + \sum_{j\neq k} A_j \bar{A}_k\, \mathrm{e}^{\mathrm{i}(S_j - S_k)/\epsilon}\, \mathrm{e}^{\mathrm{i}(\xi_j - \xi_k)y} + \mathrm{O}(\epsilon).$$

To determine the weak limit one only needs to study the crossing terms. Other terms will converge pointwise. Notice that the oscillatory terms:

$$\mathrm{e}^{\mathrm{i}(\xi_j - \xi_k)y}, \quad k \neq j,$$

has period $2\pi/|\xi_j - \xi_k|$. Following the spirit of the above theorem, the integral over any interval $[a, b]$ can be divided into the integrals over several small intervals in which the function is periodic. But since the function has mean value 0, one yields

$$\int_a^b m_0^\epsilon(x)\,\mathrm{d}x = \int_a^b \rho_1(x) + \rho_2(x) + \cdots + \rho_N(x)\,\mathrm{d}x + \mathrm{O}(\epsilon)$$

and thus

$$m_0^\epsilon \to \rho_1 + \rho_2 + \cdots + \rho_N$$

in the weak sense. Similarly one obtains, for m_l^ϵ defined in (9):

$$m_l^\epsilon \to \rho_1 \xi_1^l + \rho_2 \xi_2^l + \cdots + \rho_N \xi_N^l, \quad \text{weakly for } \ l = 1, 2, \ldots .$$

In addition, these limits satisfy the multi-phase equations given in the previous section. For multi-phase equations with more phases, see the next section.

For linear problems, this procedure can be easily extended to multi-dimensional case. In order to use Whitham's averaging technique, one needs to find sufficiently many conservation laws to generate the corresponding multi-phases.

Whitham's equations characterize *locally* the behavior of multi-phase solutions. In different regions, the number of physical phases, and thus the Whitham's equations might be different. The approach by using the Wigner distribution, to be studied in next section, provides a global characterization of the semiclassical limit.

4. Multi-phase equations via the Wigner transform and kinetic moment closure

4.1. The Wigner distribution and the semiclassical limit

For any smooth functions ϕ and ψ, rapidly decaying at infinity (more precisely, in $S(\mathrm{R}^n)$), the corresponding Wigner distribution is defined as [43]:

$$W[\phi,\psi] = \frac{1}{(2\pi)^n}\int_{\mathrm{R}^n} \mathrm{e}^{\mathrm{i}\mathbf{v}\cdot\mathbf{y}}\phi\left(\mathbf{x}-\frac{\epsilon\mathbf{y}}{2}\right)\overline{\psi}\left(\mathbf{x}+\frac{\epsilon\mathbf{y}}{2}\right)\mathrm{d}\mathbf{y}. \tag{20}$$

When ψ solves the Schrödinger equation (1), the Wigner distribution:

$$W^\epsilon(\mathbf{x},\mathbf{v},t) = W[\psi,\psi]$$

solves the Wigner equation:

$$W_t^\epsilon + \mathbf{v}\cdot W_{\mathbf{x}}^\epsilon - \Theta^\epsilon[V]W^\epsilon = 0, \tag{21}$$

where the linear operator Θ can be written as

$$\begin{aligned}\Theta^\epsilon[V]W^\epsilon &= \frac{\mathrm{i}}{(2\pi)^n\epsilon}\int_{\mathrm{R}^n}\mathrm{e}^{\mathrm{i}\mathbf{v}\cdot\mathbf{y}}\psi^\epsilon\left(\mathbf{x}-\frac{\epsilon\mathbf{y}}{2},t\right)\left[V\left(\mathbf{x}+\frac{\epsilon\mathbf{y}}{2}\right)-V\left(\mathbf{x}-\frac{\epsilon\mathbf{y}}{2}\right)\right]\mathrm{d}\mathbf{y}\\ &= \frac{\mathrm{i}}{(2\pi)^n\epsilon}\int_{\mathrm{R}^n}\int_{\mathrm{R}^n}\mathrm{e}^{\mathrm{i}(\mathbf{v}-\mathbf{k})\cdot\mathbf{y}}W^\epsilon(x,k,t)\left[V\left(\mathbf{x}+\frac{\epsilon\mathbf{y}}{2}\right)-V\left(\mathbf{x}-\frac{\epsilon\mathbf{y}}{2}\right)\right]\mathrm{d}\mathbf{y}.\end{aligned}$$

It can be shown that [18,29], as $\epsilon\to 0$:

$$\Theta^\epsilon[V]U(\mathbf{x},\mathbf{v}) \to \nabla_{\mathbf{x}}V\cdot\nabla_{\mathbf{v}}U$$

and the series $W^\epsilon(x,v,t)$ is weakly compact. Therefore, the limit of the Wigner function W^ϵ, $w(x,v,t)$, as $\epsilon\to 0$, satisfies the Vlasov or Liouville equation:

$$w_t + \mathbf{v}\cdot\nabla_{\mathbf{x}}w - \nabla_{\mathbf{x}}V\cdot\nabla_{\mathbf{v}}w = 0 \tag{22}$$

in the weak sense. In addition, the initial data

$$W^\epsilon(\mathbf{x},\mathbf{v},0) = \frac{1}{(2\pi)^n}\int_{\mathrm{R}^n} A_0\left(\mathbf{x}-\frac{\epsilon}{2}\right)\overline{A_0}\left(\mathbf{x}+\frac{\epsilon}{2}\right)\mathrm{e}^{\mathrm{i}\mathbf{v}\cdot\mathbf{y}}\,\mathrm{e}^{-\mathrm{i}(S_0(\mathbf{x}+(\epsilon\mathbf{y}/2))-S_0(\mathbf{x}-(\epsilon\mathbf{y}/2)))/\epsilon}\,\mathrm{d}\mathbf{y}$$

converges weakly to

$$w(\mathbf{x},\mathbf{v},0) = \rho_0\delta(\mathbf{v}-\mathbf{u}_0), \tag{23}$$

where $\mathbf{u}_0 = \nabla S_0$ and $\rho_0 = |A_0|^2$. This convergence will be proved in the next section for the multi-phase case.

Moreover, it was shown in [17] that

$$m_0^\epsilon = \int_{\mathrm{R}^n} W^\epsilon\,\mathrm{d}\mathbf{v} \to m_0 = \int_{\mathrm{R}^n} w(\mathbf{x},\mathbf{v},t)\,\mathrm{d}\mathbf{v} \in C_{\mathrm{b}}(\mathrm{R}_t; M^+(\mathrm{R}^n_{\mathbf{x}})w-\star),$$

$$\mathbf{m}_1^\epsilon = \int_{\mathrm{R}^n} W^\epsilon\mathbf{v}\,\mathrm{d}\mathbf{v} \to \mathbf{m}_1 = \int_{\mathrm{R}^n} w(\mathbf{x},\mathbf{v},t)\mathbf{v}\,\mathrm{d}\mathbf{v} \in C_{\mathrm{b}}(\mathrm{R}_t; M(\mathrm{R}^n_{\mathbf{x}})^n w-\star)$$

uniformly on compact subsets of R_t in $(C_0(\mathrm{R}^n_{\mathbf{x}}))^\star w-\star$ and $((C_0(\mathrm{R}^n_{\mathbf{x}}))^\star)^n w-\star$, where $M(M^+)$ represents the space of measures (positive measures). Hence the weak limits of the observables are encoded in the solution of (22). The convergence of $m_0^\epsilon \to m_0$, $\mathbf{m}_1^\epsilon \to \mathbf{m}_1$ are in measure sense in that

$$\int_{\mathrm{R}^n} m_0^\epsilon \phi \,\mathrm{d}\mathbf{x} \to \int_{\mathrm{R}^n} m_0 \phi \,\mathrm{d}\mathbf{x}, \qquad \int_{\mathrm{R}^n} \mathbf{m}_1^\epsilon \phi \,\mathrm{d}\mathbf{x} \to \int_{\mathrm{R}^n} \mathbf{m}_1 \phi \,\mathrm{d}\mathbf{x}, \quad \text{as } \epsilon \to 0$$

for any test function $\phi \in C_0(\mathrm{R}^n_{\mathbf{x}})$. This is because at caustic points where rays intersect, the solution of the Vlasov equation as well as its integrals may exhibits concentration phenomena.

With smooth initial data ρ_0 and u_0, the solution will remain in the initial form:

$$w(\mathbf{x}, \mathbf{v}, t) = \rho(\mathbf{x}, t)\delta(\mathbf{v} - \mathbf{u}(\mathbf{x}, t)), \tag{24}$$

before breaking time t_b.

Applying (24) to the Vlasov equation (22) and taking the first two moments, one yields a closed system for ρ and u as

$$\rho_t + \nabla \cdot (\rho \mathbf{u}) = 0, \qquad (\rho \mathbf{u})_t + \nabla \cdot (\rho \mathbf{u} \otimes \mathbf{u}) + \rho \nabla V = 0. \tag{25}$$

These are the pressureless gas equations, which gives a weakly hyperbolic system with only one characteristic speed $\mathbf{u}$ and the Jacobian matrix is a Jordan block. With proper initial data, solution may develop singularities—shock for $\mathbf{u}$ and delta-shock for ρ at a break time t_b [8,10,36,40]. This corresponds to the formation of caustics in geometric optics. Beyond the break time t_b the above ansatz (24) is no longer valid. Numerical approximations of the gas equations (25) using shock capturing techniques yield the viscosity solution, such as the δ-shock solution [5], which violates the superposition principle and is not the semiclassical limit of the linear Schrödinger equation.

Introduce the Hamiltonian flow:

$$\mathbf{x}'(t) = \mathbf{v}, \quad \mathbf{x}(0) = \mathbf{x}_0, \qquad \mathbf{v}'(t) = -\nabla V(\mathbf{x}), \quad \mathbf{v}(0) = \mathbf{v}_0. \tag{26}$$

We denote the solution to these ODEs by $\mathbf{x} = \mathbf{x}(\mathbf{x}_0, \mathbf{v}_0, t)$ and $\mathbf{v} = \mathbf{v}_0(\mathbf{x}_0, \mathbf{v}_0, t)$. The curves $(\mathbf{x}, \mathbf{v})$ are usually referred to as the *bicharacteristics* in phase space. Since the Hamiltonian flow is volume preserving, we have, for any $\phi(\mathbf{x}, \mathbf{v}) \in C_\mathrm{b}(\mathrm{R}^n \times \mathrm{R}^n)$:

$$\int_{\mathrm{R}^n}\int_{\mathrm{R}^n} \phi(\mathbf{x}, \mathbf{v}) w \,\mathrm{d}\mathbf{x}\,\mathrm{d}\mathbf{v} = \int_{\mathrm{R}^n}\int_{\mathrm{R}^n} w(\mathbf{x}_0, \mathbf{v}_0, 0)\phi(\mathbf{x}(\mathbf{x}_0, \mathbf{v}_0, t), \mathbf{v}(\mathbf{x}_0, \mathbf{v}_0, t)) \,\mathrm{d}\mathbf{x}_0\,\mathrm{d}\mathbf{v}_0. \tag{27}$$

Since the Vlasov equation (22) is linear, w given by (27) exists globally in time. Thus the caustics we encountered in the nonlinear problem (25) are unfolded in the phase space.

By applying the initial condition (23), the above equality becomes

$$\int_{\mathrm{R}^n}\int_{\mathrm{R}^n} \phi(\mathbf{x}, \mathbf{v}) w(\mathbf{x}, \mathbf{v}, t) \,\mathrm{d}\mathbf{x}\,\mathrm{d}\mathbf{v} = \int_{\mathrm{R}^n_{\mathbf{x}}} \rho_0(\mathbf{x})\phi(\hat{\mathbf{x}}(\mathbf{x}, t), \hat{\mathbf{v}}(\mathbf{x}, t)) \,\mathrm{d}\mathbf{x}, \tag{28}$$

where $(\hat{\mathbf{x}}(\mathbf{x}, t), \hat{\mathbf{v}}(\mathbf{x}, t))$ solve the ODEs

$$\frac{\mathrm{d}}{\mathrm{d}t}\hat{\mathbf{x}} = \hat{\mathbf{v}}, \quad \hat{\mathbf{x}}(\mathbf{x}, 0) = \mathbf{x}, \qquad \frac{\mathrm{d}}{\mathrm{d}t}\hat{\mathbf{v}} = -\nabla V(\hat{\mathbf{x}}), \quad \hat{\mathbf{v}}(\mathbf{x}, 0) = \mathbf{u}_0(\mathbf{x}). \tag{29}$$

Here $\hat{\mathbf{x}}$ are the characteristic curves of the field-driven Burger's equation:

$$\mathbf{u}_t + (\mathbf{u} \cdot \nabla)\mathbf{u} + \nabla V = 0, \tag{30}$$

which is just the momentum equation of the pressureless gas equations (25) for smooth solution, or the *rays* of the eikonal equation:

$$S_t + \tfrac{1}{2}|\nabla S|^2 + V(\mathbf{x}) = 0.$$

These two equations are equivalent for smooth solutions with $\mathbf{u} = \nabla S$.

