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Computing multi-valued physical observables for the high frequency limit of symmetric hyperbolic systems

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Abstract

We develop a level set method for the computation of multi-valued physical observables (density, velocity, energy, etc.) for the high frequency limit of symmetric hyperbolic systems in any number of space dimensions. We take two approaches to derive the method.

The first one starts with a weakly coupled system of an eikonal equation for phase S and a transport equation for density ρ:

$$\partial_t S + H(x, \nabla S) = 0, \quad (t,x) \in \mathbb{R}^+ \times \mathbb{R}^n,$$
$$\partial_t \rho + \nabla_x \cdot (\rho \nabla_p H(x, \nabla_x S)) = 0.$$

The main idea is to evolve the density near the n-dimensional bi-characteristic manifold of the eikonal (Hamiltonian–Jacobi) equation, which is identified as the common zeros of n level set functions in phase space $(x,k) \in \mathbb{R}^{2n}$. These level set functions are generated from solving the Liouville equation with initial data chosen to embed the phase gradient. Simultaneously, we track a new quantity $f = \rho(t,x,k)|\det(\nabla_k \phi)|$ by solving again the Liouville equation near the obtained zero level set $\phi = 0$ but with initial density as initial data. The multi-valued density and higher moments are thus resolved by integrating f along the bi-characteristic manifold in the phase directions.

The second one uses the high frequency limit of symmetric hyperbolic systems derived by the Wigner transform. This gives rise to Liouville equations in the phase space with measure-valued solution in its initial data. Due to the linearity of the Liouville equation we can decompose the density distribution into products of function, each of which solves the Liouville equation with L^∞ initial data on any bounded domain. It yields higher order moments such as energy and energy flux.

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The main advantages of these new approaches, in contrast to the standard kinetic equation approach using the Liouville equation with a Dirac measure initial data, include: (1) the Liouville equations are solved with L^∞ initial data, and a singular integral involving the Dirac-δ function is evaluated only in the post-processing step, thus avoiding oscillations and excessive numerical smearing; (2) a local level set method can be utilized to significantly reduce the computation in the phase space. These methods can be used to compute *all* physical observables for multi-dimensional problems.

Our method applies to the wave fields corresponding to simple eigenvalues of the dispersion matrix. One such example is the wave equation, which will be studied numerically in this paper.

Keywords: High frequency limit; Multivalued solution; Level set; Liouville equation

1. Introduction

Many wave equations arising from physical problems can be written as symmetric hyperbolic systems of the form:[1]

$$A(x)\frac{\partial \mathbf{u}_\varepsilon}{\partial t} + \sum_{j=1}^{n} D^j \frac{\partial \mathbf{u}_\varepsilon}{\partial x^j} = 0, \tag{1.1}$$

$$\mathbf{u}_\varepsilon(0,\mathbf{x}) = \mathbf{B}(\mathbf{x})e^{\frac{iS_0(\mathbf{x})}{\varepsilon}}, \tag{1.2}$$

where $\mathbf{u}_\varepsilon \in C^M$ is a complex-valued vector and $\mathbf{x} \in \mathbb{R}^d$. We assume that the matrix $A(x)$ is symmetric and positive definite and that the matrices D^j are symmetric and independent of $\mathbf{x}$ and t. Here, ε is a small parameter that characterizes the wave length of the oscillations. In most physical applications, ε is very small when compared with the domain length of the problem. Numerical computations based on direct simulation of (1.1) and (1.2) are prohibitively expensive.

An effective numerical method to resolve highly oscillatory waves is to solve the limiting problem when $\varepsilon \to 0$. This corresponds to geometric optics in wave propagation, and the semiclassical limit of the Schrödinger equation. For a smooth non-linear Hamiltonian $H(\mathbf{x},\mathbf{k})$: $\mathbb{R}^n \times \mathbb{R}^n \to \mathbb{R}^1$, the classical WKB method for high frequency wave propagation typically results in a weakly coupled system of an eikonal equation for phase S and a transport equation for density ρ, respectively:

$$\partial_t S + H(\mathbf{x}, \nabla S) = 0, \quad (t,\mathbf{x}) \in \mathbb{R}^+ \times \mathbb{R}^n, \tag{1.3}$$

$$\partial_t \rho + \nabla_\mathbf{x} \cdot (\rho \nabla_\mathbf{k} H(\mathbf{x}, \nabla_\mathbf{x} S)) = 0. \tag{1.4}$$

Examples of such systems arise in, for example, the semiclassical limit of the Schrödinger equation ($H = \frac{1}{2}|\mathbf{k}|^2 + V(\mathbf{x})$) and the geometrical limit of the wave equation ($H = c(\mathbf{x})|\mathbf{k}|$).

Instead of the oscillatory wave field, the unknowns in this approximate WKB system are the phase and the density, neither of which depends on the small scale ε. Instead they vary on a much coarser scale than the wave field. Hence they are, in principle, easier to compute numerically.

However, a well known drawback of this approach is the lack of the superposition principle when a linear system, in the limit $\varepsilon \to 0$, is replaced by a fully non-linear PDE (1.3). The solution of a non-linear eikonal equation, in general, develops singularities in finite time. Viscosity solutions were introduced in [8]

[1] The conventional summation is used here: repeated Latin indices are summed, while repeated Greek indices are not summed.

to mathematically select a unique, single valued weak solution. Unfortunately, this class of weak solutions is not appropriate in treating linear wave propagation problems. Instead, multi-valued solutions that correspond to crossing waves are the physically relevant ones. Developing efficient numerical methods for these highly oscillatory waves has become a very active area of research in recent years [1–6,9–12,15,18,19,21–24,26,28,30]. These solutions become multi-valued in the physical space, imposing tremendous numerical challenges.

Let $\mathbf{v} = \nabla_{\mathbf{x}} S$ denote the phase gradient. Then for smooth solutions, the gradient of the eikonal equation (1.3) satisfies a quasilinear hyperbolic equation with a forcing term

$$\partial_t \mathbf{v} + \nabla_{\mathbf{x}} H(\mathbf{x}, \mathbf{v}) = 0. \tag{1.5}$$

A level set method was introduced in [6,23] to compute the multi-valued solution to (1.5). In this method, the phase gradient $\mathbf{v} = \nabla_{\mathbf{x}} S$ is embedded into an n-dimensional manifold, which corresponds to the intersection of the zero level sets of n functions,

$$\phi(t, \mathbf{x}, \mathbf{k}) = 0 \quad \text{at } \mathbf{k} = \nabla_{\mathbf{x}} S,$$

satisfying the Liouville equation

$$\partial_t \phi + \nabla_{\mathbf{k}} H \cdot \nabla_{\mathbf{x}} \phi - \nabla_{\mathbf{x}} H \cdot \nabla_{\mathbf{k}} \phi = 0. \tag{1.6}$$

In general, Eq. (1.3) is not homogeneous of degree one in the gradient, and consequently, the phase value S is not a constant along the characteristics. Therefore, to compute the multi-valued phase S, satisfying (1.3) the authors in [6] suggest solving an additional level set function in the augmented space $(\mathbf{x},\mathbf{k},z)$ with $z = S(t,\mathbf{x})$.

The computation of density ρ, and other physical observables, was addressed in [22] for the linear Schrödinger equation. The advantage of this method is that we avoided the computation of the Dirac measure-valued solution. We only need to solve a Liouville equation with initial data in L^∞ space in a bounded computational domain.

In this paper, we extend our previous approaches to general symmetric hyperbolic systems (1.1) and (1.2). While the eikonal equation (1.1) can be solved using the level set method given in [6,23] for multi-valued quantities, the aim here is to solve numerically for the density ρ and other physical observables that can be defined as the moments of the Wigner function. We adopt two approaches. One begins with the transport Eq. (1.4), and follows the path of [22] to derive a Liouville equation for density in the phase space, using an appropriate initial data. The second approach is based on the derivation of the high frequency limit of the symmetric hyperbolic systems using the Wigner function [29], which yields higher moments such as energy and energy flux.

We sketch our main idea of the first approach for the 1-D setting. We use a level set function ϕ in the phase space, $(x,k) \in R^2$ with $k = v$. As shown in [6,23], the scalar level set function $\phi(t,x,k)$ satisfies a linear Liouville equation

$$\partial_t \phi + H_k \phi_x - H_x \phi_k = 0. \tag{1.7}$$

The zero level set of this function, initialized as $k - \partial_x S_0(x)$, forms a one-dimensional manifold in (x,k) space. We need to perform integration along this manifold to obtain the physical observables.

We show that the WKB systems (1.3) and (1.4) can be rewritten in phase space as:

$$\partial_t \tilde{S} + H_k \partial_x \tilde{S} - H_x \partial_k \tilde{S} = kH_k - H, \tag{1.8}$$

$$\partial_t \tilde{\rho} + H_k \partial_x \tilde{\rho} - \partial_x H \partial_k \tilde{\rho} = -\rho G, \tag{1.9}$$

where $(\tilde{S}, \tilde{\rho})(t, x, v(t, x)) = (S, \rho)(t, x)$ and

$$G = H_{kx} - H_{kk} \frac{\phi_x}{\phi_k}.$$

As we mentioned earlier, one strategy to resolve $\tilde{S}$ is to look at the graph of the function $z = \tilde{S}(x,t)$ in the whole domain and project the phase value onto the manifold $\phi = 0$, see [6].