Formal formula for solution of the pressureless gas equations (25) can be found using the method of characteristics. We use $(\mathbf{x}_0(\mathbf{x}, \mathbf{v}; t), \mathbf{v}_0(\mathbf{x}, \mathbf{v}; t))$ to denote the inverse mapping of the bicharacteristic curve given in (26). Since the solution of the Vlasov equation (22) is a constant along the bicharacteristic curve defined by (26), one has

$$w(\mathbf{x}, \mathbf{v}, t) = w(\mathbf{x}_0(\mathbf{x}, \mathbf{v}, t), \mathbf{v}_0(\mathbf{x}, \mathbf{v}, t), 0). \tag{31}$$

If $\rho, \mathbf{u}$ are (single-valued) solutions to the pressureless gas equations (25), then using (24)–(31) one gets

$$\rho(\mathbf{x}, t)\delta(\mathbf{v} - \mathbf{u}(\mathbf{x}, t)) = \rho_0(\mathbf{x}_0(\mathbf{x}, \mathbf{v}; t))\delta(\mathbf{v}_0(\mathbf{x}, \mathbf{v}, t) - \mathbf{u}_0(\mathbf{x}_0(\mathbf{x}, \mathbf{v}, t))). \tag{32}$$

Define

$$\Phi_{\mathbf{x}t}(\mathbf{v}) = \mathbf{v}_0(\mathbf{x}, \mathbf{v}, t) - \mathbf{u}_0(\mathbf{x}_0(\mathbf{x}, \mathbf{v}, t)), \tag{33}$$

then (32) implies that the zero of $\Phi_{\mathbf{x}t}(\mathbf{v})$ gives $\mathbf{u}(\mathbf{x}, t)$ and the corresponding

$$\rho(\mathbf{x}, t) = \frac{\rho_0(\mathbf{x}_0(\mathbf{x}, \mathbf{u}(\mathbf{x}, t), t))}{|\det(\partial\Phi_{\mathbf{x}t}(\mathbf{u}(\mathbf{x}, t))/\partial\mathbf{v})|}. \tag{34}$$

At caustics, one has

$$\det\frac{\partial\Phi_{\mathbf{x}t}(\mathbf{u}(\mathbf{x}, t))}{\partial\mathbf{v}} = 0$$

and one sees from (34) that the density has a concentration known as the δ-shock for pressureless gas.

4.2. Ansatz for the multi-phase solutions

Intuitively the solution will follow the Hamiltonian flow and whenever they cross the density and momentum will superimpose. Namely, the semiclassical solution should allow the exhibition of multi-phase solution once the single phase ansatz breaks down. As mentioned in the previous section, one can get the asymptotic solution:

$$\psi \approx \sum_{k=1}^{N(\mathbf{x},t)} \psi_k(\mathbf{x}, t) = \sum_{k=1}^{N(\mathbf{x},t)} A_k(\mathbf{x}, t)\, \mathrm{e}^{\mathrm{i}(S_k(\mathbf{x},t)/\epsilon)}. \tag{35}$$

In addition, we have $\mathbf{u}_k(\mathbf{x}, t) = \nabla S_k(\mathbf{x}, t) \neq \mathbf{u}_j(\mathbf{x}, t)$ for $k \neq j$ and A_k's does not vanish. This assumption ensures that at point $(\mathbf{x}, t)$ there are indeed N (rather than less) different phases. These assumptions will guarantee that the ansatz (35) is not degenerate, and consequently that the resulting moment system in the semiclassical limit is hyperbolic (the Jacobian from the moments to densities and velocities are invertible), as will be shown in Section 4.6. In A_k vanishes at a point $(\mathbf{x}, t)$, it simply means that the assumption of having N phase is not valid and one has to lower the number to the correct one. Practically if A_k is vanishingly small, it means that the branch is near vacuum. It can be numerically handled by kinetic schemes, which will be discussed in details in Section 6.

We proceed to compute the Wigner distribution for solutions of this form. To compute the weak limit of $W[\psi_k, \psi_j]$, we first integrate it with a test function $\phi(\mathbf{v}) \in D(\mathrm{R}^n_{\mathbf{v}})$:

$$\begin{aligned}
&\int_{\mathrm{R}^n} W[\psi_k, \psi_j]\phi(\mathbf{v})\,\mathrm{d}\mathbf{v} \\
&\quad = \frac{1}{(2\pi)^n}\int_{\mathrm{R}^n}\int_{\mathrm{R}^n} \mathrm{e}^{\mathrm{i}\mathbf{v}\cdot\mathbf{y}} A_k\left(\mathbf{x}-\epsilon\frac{\mathbf{y}}{2},t\right)\bar{A}_j\left(\mathbf{x}+\epsilon\frac{\mathbf{y}}{2},t\right)\mathrm{e}^{\mathrm{i}(S_k(\mathbf{x}-\epsilon(\mathbf{y}/2),t)-S_j(\mathbf{x}+\epsilon(\mathbf{y}/2),t))/\epsilon}\phi(\mathbf{v})\,\mathrm{d}\mathbf{y}\,\mathrm{d}\mathbf{v} \\
&\quad = \frac{1}{(2\pi\epsilon)^n}\int_{\mathrm{R}^n}\int_{\mathrm{R}^n} A_k\left(\mathbf{x}-\frac{\mathbf{y}}{2},t\right)\bar{A}_j\left(\mathbf{x}+\frac{\mathbf{y}}{2},t\right)\mathrm{e}^{\mathrm{i}(\mathbf{v}\cdot\mathbf{y}+S_k(\mathbf{x}-(\mathbf{y}/2),t)-S_j(\mathbf{x}+(\mathbf{y}/2),t))/\epsilon}\phi(\mathbf{v})\,\mathrm{d}\mathbf{y}\,\mathrm{d}\mathbf{v}.
\end{aligned}$$

The asymptotic limit can be carried out by the stationary phase method. Define

$$\theta(\mathbf{v},\mathbf{y}) = \mathbf{v}\cdot\mathbf{y} + S_k\left(\mathbf{x}-\frac{\mathbf{y}}{2},t\right) - S_j\left(\mathbf{x}+\frac{\mathbf{y}}{2},t\right).$$

Because of the high oscillations in the integral, the main contributions come from the vicinity of the stationary points of $\theta(\mathbf{v},\mathbf{y})$. Since

$$\nabla\theta = \left(\mathbf{y}, \mathbf{v} - \frac{1}{2}\left(\mathbf{u}_k\left(\mathbf{x}-\frac{\mathbf{y}}{2},t\right)+\mathbf{u}_j\left(\mathbf{x}+\frac{\mathbf{y}}{2}\right)\right)\right),$$

the single stationary point is located at $((1/2)(\mathbf{u}_k(\mathbf{x},t)+\mathbf{u}_j(\mathbf{x},t)),0)$. The Hessian matrix $D^2\theta$ has determinant -1. Therefore

$$\int_{\mathrm{R}^n} W[\psi_k,\psi_j]\phi(\mathbf{v})\,\mathrm{d}\mathbf{v} = A_k(\mathbf{x},t)\bar{A}_j(\mathbf{x},t)\,\mathrm{e}^{\mathrm{i}(\pi/4)\,\mathrm{sgn}(D^2\theta)}\,\mathrm{e}^{\mathrm{i}(S_k(\mathbf{x},t)-S_j(\mathbf{x},t))/\epsilon}\phi\left(\frac{1}{2}(\mathbf{u}_j(\mathbf{x},t)+\mathbf{u}_k(\mathbf{x},t))\right)+\mathrm{O}(\epsilon).$$

If $j=k$, $\mathrm{sgn}\,D^2\theta = 0$, one then has

$$\int_{\mathrm{R}^n} W[\psi_k,\psi_k]\phi(\mathbf{v})\,\mathrm{d}\mathbf{v} \to \rho_k(\mathbf{x},t)\phi(\mathbf{u}_k(\mathbf{x},t)), \quad \text{as } \epsilon\to 0.$$

For $j\neq k$, observe that the function $S_k(\mathbf{x},t)-S_j(\mathbf{x},t)$ has no stationary point because $\mathbf{u}_j(\mathbf{x},t)\neq\mathbf{u}_k(\mathbf{x},t)$. Thus the integral

$$\int_{\mathrm{R}^n}\int_{\mathrm{R}^n} W[\psi_k,\psi_j]\phi(\mathbf{v})\eta(\mathbf{x})\,\mathrm{d}\mathbf{v}\,\mathrm{d}\mathbf{x}$$

converges to 0 for any $\eta\in D(\mathrm{R}^n_{\mathbf{x}})$ again by the stationary phase method.

Hence (in the measure convergence sense), we have

$$W[\psi_k,\psi_j] \to \begin{cases} \rho_k(\mathbf{x},t)\delta(\mathbf{v}-\mathbf{u}_k(\mathbf{x},t)) & \text{for } j=k, \\ 0 & \text{for } j\neq k \end{cases} \quad \text{in } C_{\mathrm{b}}(\mathrm{R}_t, M^+(\mathrm{R}_{\mathbf{v}}\times\mathrm{R}_{\mathbf{x}})w-\star) \tag{36}$$

and the corresponding limiting Wigner function becomes

$$w(\mathbf{x},\mathbf{v},t) = \sum_{k=1}^{N(\mathbf{x},t)} \rho_k\delta(\mathbf{v}-\mathbf{u}_k) \tag{37}$$

away from the caustics.

Another derivation of the multi-phase ansatz can be obtained via (28). Let $\phi(\mathbf{x},\mathbf{v})$ be any test function. From the definitions (26) and (29):

$$\int_{\mathrm{R}^n}\rho_0(\mathbf{x}_0)\phi(\hat{\mathbf{x}}(\mathbf{x}_0,t),\hat{\mathbf{v}}(\mathbf{x}_0,t))\,\mathrm{d}\mathbf{x}_0 = \int_{\mathrm{R}^n}\int_{\mathrm{R}^n}\rho_0(\mathbf{x}_0)\phi(\mathbf{x}(\mathbf{x}_0,\mathbf{v}_0,t),\mathbf{v}(\mathbf{x}_0,\mathbf{v}_0,t))\delta(\mathbf{v}_0-\mathbf{u}_0(\mathbf{x}_0))\,\mathrm{d}\mathbf{v}_0\,\mathrm{d}\mathbf{x}_0.$$

Changing variables to the bicharacteristic curves $(\mathbf{x}, \mathbf{v})$ defined in (26), using the definition of $\Phi_{\mathbf{x}t}$ (which has zeroes $\mathbf{u}_k(\mathbf{x}, t)$, $1 \le k \le N(\mathbf{x}, t)$), and the volume-preserving property of the Hamiltonian flow, the above integrals equal to

$$\begin{aligned}
&\int_{\mathrm{R}^n}\int_{\mathrm{R}^n} \rho_0(\mathbf{x}_0(\mathbf{x}, \mathbf{v}, t))\phi(\mathbf{x}, \mathbf{v})\delta(\Phi_{\mathbf{x}t}(\mathbf{v}))\,\mathrm{d}\mathbf{v}\,\mathrm{d}\mathbf{x}\\
&\quad= \int_{\mathrm{R}^n} \sum_{k=1}^{N(\mathbf{x},t)} \frac{\rho_0(\mathbf{x}_0(\mathbf{x}, \mathbf{u}_k(\mathbf{x}, t), t))}{|\det(\partial\Phi_{\mathbf{x}t}(\mathbf{u}_k(\mathbf{x}, t))/\partial\mathbf{v})|}\phi(\mathbf{x}, \mathbf{u}_k(\mathbf{x}, t))\,\mathrm{d}\mathbf{x}\\
&\quad= \int_{\mathrm{R}^n}\int_{\mathrm{R}^n} \sum_{k=1}^{N(\mathbf{x},t)} \frac{\rho_0(\mathbf{x}_0(\mathbf{x}, \mathbf{u}_k(\mathbf{x}, t), t))}{|\det(\partial\Phi_{\mathbf{x}t}(\mathbf{u}_k(\mathbf{x}, t))/\partial\mathbf{v})|}\delta(\mathbf{v} - \mathbf{u}_k(\mathbf{x}, t))\phi(\mathbf{x}, \mathbf{v})\,\mathrm{d}\mathbf{v}\,\mathrm{d}\mathbf{x}\\
&\quad= \int_{\mathrm{R}^n}\int_{\mathrm{R}^n} \sum_{k=1}^{N(\mathbf{x},t)} \rho_k(\mathbf{x}, t)\delta(\mathbf{v} - \mathbf{u}_k(\mathbf{x}, t))\phi(\mathbf{x}, \mathbf{v})\,\mathrm{d}\mathbf{v}\,\mathrm{d}\mathbf{x}
\end{aligned}$$

with ρ_k connected with u_k by (34). The above equalities hold as long as

$$\det\frac{\partial\Phi_{\mathbf{x}t}(\mathbf{u}_k(\mathbf{x}, t))}{\partial\mathbf{v}} \neq 0, \quad k = 1, \ldots, N,$$

namely, away from the caustics. This proves that w given in (37) satisfies the Vlasov equation (22) with initial condition (23) in the distributional sense, while each $(\rho_k, \mathbf{u}_k)$ is the classical solution to the pressureless gas equations (25).

We summarize our results in the following theorem.

Theorem 3. *If ψ satisfies (1) and (2), then the Wigner transform $W[\psi, \psi]$ converges in the measure sense to (37) away from the caustics, where $(\rho_k, \mathbf{u}_k)$'s are the classical solution of the pressureless gas equations (25). The solution of the Vlasov equation (22) in the multi-phase domain is given by (37) in the distributional sense.*

Remark 1. Since the physical observables can be represented by the moments of the solutions of (22), the convergence in (36) also implies that in the single phase domain, the convergence of these observables are in the strong sense.

Remark 2. The zeroes of $\Phi_{\mathbf{x}t}(\mathbf{v})$ are the multi-valued velocities. Therefore, one can get a bound of the number of possible phases $N(\mathbf{x}, t)$. For instance, in one dimension one immediately sees that

$$N(x, t) \le n \quad \text{if} \quad \frac{\mathrm{d}^n}{\mathrm{d}v^n}\Phi_{xt}(v) \neq 0 \ \ \forall v \in R.$$

Especially in the zero potential case, $\Phi_{xt}(v) = v - u_0(x - vt)$, a sufficient condition for $N(x, t) \le n$ $(n \ge 2)$ is

$$\frac{\mathrm{d}^n}{\mathrm{d}x^n}u_0 \neq 0.$$

Interestingly this agrees with the phase number estimate for the KdV equation in the zero-dispersion limit [21].

4.3. One-dimensional moment equations for multi-phase solutions

Next we will apply this multi-phase ansatz (37) to obtain moment equations for multi-phase solutions. To compare with the results from Whitham's averaging technique, we first derive the equations in one space dimension.

Define the moments

$$m_l = \int_R w(x, v, t) v^l \, \mathrm{d}v, \quad l = 0, 1, \ldots, 2N.$$

In addition, we define the density and velocity by

$$\rho(x, t) = m_0, \quad u(x, t) = \frac{m_1}{m_0}.$$

Multiplying the Vlasov equation (22) in one-dimensional by v^l, $l = 0, 1, \ldots, 2N-1$ and integrating over v, one obtains the moment equations in the physical space

$$\begin{aligned} &\partial_t m_0 + \partial_x m_1 = 0, \\ &\partial_t m_1 + \partial_x m_2 = -m_0 \partial_x V, \\ &\vdots \\ &\partial_t m_{2N-1} + \partial_x m_{2N} = -(2N-1) m_{2N-2} \partial_x V. \end{aligned} \tag{38}$$

With the ansatz (37) for the N phase solution, one has

$$m_l = \sum_{k=1}^{N} \rho_k u_k^l, \quad l = 0, 1, \ldots, 2N. \tag{39}$$

With these one can close the moment system (38) by expressing m_{2N} as a function of $m_0, \ldots, m_{2N-1}$:

$$m_{2N} = F(m_0, m_1, \ldots, m_{2N-1}), \tag{40}$$

provided the $2N \times 2N$ system

$$m_l = \sum_{k=1}^{N} \rho_k u_k^l, \quad l = 0, 1, \ldots, 2N-1 \tag{41}$$

is invertible, allowing us to express $(\rho_k, u_k, k = 1, \ldots, N)$ in terms of $m_0, m_1, \ldots, m_{2N-1}$. If this is true, the function F in (40) can be defined and consequently the multi-phase equations (38) and (40) are equivalent to the N pressureless gas equations (25) satisfied by each (ρ_k, u_k). This will be provide in Section 3.6. A general way to obtain and compute F is given in Appendix A.

4.4. Two phase equations

If $N = 2$, then one obtains four moment equations:

$$\begin{aligned} &\partial_t m_0 + \partial_x m_1 = 0, \qquad \partial_t m_1 + \partial_x m_2 = -m_0 \partial_x V, \\ &\partial_t m_2 + \partial_x m_3 = -2 m_1 \partial_x V, \qquad \partial_t m_3 + \partial_x m_4 = -3 m_2 \partial_x V \end{aligned} \tag{42}$$

with

$$m_4 = \frac{m_3^2 m_0 - 2 m_1 m_2 m_3 + m_2^3}{m_0 m_2 - m_1^2}. \tag{43}$$

This system governs the evolution of two phase solutions, which coincides with the Whitham's two phase equations derived in Section 2. It breaks down if more than two phases emerge.

Clearly, (43) is well-defined if and only if $(m_0m_2 - m_1^2)/\rho_1\rho_2\ (= (u_2 - u_1)^2) \neq 0$. Otherwise, the two phase solution does not exist at this point and one has to use the single phase equations (16) and (17). In order to have a system of PDEs that governs *both* the double phase and single phase solution we define m_4 as follows:

$$m_4 = \begin{cases} \dfrac{m_3^2 m_0 - 2m_1m_2m_3 + m_2^3}{m_0m_2 - m_1^2} & \text{if } m_0m_2 - m_1^2 \neq 0, \\ \dfrac{m_2^2}{m_0} & \text{otherwise.} \end{cases} \tag{44}$$

It is easy to verify that when $m_0m_2 = m_1^2$, this definition of m_4 makes the double phase equation (42) equivalent to the single phase equations (16) and (17). Namely, by solving (42) with a discontinuous flux defined in (44), we obtain both single and double phase solutions, whichever emerges.

The double phase system can be written in another way. Define

$$p = \begin{cases} \dfrac{m_3m_0 - m_1m_2}{m_0m_2 - m_1^2} (= u_1 + u_2) & \text{if } m_0m_2 - m_1^2 \neq 0, \\ \dfrac{m_1}{m_0} & \text{otherwise,} \end{cases} \tag{45}$$

$$q = \begin{cases} \dfrac{m_1m_3 - m_2^2}{m_0m_2 - m_1^2} (= u_1u_2) & \text{if } m_0m_2 - m_1^2 \neq 0, \\ 0 & \text{otherwise.} \end{cases} \tag{46}$$

Then

$$m_4 = pm_3 - qm_2, \qquad m_3 = pm_2 - qm_1, \qquad m_2 = pm_1 - qm_0$$

and the system becomes

$$\partial_t \mathbf{m} + \partial_x (A(p, q)\mathbf{m}) = S(\mathbf{m}), \tag{47}$$

where

$$A = \begin{bmatrix} 0 & 1 & 0 & 0 \\ -q & p & 0 & 0 \\ 0 & -q & p & 0 \\ 0 & 0 & -q & p \end{bmatrix}$$

and

$$S(\mathbf{m}) = (0, m_0\partial_x V, 2m_1\partial_x V, 3m_2\partial_x V)^{\mathrm{T}}.$$

For this system, the Jacobian is

$$\begin{bmatrix} 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ -u_1^2u_2^2 & 2(u_1 + u_2)u_1u_2 & -(u_1^2 + u_2^2 + 4u_1u_2) & 2(u_1 + u_2) \end{bmatrix}.$$

The eigenvalues are u_1 and u_2, with eigenvectors

$$(1, u_1, u_1^2, u_1^3) \quad \text{and} \quad (1, u_2, u_2^2, u_2^3),$$

respectively. Hence the Jacobian is similar to a Jordan form and the systems (42) and (44) are *weakly* hyperbolic.

We can see that this hyperbolic system is also homogeneous. One may take this fact into consideration when designing numerical schemes for this system.

4.5. Three phase equations

For the triple phase case, $N = 3$, the moment equations can still be written in homogeneous form:

$$\partial_t \mathbf{m} + \partial_x (A\mathbf{m}) = S(\mathbf{m}) \tag{48}$$

with

$$S(\mathbf{m}) = (0, m_0 \partial_x V, 2m_1 \partial_x V, 3m_2 \partial_x V, 4m_3 \partial_x V)^{\mathrm{T}}$$

and

$$A = \begin{bmatrix} 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ p_3 & -p_2 & p_1 & & & \\ & p_3 & -p_2 & p_1 & & \\ & & p_3 & -p_2 & p_1 & \\ & & & p_3 & -p_2 & p_1 \end{bmatrix},$$

where

$$p_1 = u_1 + u_2 + u_3 = \frac{m_5 m_1^2 - m_5 m_2 m_0 + m_4 m_3 m_0 - m_4 m_1 m_2 + m_3 m_2^2 - m_1 m_3^2}{m_4 m_1^2 - m_4 m_2 m_0 + m_3^2 m_0 - 2m_1 m_2 m_3 + m_2^3},$$

$$p_2 = u_1 u_2 + u_1 u_3 + u_2 u_3 = -\frac{m_5 m_3 m_0 - m_5 m_2 m_1 + m_4 m_2^2 - m_4^2 m_0 + m_4 m_3 m_1 - m_2 m_3^2}{m_4 m_1^2 - m_4 m_2 m_0 + m_3^2 m_0 - 2m_1 m_2 m_3 + m_2^3},$$

$$p_3 = u_1 u_2 u_3 = -\frac{m_5 m_1 m_3 - m_5 m_2^2 - m_4^2 m_1 + 2m_4 m_3 m_2 - m_3^3 - m_4^2 m_1}{m_4 m_1^2 - m_4 m_2 m_0 + m_3^2 m_0 - 2m_1 m_2 m_3 + m_2^3}.$$

In order to include also the double and single phase solutions in (48), we use the following quantities:

$$\phi_1 = m_0 m_2 - m_1^2, \tag{49}$$

$$\phi_2 = m_4 m_1^2 - m_4 m_2 m_0 + m_3^2 m_0 - 2m_1 m_2 m_3 + m_2^3, \tag{50}$$

as phase indicators. Here $\phi_1 > 0$ if at least two phases of the solution superimpose and $\phi_2 < 0$ if the solution splits into at least three phases. In the case of two phases we define

$$p_1 = p, \qquad p_2 = q, \qquad p_3 = 0 \quad \text{when} \quad \phi_2 = 0 \tag{51}$$

with p and q defined in (45) and (46). Then the matrix A can be used to compute solutions containing one to three phases.

The case when $N > 3$ can also be derived in the same way. We have found the expression of M_{2N} for N up to 5 (see [26]).

4.6. Hyperbolicity of the N phase equations

To show the (weak) hyperbolicity of the N phase equations (38) and (40), one just needs to prove that the Jacobian matrix:

$$A_N = \frac{\partial(m_0, m_1, \ldots, m_{2N-1})}{\partial(\rho_1, \rho_2, \ldots, \rho_N, u_1, \ldots, u_N)}$$

has rank $2N$. Then one can invert system (41) to express ρ_k, u_k as functions of $m_0, \ldots, m_{2N-1}$. Since each (ρ_i, u_i) satisfies the pressureless gas equations which are weakly hyperbolic, as a consequence, systems (38) and (40) are then (weakly) hyperbolic. By direct differentiation one has

$$A_N(\rho_1, \rho_2, \ldots, \rho_N, u_1, u_2, \ldots, u_N) \times \begin{bmatrix} 1 & 1 & \cdots & 1 & 0 & 0 & \cdots & 0 \\ u_1 & u_2 & \cdots & u_N & 1 & 1 & \cdots & 1 \\ u_1^2 & u_2^2 & \cdots & u_N^2 & 2\rho_1 u_1 & 2\rho_2 u_2 & \cdots & 2\rho_N u_N \\ \vdots & \vdots & \cdots & \vdots & \vdots & \vdots & \cdots & \vdots \\ u_1^{2N-1} & u_2^{2N-1} & \cdots & u_N^{2N-1} & (2N-1)\rho_1 u_1^{2N-2} & (2N-1)\rho_2 u_2^{2N-2} & \cdots & (2N-1)\rho_N u_2^{2N-2} \end{bmatrix}.$$

Then one can use the standard technique for Vandermonde type of matrices:

$$\begin{aligned} &\det(A_N) \\ &\quad = \rho_1 \times \cdots \times \rho_N \\ &\qquad \times \det \begin{bmatrix} 1 & 1 & \cdots & 1 & 0 & 0 & \cdots & 0 \\ u_1 & u_2 & \cdots & u_N & \rho_1 & \rho_2 & \cdots & \rho_N \\ u_1^2 & u_2^2 & \cdots & u_N^2 & 2u_1 & 2u_2 & \cdots & 2u_N \\ \vdots & \vdots & \cdots & \ddots & \vdots & \vdots & \ddots & \vdots \\ u_1^{2N-1} & u_2^{2N-1} & \cdots & u_N^{2N-1} & (2N-1)u_1^{2N-2} & (2N-1)u_2^{2N-2} & \cdots & (2N-1)u_2^{2N-2} \end{bmatrix} \\ &\quad = \rho_1 \times \cdots \times \rho_N \times (u_2 - u_1) \times \cdots \times (u_N - u_1) \\ &\qquad \times \det \begin{bmatrix} 1 & \cdots & 1 & 1 & 1 & \cdots & 1 \\ u_2 & \cdots & u_N & u_1 & 2u_2 - u_1 & \cdots & 2u_N - u_1 \\ u_2^2 & \cdots & u_N^2 & u_1^2 & 3u_2^2 - 2u_2 u_1 & \cdots & 3u_N^2 - 2u_N u_1 \\ \vdots & \ddots & \vdots & \vdots & \vdots & \ddots & \vdots \\ u_2^{2N-2} & \cdots & u_N^{2N-2} & u_1^{2N-2} & (2N-1)u_2^{2N-2} - (2N-2)u_2^{2N-3} & \cdots & (2N-1)u_N^{2N-2} - (2N-2)u_N^{2N-3} \end{bmatrix} \\ &\quad = \rho_1 \times \cdots \times \rho_N \times (u_2 - u_1)^2 \times \cdots \times (u_N - u_1)^2 \\ &\qquad \times \det \begin{bmatrix} 1 & \cdots & 1 & 2u_2 - 2u_1 & \cdots & 2u_N - 2u_1 \\ u_2 & \cdots & u_N & (3u_2 - u_1)(u_2 - u_1) & \cdots & (3u_N - u_1)(u_N - u_1) \\ u_2^2 & \cdots & u_N^2 & (4u_2 - 2u_1)u_2(u_2 - u_1) & \cdots & (4u_N - 2u_1)u_N(u_N - u_1) \\ \vdots & \ddots & \vdots & \vdots & \ddots & \vdots \\ u_2^{2N-3} & \cdots & u_N^{2N-3} & ((2N-1)u_2 - (2N-3)u_1)u_2^{2N-4}(u_2 - u_1) & \cdots & ((2N-1)u_N - (2N-3)u_1)u_N^{2N-4}(u_N - u_1) \end{bmatrix} \end{aligned}$$

$$
\begin{aligned}
&= (-1)^{N+1}\rho_1 \times \cdots \times \rho_N \times (u_2-u_1)^3 \times \cdots \times (u_N-u_1)^3 \\
&\times \det \begin{bmatrix}
1 & \cdots & 1 & 2 & \cdots & 2 \\
u_2 & \cdots & u_N & 3u_2-u_1 & \cdots & 3u_N-u_1 \\
u_2^2 & \cdots & u_N^2 & (4u_2-3u_1)u_2 & \cdots & (4u_N-2u_1)u_N \\
\vdots & \ddots & \vdots & \vdots & \ddots & \vdots \\
u_2^{2N-3} & \cdots & u_N^{2N-3} & ((2N-1)u_2-(2N-3)u_1)u_2^{2N-4} & \cdots & ((2N-1)u_N-(2N-3)u_1)u_N^{2N-4}
\end{bmatrix} \\
&= (-1)^{N+1}\rho_1 \times (u_2-u_1)^4 \times \cdots \times (u_N-u_1)^4 \times \det(A_{N-1}(\rho_2,\ldots,\rho_N,u_2,\ldots,u_N)).
\end{aligned}
$$

Obviously, $\det(A_1)=\rho_1$. Hence, by induction one has

$$
\det(A_N) = (-1)^{N(N+3)/2} \prod_{l=1}^{N} \rho_l \prod_{1\le j<k\le N} (u_j-u_k)^4.
$$

This shows that the determinant does not vanish as long as the u_k's are distinct and the ρ_k's are positive. Under these conditions, system (41) is invertible and consequently, systems (38) and (40) are weakly hyperbolic.

4.7. Two-dimensional multi-phase equations

In two-dimensional, to describe an N phase solution, we need $3N$ moments. One has to select the moment equations very carefully to avoid the degeneracy of the resulting system. For instance, in the double phase case, if we define the moments by multiplying w with $(1, v_1, v_2, v_1^2, v_1v_2, v_2^2)$, the moments are

$$
(\rho_1+\rho_2, \rho_1u_1^{(1)}+\rho_2u_2^{(1)}, \rho_1u_1^{(2)}+\rho_2u_2^{(2)}, \rho_1u_1^{(1)^2}+\rho_2u_2^{(1)^2}, \rho_1u_1^{(1)}u_1^{(2)}+\rho_2u_2^{(1)}u_2^{(2)}, \rho_1u_1^{(2)^2}+\rho_2u_2^{(2)^2}),
$$

where $\mathbf{u}=(u^{(1)},u^{(2)})$. One can easily check that the corresponding moment equations are degenerate in that the Jacobian has determinant 0 and so the mapping from $(\rho_1,\mathbf{u}_1,\rho_2,\mathbf{u}_2)$ to the moments is not invertible.

Instead, we let

$$
(c,s) = \frac{\mathbf{u}}{\|\mathbf{u}\|}
$$

in which $\|\cdot\|$ is the Cartesian distance. This vector can be interpreted as the direction of the rays. We select the first $2N$ moments in the following way:

$$
\begin{aligned}
m_{j,0} &= \int w \left(\frac{v_1}{\|\mathbf{v}\|}\right)^{2j-1} \mathrm{d}\mathbf{v} = \sum_{k=1}^{N} \rho_k c_k^{2j-1}, \\
m_{0,j} &= \int w \left(\frac{v_2}{\|\mathbf{v}\|}\right)^{2j-1} \mathrm{d}\mathbf{v} = \sum_{k=1}^{N} \rho_k s_k^{2j-1}, \quad j=1,\ldots,N,
\end{aligned} \tag{52}
$$

where the multi-phase ansatz (37) has been used.

In [12], it was proven that as long as c_k's are distinct, the mapping

$$
(\rho_1c_1, \rho_1s_1, \ldots, \rho_Nc_N, \rho_Ns_N) \to (m_{1,0}, m_{0,1}, \ldots, m_{N,0}, m_{0,N}) \tag{53}
$$

is invertible. This is certainly the case if rays do not follow the same directions or run into each other head-to-head. Otherwise, one has to choose different coordinate to close the system. Since $c^2+s^2=1$, there are $2N$ independent

variables on the left-hand side of (53), thus one can recover the density ρ_k's and the direction of the rays from the moment variables $(m_{0,j}, m_{j,0})$.

The next N moments are chosen to be the strength of the rays:

$$m_{j,j} = \int w \frac{v_1^j}{\|\mathbf{v}\|^{j-1}} \,\mathrm{d}\mathbf{v} = \sum_{k=1}^{N} \rho_k \|\mathbf{u}_k\| c_k^j, \quad j = 1, 2, \ldots, N.$$

Clearly, one can solve $\rho_k\|\mathbf{u}_k\|$ from these equations because the linear system is of the Vandermonde type. Hence the multi-phase equations are

$$\partial_t \sum_{j=1}^{N} \rho_j c_j + \partial_x \sum_{j=1}^{N} \rho_j \|\mathbf{u}_j\| c_j^2 + \partial_y \sum_{j=1}^{N} \rho_j \|\mathbf{u}_j\| c_j s_j = -\sum_{j=1}^{N} \left(\rho_j \frac{s_j^2}{\|\mathbf{u}_j\|} \partial_x V - \rho_j \frac{c_j s_j}{\|\mathbf{u}_j\|} \partial_y V \right),$$

$$\partial_t \sum_{j=1}^{N} \rho_j s_j + \partial_x \sum_{j=1}^{N} \rho_j \|\mathbf{u}_j\| c_j s_j + \partial_y \sum_{j=1}^{N} \rho_j \|\mathbf{u}_j\| s_j^2 = \sum_{j=1}^{N} \left(\rho_j \frac{c_j s_j}{\|\mathbf{u}_j\|} \partial_x V - \rho_j \frac{c_j^2}{\|\mathbf{u}_j\|} \partial_y V \right), \cdots$$

$$\partial_t \sum_{j=1}^{N} \rho_j c_j^{2N-1} + \partial_x \sum_{j=1}^{N} \rho_j \|\mathbf{u}_j\| c_j^{2N} + \partial_y \sum_{j=1}^{N} \rho_j \|\mathbf{u}_j\| c_j^{2N-1} s_j$$
$$= -(2N-1) \sum_{j=1}^{N} \left(\rho_j \frac{s_j^2 c_j^{2N-2}}{\|\mathbf{u}_j\|} \partial_x V - \rho_j \frac{c_j^{2N-1} s_j}{\|\mathbf{u}_j\|} \partial_y V \right),$$

$$\partial_t \sum_{j=1}^{N} \rho_j s_j^{2N-1} + \partial_x \sum_{j=1}^{N} \rho_j \|\mathbf{u}_j\| c_j s_j^{2N-1} + \partial_y \sum_{j=1}^{N} \rho_j \|\mathbf{u}_j\| s_j^{2N}$$
$$= (2N-1) \sum_{j=1}^{N} \left(\rho_j \frac{c_j s_j^{2N-1}}{\|\mathbf{u}_j\|} \partial_x V - \rho_j \frac{c_j^2 s_j^{2N-2}}{\|\mathbf{u}_j\|} \partial_y V \right),$$

$$\partial_t \sum_{j=1}^{N} \rho_j \|\mathbf{u}_j\| + \partial_x \sum_{j=1}^{N} \rho_j \|\mathbf{u}_j\|^2 c_j + \partial_y \sum_{j=1}^{N} \rho_j \|\mathbf{u}_j\|^2 s_j = \sum_{j=1}^{N} \rho_j \partial_x V, \cdots$$

$$\partial_t \sum_{j=1}^{N} \rho_j \|\mathbf{u}_j\| c_j^{N-1} + \partial_x \sum_{j=1}^{N} \rho_j \|\mathbf{u}_j\|^2 c_j^N + \partial_y \sum_{j=1}^{N} \rho_j \|\mathbf{u}_j\|^2 c_j^{N-1} s_j$$
$$= \sum_{j=1}^{N} (\rho_j (N c_j^{N-1} - (j-1) c_j^{N+1}) \partial_x V - \rho_j (N-1) c_j^N s_j).$$

5. Other related problems

The above study on multi-phase solutions can be carried out for other related equations, for which we will show that the Whitham averaging technique and the Wigner transform and kinetic moment closure methods produce the same multi-phase equations. To simplify the presentation, we only show the derivation of the single phase equations for Whitham's method. For multi-phase equations, one has to use more balance equations in Whitham's method, or take more moments in the Wigner approach.

5.1. The Linearized Korteweg–de Vries equation

We consider the linear KdV equation:

$$u_t + cu_x + \epsilon^2 u_{xxx} = 0, \quad x \in \mathrm{R}. \tag{54}$$

5.1.1. Whitham's averaging method

Starting from (54), one can consider the wave train:

$$u(x,t) = a\cos\left(\frac{\xi x - \omega(\xi)t}{\epsilon}\right),$$

where

$$\omega(\xi) = c\xi - \xi^3$$

is the dispersive relation, and a and ξ depend on x and t. When integrating over a small range, they can be held as constants.

Note that the equation is endowed with the following conservation laws:

$$(u^2)_t + (cu^2 + 2\epsilon^2 uu_{xx} - \epsilon^2 u_x^2)_x = 0, \qquad (\epsilon^2 u_t u_x + c\epsilon^2 \tfrac{1}{2}u_x^2 - \tfrac{1}{2}\epsilon^4 u_{xx}^2)_t + (\epsilon^4 u_x u_{xxt} - \tfrac{1}{2}\epsilon^2 u_t^2)_x = 0.$$

Averaging the equations over one period gives

$$\overline{u^2} = \frac{1}{2}a^2, \qquad \overline{\epsilon^2 uu_{xx}} = -\frac{1}{2}a^2\xi^2, \qquad \overline{\epsilon^2 u_x^2} = \frac{1}{2}a^2\xi^2, \qquad \overline{\epsilon^2 u_t u_x} = -\omega\xi\frac{a^2}{2},$$
$$\overline{\epsilon^4 u_{xx}^2} = \xi^4\frac{a^2}{2}, \qquad \overline{\epsilon^4 u_x u_{xxt}} = -\xi^3\omega\frac{a^2}{2}, \qquad \overline{\epsilon^2 u_t^2} = \omega^2\frac{a^2}{2}.$$

Therefore, one gets the following equations:

$$(a^2)_t + (C(\xi)a^2)_x = 0, \qquad (a^2\xi\omega(\xi))_t + (a^2\xi\omega(\xi)C(\xi))_x = 0, \tag{55}$$

where

$$C(\xi) = \omega'(\xi) = c - 3\xi^2$$

is the group velocity.

(55) can be rewritten as

$$(a^2)_t + (C(\xi)a^2)_x = 0, \qquad \xi_t + (\omega(\xi))_x = 0. \tag{56}$$

It is easy to see that the only eigenvalue is $C(\xi)$, and this system is weakly hyperbolic.

5.1.2. Wigner function approach

We now use the Wigner transform to obtain the single and multi-phase equations. Let

$$W^\epsilon(x,v,t) = W[u,u] = \frac{1}{2\pi}\int_{\mathrm{R}} \mathrm{e}^{\mathrm{i}vy} u\left(t, x - \frac{\epsilon y}{2}\right) u\left(t, x + \frac{\epsilon y}{2}\right) \mathrm{d}y.$$

Then, the Wigner function $W(x,v,t)$ satisfies:

$$W_t^\epsilon + (c - 3v^2)W_x^\epsilon + \frac{\epsilon^2}{4}W_{xxx}^\epsilon = 0.$$

Therefore its limiting distribution $w(x, v, t)$ solves the transport equation:

$$w_t + (c - 3v^2)w_x = 0. \tag{57}$$

One can see that $c - 3v^2$ is nothing but the group velocity $C(v)$.

We assume the WKB initial condition

$$u_0(x) = a\,\mathrm{e}^{\mathrm{i}(S(x,0)/\epsilon)}$$

and the solution remains in this form up to the breaking time. Then

$$w(x, v, 0) = a^2\delta(v - \partial_x S(x, 0)).$$

When $w(x, v, t)$ remains in this form, we can integrate the transport equation (57) and immediately end up with (56) and ξ can be identified as $\partial_x S$.

For multi-phase equations, we define

$$m_j = \int w v^j \,\mathrm{d}v, \qquad n_j = \int w C(v) v^j \,\mathrm{d}v, \quad j = 1, 2, \ldots, N.$$

Then the moments satisfy

$$\partial_t m_j + \partial_x n_j = 0, \quad j = 1, 2, \ldots, N. \tag{58}$$

Obviously

$$n_j = m_j - 3m_{j+2}.$$

Let

$$w(x, v, t) = \sum_{k=1}^{N} a_k^2 \delta(v - \partial_x S_k),$$

then

$$m_j = \sum_{k=1}^{N} a_k^2 u_k^i$$

with $u_k = \partial_x S_k$. Therefore, we can close the system as we did in Section 2. For instance, when $N = 2$, we define

$$p = \frac{m_3 m_0 - m_1 m_2}{m_0 m_2 - m_1^2}, \qquad q = \frac{m_3 m_1 - m_2^2}{m_0 m_2 - m_1^2}.$$

Then one has

$$m_4 = pm_3 - qm_2, \qquad m_5 = (p^2 - q)m_3 - pqm_2,$$

which can close the system.

5.2. The linear wave equation

Consider the wave equation:

$$u_{tt} = c(\mathbf{x})^2 \Delta u, \quad \mathbf{x} \in \mathrm{R}^2. \tag{59}$$

5.2.1. Whitham's approach

The initial condition and the solution (before caustics form) are again assumed to be in the WKB form:

$$u = A\,\mathrm{e}^{\mathrm{i}(S/\epsilon)}. \tag{60}$$

The standard WKB analysis shows that S satisfies the eikonal equation:

$$S_t \pm c|\nabla S| = 0. \tag{61}$$

We will choose the "+" sign to avoid ambiguous computations.

First the following balance equations hold:

$$\left(\epsilon^2\frac{(u_t)^2}{2c^2} + \epsilon^2\frac{|\nabla u|^2}{2}\right)_t + \nabla\cdot(-\epsilon^2 u_t\nabla u) = 0,$$
$$(\epsilon^3 c^{-2}u_{tt}\nabla u)_t - \nabla\cdot(\epsilon^3\nabla u\otimes\nabla u_t + \epsilon^3\nabla u_t\otimes\nabla u - \epsilon^3(\nabla u\cdot\nabla u_t)I) = 0.$$

Let $\xi = \nabla S$ and $\omega = c|\xi|$. A direct calculation gives

$$\overline{\epsilon^2 u_t^2} = \frac{\omega^2 A^2}{2}, \qquad \overline{\epsilon^2|\nabla u|^2} = \frac{|\xi|^2 A^2}{2}, \qquad \overline{-\epsilon^2 u_t\nabla u} = \frac{A^2\omega(\xi)\xi}{2},$$
$$\overline{\epsilon^3 u_{tt}\nabla u} = -\mathrm{i}A^2|\xi|^2 c^2\xi, \qquad \overline{\epsilon^3\nabla u\cdot\nabla u_t} = \overline{\mathrm{i}A^2 c|\xi|^3}, \qquad \overline{\epsilon^3\nabla u\otimes\nabla u_t} = \overline{\mathrm{i}A^2 c|\xi|\xi\otimes\xi}.$$

Therefore, averaging procedure will lead to the equations:

$$(A^2|\xi|^2)_t + \nabla\cdot(A^2 c(x)|\xi|\xi) = 0, \qquad (A^2|\xi|^2\xi)_t + \nabla\cdot(2A^2|\xi|\xi\otimes\xi - A^2|\xi|^3 cI) = 0. \tag{62}$$

These equations can be simplified to be

$$\xi_t + \nabla(c(x)|\xi|) = 0, \qquad (A^2)_t + c\frac{\xi}{|\xi|}\cdot\nabla(A^2) - A^2\nabla c\cdot\frac{\xi}{|\xi|} = 0. \tag{63}$$

These equations possess classical solutions before caustics. From the first equation, one finds that $\nabla\times\xi$ is invariant of time. Since $\xi_0 = \nabla S_0$ at $t = 0$, it remains as a gradient as time progresses. Thus these equations agree with the classical WKB results [41]:

$$S_t + c(\mathbf{x})|\nabla S| = 0, \qquad (A^2)_t + c\frac{\nabla S}{|\nabla S|}\cdot\nabla(A^2) - A^2\nabla c\cdot\frac{\nabla S}{|\nabla S|} = 0. \tag{64}$$

For multi-phase solutions, the Fourier integral method shows that these equations are satisfied by each individual branch [9].

5.2.2. The Wigner function approach

We define

$$f = \epsilon u_t, \qquad \mathbf{g} = \epsilon\nabla u.$$

Then the wave equation can be written as

$$\eta^2 f_t = \nabla\cdot\mathbf{g}, \qquad \mathbf{g}_t = \nabla(f) \tag{65}$$

with $\eta = c^{-1}$.

This kind of symmetric hyperbolic system has been analyzed, using the Wigner distribution, in [34] by a perturbation technique. One introduces a vector-valued function:

$$\mathbf{u}(\mathbf{x}, t) = (f, \mathbf{g}).$$

Then the system becomes

$$\frac{\partial \mathbf{u}}{\partial t} + A \sum_j D_j \frac{\partial \mathbf{u}}{\partial x_j} = 0, \tag{66}$$

where

$$A = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & c^2 \end{pmatrix}, \qquad D_1 = \begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ 1 & 0 & 0 \end{pmatrix}, \qquad D_2 = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}.$$

The matrix-valued Wigner distribution is defined by

$$W^\epsilon(\mathbf{x}, \mathbf{v}, t) = \frac{1}{(2\pi)^2} \int \mathrm{e}^{\mathrm{i}\mathbf{v}\cdot\mathbf{y}} \mathbf{u}\left(\mathbf{x} - \frac{\epsilon \mathbf{y}}{2}, t\right) \mathbf{u}^*\left(\mathbf{x} + \frac{\epsilon \mathbf{y}}{2}, t\right) \mathrm{d}\mathbf{y} \tag{67}$$

in which $\mathbf{u}^*$ denotes the transpose of $\mathbf{u}$. Then $W^\epsilon(\mathbf{x}, \mathbf{v}, t)$ satisfies the following equation:

$$\frac{\partial W^\epsilon}{\partial t} + Q_1 W^\epsilon + \frac{1}{\epsilon} Q_2 W^\epsilon = 0, \tag{68}$$

where

$$\begin{aligned} Q_1 W^\epsilon = {} & \frac{1}{2} \int \mathrm{e}^{-\mathrm{i}\mathbf{x}\cdot\xi} \sum_j \left(\hat{A}(\xi) D_j \frac{\partial W^\epsilon}{\partial x_j}\left(\mathbf{x}, \mathbf{v} + \frac{\epsilon\xi}{2}\right) + \frac{\partial W^\epsilon}{\partial x_j}\left(\mathbf{x}, \mathbf{v} - \frac{\epsilon\xi}{2}\right) D_j \hat{A}(\xi) \right) \mathrm{d}\xi \\ & + \frac{1}{2} \int \mathrm{e}^{-\mathrm{i}\mathbf{x}\cdot\xi} \mathrm{i}\xi_j \sum_j \left(\hat{A}(\xi) D_j W^\epsilon\left(\mathbf{x}, \mathbf{v} + \frac{\epsilon\xi}{2}\right) + W^\epsilon\left(\mathbf{x}, \mathbf{v} - \frac{\epsilon\xi}{2}\right) D_j \hat{A}(\xi) \right) \mathrm{d}\xi \end{aligned}$$

and

$$Q_2 W^\epsilon = \int \mathrm{e}^{-\mathrm{i}\mathbf{x}\cdot\xi} \sum_j \mathrm{i} v_j \left(\hat{A}(\xi) D_j W^\epsilon\left(\mathbf{x}, \mathbf{v} + \frac{\epsilon\xi}{2}\right) + W^\epsilon(\mathbf{x}, \mathbf{v} - \frac{\epsilon\xi}{2}) D_j \hat{A}(\xi) \right) \mathrm{d}\xi.$$

We first expand the operator Q_2 as

$$Q_2 = Q_2^{(0)} + \epsilon Q_2^{(1)} + \mathrm{o}(\epsilon).$$

As $\epsilon \to 0$, the limits of these operator are of

$$Q_2^{(0)} Z = \sum_j \mathrm{i} A v_j D_j Z - \mathrm{i} Z v_j D_j A, \qquad Q_2^{(1)} Z = -\sum_{j,k} \frac{1}{2} \left(\frac{\partial A}{\partial x_k} k_j D_j \frac{\partial Z}{\partial v_k} + \frac{\partial Z}{\partial v_k} k_j D_j \frac{\partial A}{\partial x_k} \right),$$

$$Q_1 Z = \sum_j \frac{1}{2} \left(A D_j \frac{\partial Z}{\partial x_j} + \frac{\partial Z}{\partial x_j} D_j A \right) - \frac{1}{2} \left(\frac{\partial A}{\partial x_j} D_j Z + Z D_j \frac{\partial A}{\partial x_j} \right)$$

for matrix-valued function $Z(\mathbf{x}, \mathbf{v})$.

Next we seek the solution with the expansion:

$$W^\epsilon(\mathbf{x},\mathbf{v},t) = W_0(\mathbf{x},\mathbf{v},t) + \epsilon W_1(\mathbf{x},\mathbf{v},t) + \cdots .$$

Substituting this in (68), one has

$$Q_2^{(0)} W_0 = 0, \tag{69}$$

$$Q_2^{(0)} W_1 = -\frac{\partial W_0}{\partial t} - Q_2^{(1)} W_0 - Q_1 W_0. \tag{70}$$

(69) implies that W_0 has to be in the kernel of the linear operator $Q_2^{(0)}$. In [34], the following dispersion matrix is introduced:

$$L(\mathbf{x},\mathbf{v}) = \sum_j A v_j D_j.$$

Let $\langle , \rangle_A$ be the inner product such that $\langle a, b\rangle_A = aAb^*$. Then L is self-adjoint with respect to this inner product, and has eigenvalues:

$$\lambda_0 = 0, \qquad \lambda_1 = c\|\mathbf{v}\|, \qquad \lambda_2 = -c\|\mathbf{v}\|$$

and eigenvectors:

$$b_0 = \begin{pmatrix} -\dfrac{v_2}{\|\mathbf{v}\|} \\ \dfrac{v_1}{\|\mathbf{v}\|} \\ 0 \end{pmatrix}, \qquad b_1 = \begin{pmatrix} \dfrac{v_1}{\sqrt{2}\|\mathbf{v}\|} \\ \dfrac{v_2}{\sqrt{2}\|\mathbf{v}\|} \\ \dfrac{c}{\sqrt{2}} \end{pmatrix}, \qquad b_2 = \begin{pmatrix} \dfrac{v_1}{\sqrt{2}\|\mathbf{v}\|} \\ \dfrac{v_2}{\sqrt{2}\|\mathbf{v}\|} \\ -\dfrac{c}{\sqrt{2}} \end{pmatrix}.$$

Since $Q_2^{(0)} Z = \mathrm{i}(LZ - ZL)$, $B_i = b_i b_i^*$'s form a basis for the null space of $Q_2^{(0)}$, one can decompose W_0 as

$$W_0 = \sum_i a_i(t,\mathbf{x},\mathbf{v}) B_i(\mathbf{x},\mathbf{v}).$$

The function $a_i(\mathbf{x},\mathbf{v},t)$ can be obtained by projection:

$$a_i(\mathbf{x},\mathbf{v},t) = \mathrm{Tr}(AW_0^* A B_i). \tag{71}$$

Meanwhile, the solvability condition of (70) forces its right-hand side to be perpendicular to the null space of $Q_2^{(1)}$. This leads to the equations for the functions a_i's:

$$\frac{\partial a_i}{\partial t} + \nabla_{\mathbf{v}}\lambda_i \cdot \nabla_{\mathbf{x}} a_i - \nabla_{\mathbf{x}}\lambda_i \cdot \nabla_{\mathbf{v}} a_i = 0. \tag{72}$$

In particular, we use the equation for $w = a_1$:

$$w_t + c\frac{\mathbf{v}}{\|\mathbf{v}\|} \cdot \nabla_{\mathbf{x}} w - \|\mathbf{v}\| \nabla_{\mathbf{x}} c \cdot \nabla_{\mathbf{v}} w = 0. \tag{73}$$

To compute initial distribution for w, we observe that

$$\begin{aligned} w^\epsilon &= \mathrm{Tr}(A(W^\epsilon)^* A B_1) \\ &= \frac{1}{2}\eta(\mathbf{x})^2 W[f,f] + \frac{1}{2} W\left[g\cdot\frac{\mathbf{v}}{\|\mathbf{v}\|}, g\cdot\frac{\mathbf{v}}{\|\mathbf{v}\|}\right] - \frac{1}{2}\eta(x)\frac{\mathbf{v}}{\|\mathbf{v}\|}(W[f,g] + W[g,f]). \end{aligned} \tag{74}$$

In light of (60), we have

$$f = -Ac(\mathbf{x})|\nabla_{\mathbf{x}} S|\, \mathrm{e}^{\mathrm{i}(S(\mathbf{x},t)/\epsilon)} + \mathrm{O}(\epsilon), \qquad g = A\nabla_{\mathbf{x}} S\, \mathrm{e}^{\mathrm{i}(S(\mathbf{x},t)/\epsilon)} + \mathrm{O}(\epsilon)$$

and the initial condition for w:

$$w(\mathbf{x}, \mathbf{v}, 0) = 2A_0^2 |\nabla_{\mathbf{x}} S_0|^2 \delta(\mathbf{v} - \nabla_{\mathbf{x}} S_0).$$

Integrating Eq. (73) together with above ansatz, one gets the moment equations which are equivalent to (62). For multi-phase solutions, one can use linear superpositions and more moment equations to close the system.

The Vlasov equation can be reduced if one only needs to track the wave front. Since the Hamiltonian

$$H(x, \mathbf{v}) = c(x)|\mathbf{v}|$$

is conserved along the bicharacteristics, if one restricts $\mathbf{v}$ to be on the sphere $|\mathbf{v}| = 1/c(x)$ initially, it will remain so all the time. Based on this fact, in [12], the following ansatz was used:

$$w(\mathbf{x}, \mathbf{v}, t) = \sum_{k=1}^{N} \rho_k \delta(\mathbf{v} - \boldsymbol{\nu}(\theta_k)),$$

where $\nu(\theta) = (\cos(\theta), \sin(\theta))$.

Remark. The multi-phase equations for all the problems studied in this paper bear several similarities. For instance, the resulting moment equations are all weakly hyperbolic. Moreover, one always gets the transport or Vlasov equation with the characteristic speed $C(v) = \omega'(v)$. This also explains that the 'energy' propagates with group velocity $\omega'(v)$ for dispersive waves. This can be easily seen by using the Weyl-quantized operators as in [37,38].

6. Numerical schemes

A kinetic scheme will be used in this section for the multi-phase system of the Schrödinger equation, with the phase number set to be $\mathcal{N}$ beforehand. A kinetic scheme for such problem is the most natural since for $\mathcal{N}$ large, the definition of the flux becomes complicated. The kinetic scheme also outperforms a Lax–Friedrichs type schemes for such systems, as will be demonstrated numerically. We briefly present the one-dimensional scheme here. Extension to higher dimension follows the line of [5].

We start from the transport equation:

$$w_t + v\partial_x w = 0. \tag{75}$$

A single phase solution for $w(x, v, t)$ has the form of

$$w(x, v, t) = \rho(x, t)\delta(v - u(x, t))$$

which produces zero temperature equation in gas dynamics. A second order kinetic scheme was introduced in [5] to solve the pressureless gas equation. Extensions of this scheme to multi-phase equations is straightforward.

There are several different interpretations for kinetic scheme. For instance, since the exact solution for (75), within one time step, is

$$w(x, v, t) = w(x - vt, v, t_n)$$

and one can use the ansatz

$$w(x, v, t) = \sum_{k=1}^{\mathcal{N}} \rho_k \delta(v - u_k),$$

to integrate (75) over $(x_{j-1/2}, x_{j+1/2}) \times R_v \times (t_n, t_{n+1})$ to get

$$(m_l)_j^{n+1} - (m_l)_j^n = \frac{\Delta t}{\Delta x}(f_{j+1/2}^{(l)} - f_{j-1/2}^{(l)}), \tag{76}$$

where

$$(m_l)_j^n = \frac{1}{\Delta x}\int_{x_{j-1/2}}^{x_{j+1/2}} m_l \,\mathrm{d}x$$

and

$$f_{j+1/2}^{(l)} = \frac{1}{\Delta t}\int_{\mathrm{R}}\int_{t_n}^{t_{n+1}} w(x_{j+1/2} - vt, v, t_n) v^l \,\mathrm{d}t \,\mathrm{d}v. \tag{77}$$

For first order scheme, one can compute (77) to get

$$f_{j+1/2}^{(l)} = \sum_{k=1}^{\mathcal{N}} (\rho_k u_k^{l-1} u_k^+)_j - (\rho_k u_k^{l-1} u_k^-)_{j+1} \tag{78}$$

Here we use the conventional notations:

$$w^+ = \tfrac{1}{2}(|w| + w), \qquad w^- = \tfrac{1}{2}(|w| - w).$$

One can use piecewise linear construction for (ρ_k, u_k) to obtain a second order scheme (the index k is dropped for convenience):

$$\rho(x) = (\rho)_j + D\rho_j(x - x_j), \qquad u(x) = \bar{u}_j + Du_j(x - x_j) \quad \text{for } x_{j-1/2} < x < x_{j+1/2}, \tag{79}$$

where $\bar{u}_j$ is chosen as

$$\bar{u}_j = u_j - \frac{D\rho_j Du_j}{12\rho_j}\Delta x^2 \tag{80}$$

in order to have the conservation property. Namely, the cell average of $q(x) = \rho(x)u(x)$ must be $q_j = (1/\Delta x)\int_{x_{j-1/2}}^{x_{j+1/2}} \rho(x)u(x)\,\mathrm{d}x$.

After a direct calculation, we have

$$f_{j+1/2}^{(l)} = \sum_{k=1}^{\mathcal{N}} \frac{1}{\Delta t}\int_{x_{j+1/2}^L}^{x_{j+1/2}} \rho_k(x)u_k(x)^{l-1}\,\mathrm{d}x - \frac{1}{\Delta t}\int_{x_{j+1/2}}^{x_{j+1/2}^R} \rho_k(x)u_k(x)^{l-1}\,\mathrm{d}x, \tag{81}$$

where

$$x_{j+1/2}^L = x_{j+1/2} - \Delta t \frac{(\bar{u}_j + \frac{\Delta x}{2}Du_j)^+}{1 + \Delta t Du_j} \tag{82}$$

and

$$x_{j+1/2}^R = x_{j+1/2} + \Delta t \frac{(u_{j+1/2}^R)^-}{1 + \Delta t Du_{j+1}}. \tag{83}$$

From (79), one can rewrite the numerical flux in more explicit forms:

$$
\begin{aligned}
f^{(l)}_{j+1/2} &= \sum_{k=1}^{\mathcal{N}} \sum_{s=0}^{l-1} C^s_{l-1}(u_k)^s_j (Du_k)^{l-s-1}_j \\
&\quad \times \left[\frac{1}{(l-s)\Delta t}(\rho_k)_j \left(\left(\frac{1}{2}\Delta x\right)^{l-s} - (x^L_{j+1/2} - x_j)^{l-s} \right) \right. \\
&\quad \left. + \frac{1}{(l-s+1)\Delta t}(D\rho_k)_j \left(\left(\frac{1}{2}\Delta x\right)^{l-s+1} - (x^L_{j+1/2} - x_j)^{l-s+1} \right) \right] \\
&\quad + \sum_{k=1}^{\mathcal{N}} \sum_{s=0}^{l-1} C^s_{l-1}(u_k)^s_{j+1} (Du_k)^{l-s-1}_{j+1} \\
&\quad \times \left[\frac{1}{(l-s)\Delta t}(\rho_k)_{j+1} \left((x^R_{j+1/2} - x_{j+1})^{l-s} - \left(-\frac{1}{2}\Delta x\right)^{l-s} \right) \right. \\
&\quad \left. + \frac{1}{(l-s+1)\Delta t}(D\rho_k)_{j+1} \left((x^R_{j+1/2} - x_{j+1})^{l-s+1} - \left(-\frac{1}{2}\Delta x\right)^{l-s+1} \right) \right].
\end{aligned}
$$

The slope limiters are chosen in the following way to ensure several relevant properties (see [5]):

$$
\begin{aligned}
D\rho_j &= \frac{1}{2}(\operatorname{sgn}(\rho_{j+1} - \rho_j) + \operatorname{sgn}(\rho_j - \rho_{j-1})) \times \min\left\{ \frac{|\rho_{j+1} - \rho_j|}{\Delta x}, \frac{|\rho_j - \rho_{j-1}|}{\Delta x}, \frac{2\rho_j}{\Delta x} \right\}, \\
Du_j &= \frac{1}{2}(\operatorname{sgn}(u_{j+1} - u_j) + \operatorname{sgn}(u_j - u_{j-1})) \times \min\left\{ \frac{|u_{j+1} - u_j|}{(1 - \Delta x D\rho_j/6\rho_j)\Delta x}, \frac{|u_j - u_{j-1}|}{(1 + \Delta x D\rho_j/6\rho_j)\Delta x}, \frac{1}{\Delta t} \right\}.
\end{aligned} \tag{84}
$$

If the potential term $V(x) \neq 0$, we discretize the source term by

$$
-(l+1)\left(\frac{m^n_l + m^{n+1}_l}{2} \nabla V \right)_k, \quad l = 0, 1, \ldots, 2\mathcal{N} - 2.
$$

Since m^{n+1}_l can be computed from the previous equation, this implicit scheme can be solved explicitly.

One can also use the Lax–Friedrichs scheme. Let a be a constant such that $a \geq \sup\{u(x,t) : x \in \mathrm{R}, t \geq 0\}$, then the numerical flux for Lax–Friedrichs scheme can be written as

$$
f^{(l)}_{j+1/2} = \sum_{k=1}^{\mathcal{N}} \frac{1}{2}(\rho_k u^{l-1}_k (a + u^+_k))_j - \frac{1}{2}(\rho_k u^{l-1}_k (a - u^-_k))_{j+1}. \tag{85}
$$

In our numerical implementation, the following procedure is used in one computational loop to solve a $\mathcal{N}$ phase system. Namely from t_n to t_{n+1}:

(1) Given $m_l(x, t_n)$, compute the indicator functions (49) to determine the number of branches $N(x,t)$, and solve for (ρ_k, u_k)'s from this moments by the procedure described in Appendix A. If $N(x,t) < \mathcal{N}$, one can set $\rho_k(x,t) = 0$, $u_k(x,t) = u(x,t)$, for $k = N(x,t) + 1, \ldots, \mathcal{N}$.
(2) Evaluate the numerical flux (81).
(3) Apply the conservative scheme (76) to advance the system to $t = t_{n+1}$.

In our tests we use the thresholds ϵ_1 and ϵ_2 for the indicator functions ϕ_1 and ϕ_2, respectively.

7. Numerical results

In this section, we present some one-dimensional numerical experiments on the multi-phase equations for the Schrödinger equation. In most test problems, exact solutions $\rho = m_0$ and $u = m_1/m_0$ are provided and compared to the numerical ones.

Example 1. $u_0 = \chi_{\{x<0\}} - 0.5\chi_{\{x>0\}}$, $\rho_0 = \chi_{\{x<0\}} + 0.5\chi_{\{x>0\}}$, $V = 0$. The multi-valued solution (for Burgers equation) has two branches with constant values 1 and -0.5, which move toward each other and create double phase solutions. The exact solution at time t is

$$\rho(x,t) = 1.5\chi_{\{x\in[-0.5t,t)\}} + \chi_{\{x<-0.5t\}} + 0.5\chi_{\{x\geq t\}}, \qquad u(x,t) = 0.5\chi_{\{x\in[-0.5t,t)\}} + \chi_{\{x<-0.5t\}} - 0.5\chi_{\{x\geq t\}}.$$

We remark that such a two-branch solution is unstable. For example, if one connects the initial two-constants by a line with a large slope, the solution at a later time will become triple-valued.

Example 2. $u_0 = \chi_{\{x<0\}} - \chi_{\{x>0\}}$, $\rho_0 = 1$, $V = x^2/2$ (Harmonic Oscillator). The multi-valued solution has two branches

$$u_{1,2}(x,t) = -x\tan(t) \pm \sec(t)$$

and as they characteristic curves cross the density will increase. The exact solution is

$$\rho(x,t) = \frac{2}{\cos(t)}\chi_{[-\sin(t),\sin(t))} + \frac{1}{\cos(t)}\chi_{(-\infty,-\sin(t)\cup[\sin(t),+\infty)},$$

$$u(x,t) = (-x\tan(t))\chi_{[-\sin(t),\sin(t))} + (\sec(t) - x\tan(t))\chi_{(-\infty,-\sin(t))} - (x\tan(t) + \sec(t))\chi_{[\sin(t),+\infty)}.$$

Example 3. $u_0 = 1\chi_{\{x<-0.5\}} + (0.3 - x)\chi_{\{-0.5<x<0\}} + 0.1\chi_{\{x>0\}}$, $\rho_0 = 1$, $V = 0$. There are two branches in the multi-valued solution from the beginning until $t = 5/9$. The exact solution is given as follows:

$$\rho(x,t) = \begin{cases} 1 + \dfrac{1}{1-t}, & x \in [-0.5 + 0.8t, -0.5 + t), \\ \dfrac{1}{1-t}, & x \in [-0.5 + t0.1t), \\ 1 + \dfrac{1}{1-t}, & x \in [0.1t, 0.3t), \\ 1 & \text{otherwise}, \end{cases}$$

$$u(x,t) = \begin{cases} 1, & x \in (-\infty, -0.5 + t), \\ \dfrac{1.3 - 2t + t^2 - x}{(1-t)(2-t)}, & x \in [-0.5 + 0.8t, -0.5 + t), \\ \dfrac{x - 0.6t + 0.3}{1-t}, & x \in [-0.5 + t, 0.1t), \\ \dfrac{0.4 - 0.2t + 0.1t^2 - x}{(1-t)(2-t)}, & x \in [0.1t, 0.3t), \\ 0.1, & x \in [0.3t, +\infty). \end{cases}$$

Then they split into three. The exact solution at time $t < 1$ is

$$\rho(x,t) = \begin{cases} 2 + \dfrac{1}{(1-t)}, & x \in [0.1t, -0.5+t), \\ 1 + \dfrac{1}{(1-t)}, & x \in [-0.5+0.8t, 0.1t) \cup [-0.5+t, 0.3t), \\ 1 & \text{otherwise}, \end{cases}$$

$$u(x,t) = \begin{cases} 1, & x \in (-\infty, -0.5+0.8t), \\ \dfrac{1.3-2t+t^2-x}{(1-t)(2-t)}, & x \in [-0.5+0.8t, 0.1t), \\ \dfrac{1.4-x+1.1t^2-2.2t}{(2t-3)(t-1)}, & x \in [0.1t, -0.5+t), \\ \dfrac{0.4-0.2t+0.1t^2-x}{(1-t)(2-t)}, & x \in [-0.5+t, 0.3t), \\ 0.1, & x \in [0.3t, +\infty) \end{cases}$$

and the multi-valued solutions are

$$u_2(x,t) = \frac{x-0.3}{t-1}, \quad x \in [-0.5+0.8t, 0.1t), \qquad u_3(x,t) = 1, \quad x \in (-\infty, -0.5+t),$$
$$u_1(x,t) = 0.1, \quad x \in [0.1t, +\infty).$$

We displayed the numerical results for solutions at $t = 0.6$.

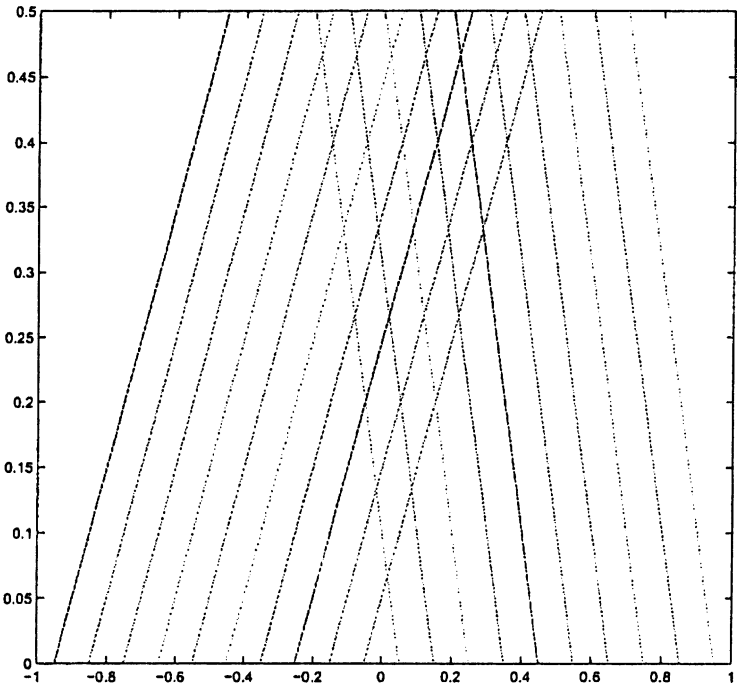

Fig. 1. Characteristic curves for Example 1.

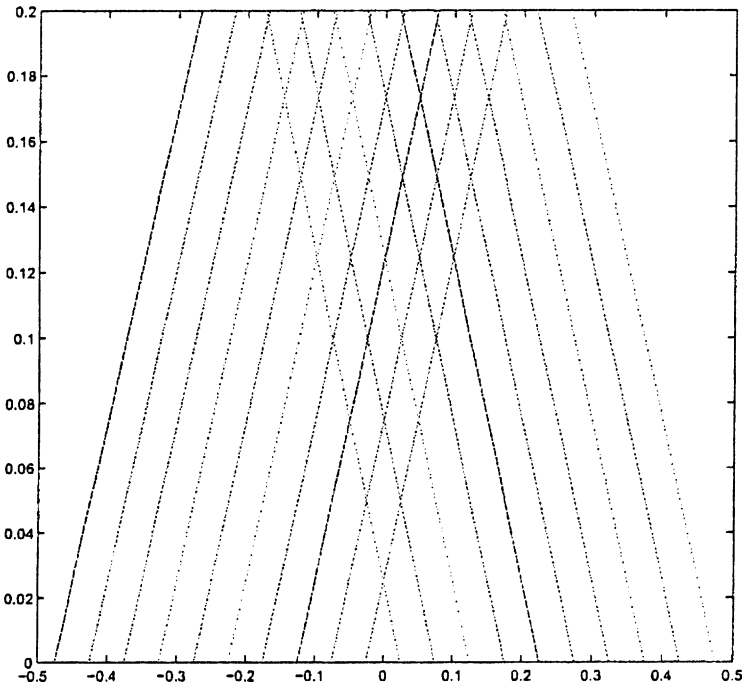

Fig. 2. Characteristic curves for Example 2.

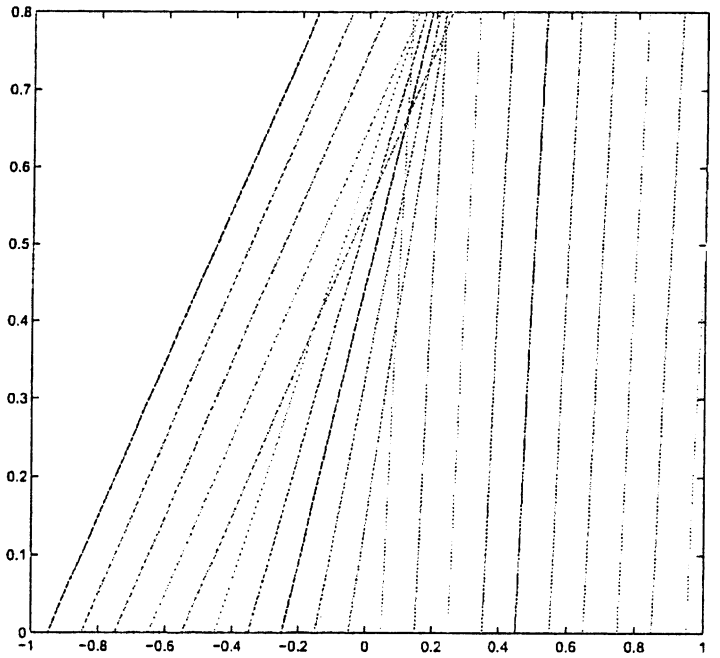

Fig. 3. Characteristic curves for Example 3.

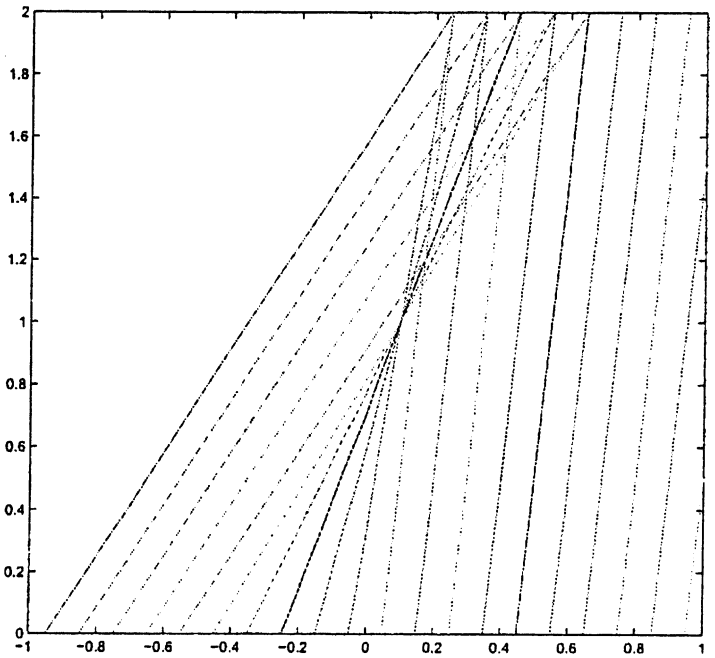

Fig. 4. Characteristic curves for Example 4.

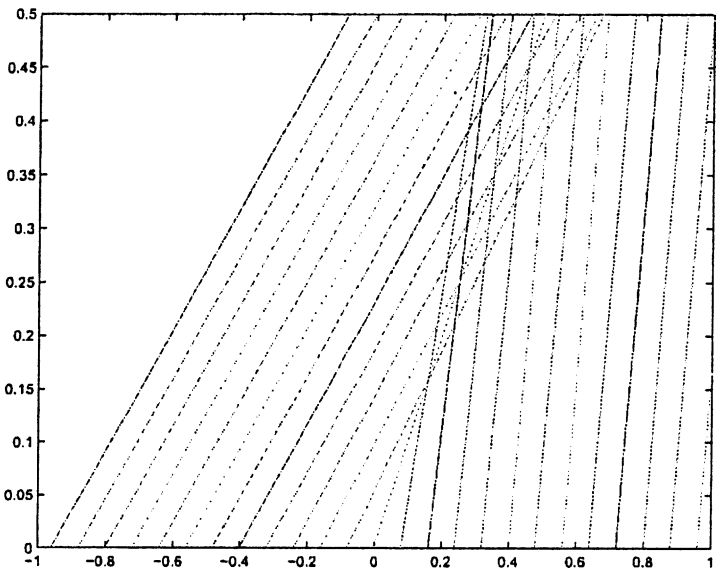

Fig. 5. Characteristic curves for Example 5.

Example 4. $u_0 = 0.6\chi_{\{x<0.5\}} + (0.1 - x)\chi_{\{-0.5<x<0\}} + 0.1\chi_{\{x>0\}}$, $\rho_0 = 1$, $V = 0$. All the characteristic lines starting from $(-0.5, 0)$ will cross at time 1 and form a focusing point where uncountably many characteristic curves meet. Then they immediately split into three branches. For $t < 1$ the solution remain classical:

$$\rho(x,t) = \begin{cases} 1, & x \in (-\infty, 0.6t - 0.5), \\ \dfrac{1}{1-t}, & x \in [0.6t - 0.5, 0.1t), \\ 1, & x \in [0.1t, +\infty) \end{cases}$$

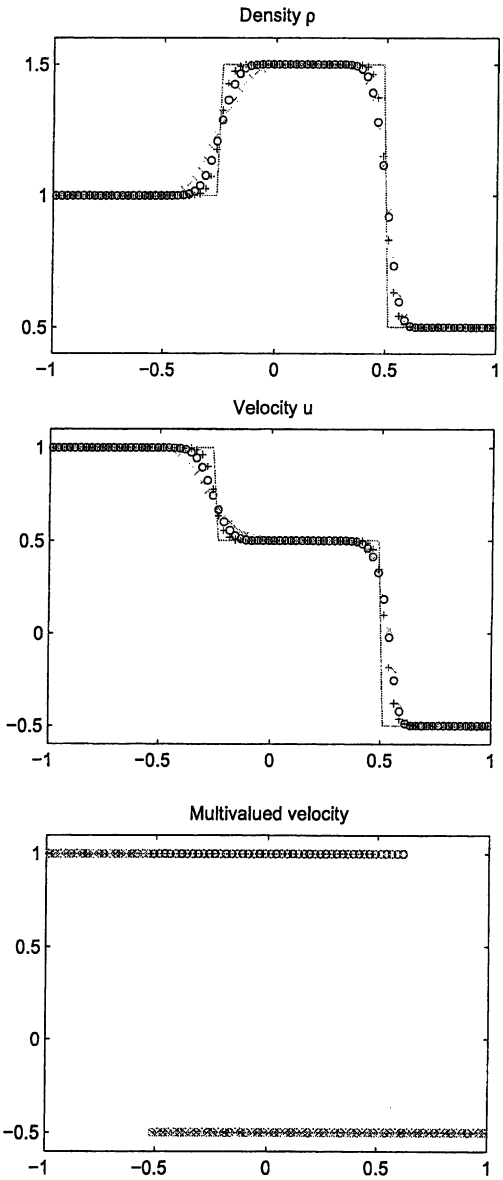

Fig. 6. Example 1, $\Delta x = 1/40$, $t = 0.5$, $\epsilon_1 = 10^{-5}$. The exact solutions are given by solid lines. ($\times$) the Lax–Friedrichs scheme; ($\bigcirc$) the first order kinetic scheme; ($+$) the second order kinetic scheme.

and

$$u(x,t) = \begin{cases} 0.6, & x \in (-\infty, 0.6t - 0.5), \\ \dfrac{0.1 - x}{1 - t}, & x \in [0.6t - 0.5, 0.1t), \\ 0.1, & x \in [0.1t, +\infty). \end{cases}$$

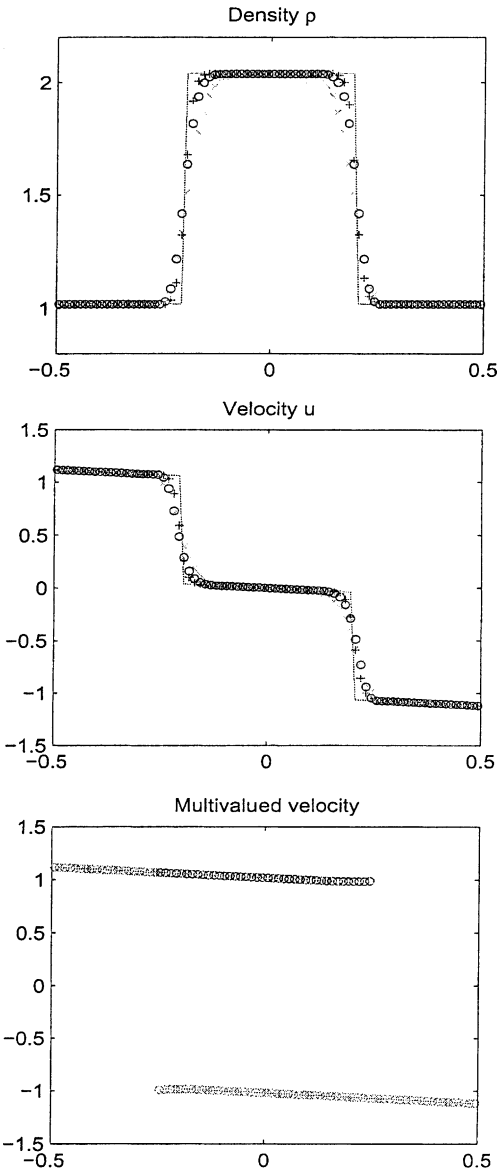

Fig. 7. Example 2, $\Delta x = 1/40$, $t = 0.2$, $\epsilon_1 = 10^{-5}$. The exact solutions are represented by solid lines. ($\times$) the Lax–Friedrichs scheme; ($\bigcirc$) the first order kinetic scheme; ($+$) the second order kinetic scheme.

At $t = 1$ the solution develops a concentration:

$$\rho(x) = 1 + \delta(x - 0.1), \qquad u(x) = 0.6\chi_{x<0.1} + 0.1\chi_{x>0.1}.$$

The exact solution at time $t > 1$ is

$$\rho(x,t) = \begin{cases} 1, & x \in (-\infty, 0.1t), \\ 2 + \dfrac{1}{t-1}, & x \in [0.1t, -0.5 + 0.6t), \\ 1, & x \in [-0.5 + 0.6t, +\infty), \end{cases}$$

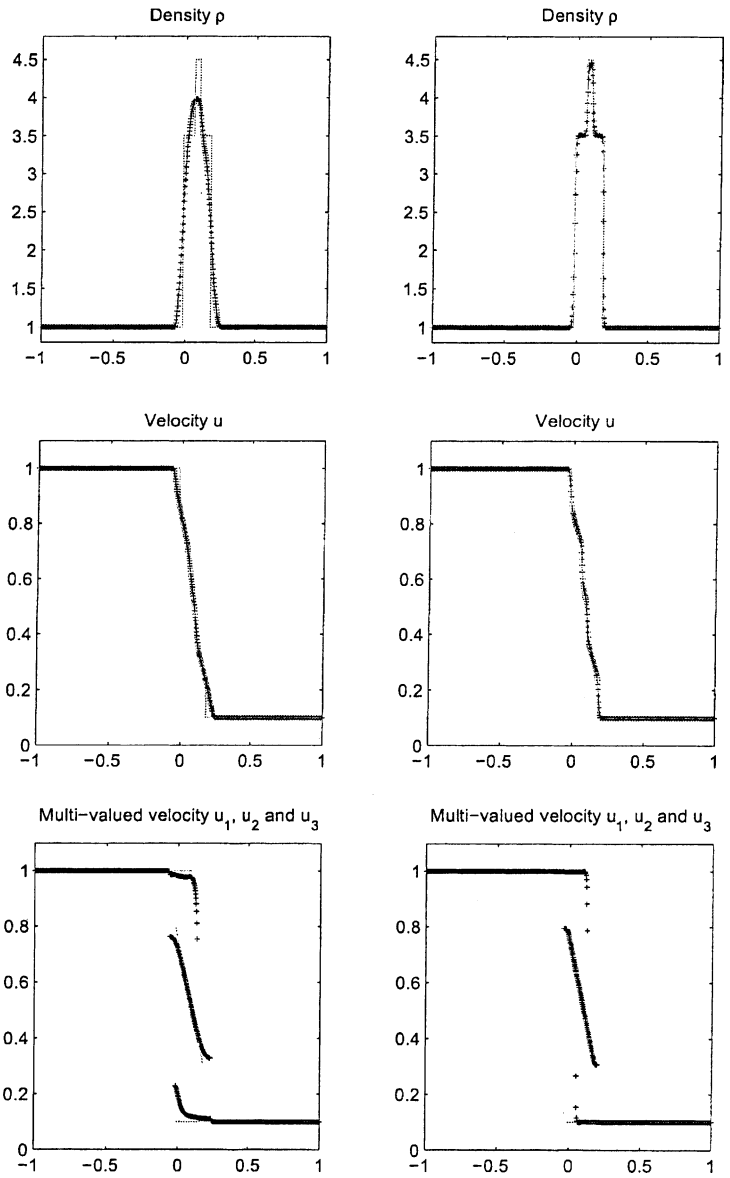

Fig. 8. Example 3, $\Delta x = 1/400$, $t = 0.8$. $\epsilon_1 = 10^{-5}$, $\epsilon_2 = -10^{-8}$. The exact solutions are given by the solid lines. Left: the Lax–Friedrichs scheme. Right: the second order kinetic scheme.

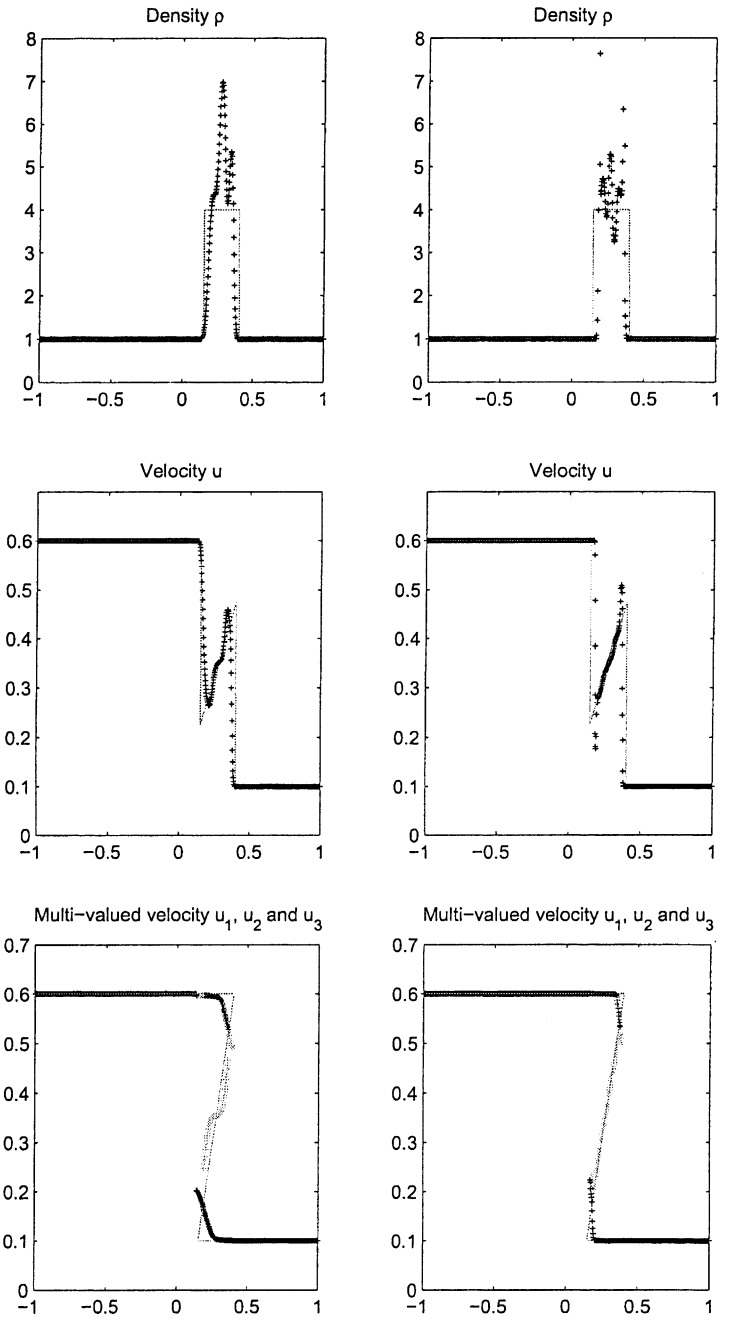

Fig. 9. Example 4, $\Delta x = 1/400$, $t = 0.8$. $\epsilon_1 = 10^{-5}$, $\epsilon_2 = -10^{-7}$. The exact solutions are given by the solid lines. Left: the Lax–Friedrichs scheme. Right: the second order kinetic scheme.

$$u(x,t) = \begin{cases} 0.6, & x \in (-\infty, 0.1t), \\ \dfrac{x + 0.6 + 0.7t^2 - 1.4t}{(2t-1)(t-1)}, & x \in [0.1t, -0.5 + 0.6t), \\ 0.1, & x \in [-0.5 + 0.6t, +\infty) \end{cases}$$

and the multi-valued velocity inside $(0.1t, -0.5 + 0.6t)$

$$u_1(x,t) = 0.6, \qquad u_2(x,t) = \frac{x - 0.1}{t - 1}, \qquad u_3(x,t) = 0.1.$$

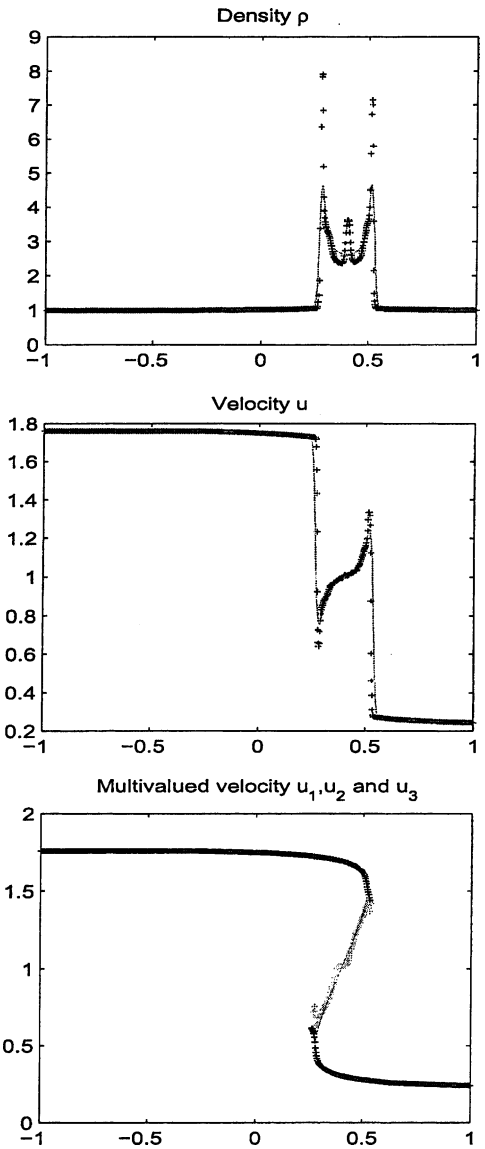

Fig. 10. Example 5, the solution at $t = 0.4$, $\Delta x = 1/400$, $\epsilon_1 = 10^{-5}$, $\epsilon_2 = -10^{-7}$. (—) the 'exact' solutions obtained by numerically solving the Vlasov equation using a second order upwind scheme; (+) computed solutions.

Example 5. $u_0 = 1.0 - (\tan^{-1}(20x)/2)$, $\rho_0 = 1.0$, $V(x) = 0$. Triple phase solution arises after time $t = 0.075$. Unlike the previous example, there is no caustic point. We do not have the analytic solution to this problem. The 'exact' solution is obtained by numerically solving the Vlasov equation with a upwind finite difference scheme.

Examples 1, 2 and 4 were used in [17]. Some additional numerical experiments were carried out in [19].

In Examples 1 and 2, we use the first and second order kinetic schemes and the Lax–Friedrichs scheme. In Examples 3 and 4, the Lax–Friedrichs scheme and the second order kinetic schemes are used. As usual, the second order kinetic scheme gives the best resolution while the Lax–Friedrichs scheme gives the poorest resolution. In all the pictures, the multi-valued velocities are ordered as $u_1 > u_2 > u_3$.

As can be observed from the figures, the numerical solutions obtained from the kinetic schemes are less smeared. In the triple phase solutions with smooth initial data, as in Example 5, the multi-valued velocity solutions are usually smoothed out near the intersections. Since in the evolution of the zero temperature equation, large gradient of the velocity will lead to concentration of the density, the rounded corners of the multi-valued velocity will result in peaks in the density approximations (Figs. 1–10).

Noticeably, the solution in Example 4 contains a focusing point at which there are infinitely many phases (not even countable). Beyond this point the solution develops three phases. At the focusing point, the assumption on finitely many phases become invalid. As a result, the three phase equations may not be appropriately initialized thereafter, causing the deterioration of the numerical solutions beyond this point. Despite this problem, the multi-valued velocity u_i's are still reasonably produced. This problem can fixed by backward ray tracing [20].

8. Conclusions

In this paper, we studied the multi-phase phenomenon in the semiclassical limit of the Schrödinger equation. The governing multi-phase equations can be derived using two different techniques: the Whitham's averaging method, and the Wigner transform with kinetic moment closure. In the latter case, the ansatz for the multi-phase Wigner distribution is derived and proved to satisfy a Vlasov equation, while the moments of the Wigner distribution solve a system of weakly hyperbolic equations. We found that this set of multi-phase equations coincides with the modulation equations derived by Whitham's averaging method. These moment equation provides an Eulerian formulation for the computation of multi-phase solutions. We utilize a kinetic scheme to approximate the multi-phase equations and present numerical experiments to validate the theory. Similar results for the linear KdV equation and the linear wave equation are also briefly presented.

The moment approach has some advantages when the number of phases is low. When the moment number becomes high the moment system becomes rather complex. An ideal solution would be a hybrid method that combines the globally defined Vlasov equation with the moment system. A most efficient numerical method of this type remains to be found.

Finally we point out that in our new work [20], the numerical schemes have been improved, and theoretical and numerical comparisons between the Wigner approach given here and that by Brenier and Corrias in [6,7] are also carried out.

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Appendix A

In this section, we show how to invert the system:

$$m_l = \sum_{k=1}^{N} \rho_k u_k^l, \quad l = 0, 2, \ldots, 2N-1. \tag{A.1}$$

First we define the following coefficients:

$$p_k = \sum_{1 \le j_1 < j_2 < \cdots < j_k \le N} u_{j_1} \cdots u_{j_k}.$$

Obviously $\{u_k\}_1^N$ can be computed from these coefficients since they are the roots of the polynomial:

$$x^N - p_1 x^{N-1} + \cdots + (-1)^N p_N.$$

We set up a system of equations for $\{p_i\}_{i=1}^N$:

$$A \begin{bmatrix} m_0 \\ m_1 \\ \vdots \\ m_{N-1} \end{bmatrix} = \begin{bmatrix} m_N \\ m_{N+1} \\ \vdots \\ m_{2N-1} \end{bmatrix}, \tag{A.2}$$

where the matrix $A = (a_{k,j})_{N\times N}$ only depends on p_i's.

We generate the matrix row by row recursively:

$$a_{1,j} = (-1)^{j-1} p_{N-j+1}, \quad j = 1, \ldots, N.$$

The kth row can be created from the $(k-1)$th row:

$$a_{k,1} = p_N a_{k-1,N}, \quad a_{k,j} = a_{1,j} a_{k-1,N} + a_{k-1,j-1}, \quad j = 2, \ldots, N.$$

By induction one can show that (A.2) is satisfied for any integer N. Once A is determined by the above procedure, (A.2) is a nonlinear system, which may be solved explicitly by some Mathematical software. We have found explicit solution for N up to 5 [26].

After u_k's are solved, we can obtain ρ_k from first N equations in (A.1) since it is a linear system and the matrix is of Vandermonde type.

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