An obvious difficulty in resolving $\tilde{\rho}$ is the need to handle the singularity in G when ϕ_k becomes null. Following [22], we shall track the new quantity

$$f(t,x,k) := \tilde{\rho}(t,x,k)|\partial_k\phi|,$$

which is shown to satisfy again the Liouville equation

$$\partial_t f + H_k\partial_x f - H_x\partial_k f = 0, \quad f(0,x,k) = \rho_0(x),$$

i.e., the concentration singularities in ρ are cancelled out by the zeros of $\partial_k\phi$!

The combination of the level set function ϕ and the function f enables us to compute the desired density and the velocity via integrations:

$$\bar{\rho}(x,t) = \int f(t,x,k)\delta(\phi)\,\mathrm{d}k, \tag{1.10}$$

$$\bar{v}(x,t) = \frac{1}{\bar{\rho}}\int kf(t,x,k)\delta(\phi)\,\mathrm{d}k. \tag{1.11}$$

This paper is organized as follows. Section 2 is devoted to a derivation of the equation for the new quantity f as well as the justification of the integration procedure. In Section 3, we discuss several wave equations to which the approach introduced in Section 2 applies. In Section 4, we study general symmetric hyperbolic systems using the Wigner approach introduced in [29]. In Section 5, we describe the numerical strategy explored in this paper and present some numerical results.

2. Level set formulation

The first part of our method consists of tracking the bi-characteristics of Hamilton–Jacobi equation (1.3) in the phase space, using the level set method developed in [6,23].

The bi-characteristics for the phase equation (1.3), or (1.5), are governed by the Hamiltonian system:

$$\frac{\mathrm{d}\mathbf{x}}{\mathrm{d}t} = \nabla_{\mathbf{k}}H(\mathbf{x},\mathbf{k}), \quad \mathbf{x}(0) = \alpha, \tag{2.1}$$

$$\frac{\mathrm{d}\mathbf{k}}{\mathrm{d}t} = -\nabla_{\mathbf{x}}H(\mathbf{x},\mathbf{k}), \quad \mathbf{k}(0) = \nabla_{\mathbf{x}}S_0(\alpha) \equiv \mathbf{v}_0(\alpha). \tag{2.2}$$

In this section, we first review our previous level set equations for multi-valued velocity and phases, and then develop a new method for computing multi-valued density and other physical observables via the solution of the Liouville equation.

2.1. Multi-valued velocity and phase

As we mentioned in Section 1, the multi-valued phase gradient or velocity may be implicitly realized as the zero vector level set of the functions $\phi(t,\mathbf{x},\mathbf{k}) \in \mathbb{R}^n$, satisfying the Liouville equation

$$\partial_t\phi + \nabla_{\mathbf{k}}H\cdot\nabla_{\mathbf{x}}\phi - \nabla_{\mathbf{x}}H\cdot\nabla_{\mathbf{k}}\phi = 0, \tag{2.3}$$

subject to initial data $\phi(0,\mathbf{x},\mathbf{k}) = \mathbf{k} - \nabla_{\mathbf{x}}S_0(x)$ or its smooth approximation. Such a zero level set represents the n-dimensional bi-characteristic manifold in phase space $(\mathbf{x},\mathbf{k}) \in \mathbb{R}^{n\times n}$ and gives implicitly the multi-valued phase gradient; i.e.

$$\phi(t,\mathbf{x},\mathbf{k}) = 0, \quad \mathbf{k} = \nabla_{\mathbf{x}}S.$$

However, the phase S cannot be obtained from solving the Liouville equation (2.3), since S is usually not preserved along the Hamiltonian flow. Instead, in the phase space $(\mathbf{x},\mathbf{k})$ the phase solves a forced transport equation

$$\partial_t\tilde{S} + \nabla_{\mathbf{k}}H\cdot\nabla_{\mathbf{x}}\tilde{S} - \nabla_{\mathbf{x}}H\cdot\nabla_{\mathbf{k}}\tilde{S} = \mathbf{k}\cdot\nabla_{\mathbf{k}}H - H, \tag{2.4}$$

for further details see [6], where the authors solve this linear transport equation and then project the obtained phase value onto the n-dimensional manifold $\phi = 0$, and thus resolve the multi-valued phase in the physical space.

2.2. Multi-valued density

In the physical space, we rewrite the density equation (1.3) as

$$\partial_t\rho + \nabla_{\mathbf{k}}H\cdot\nabla_{\mathbf{x}}\rho = -\rho G, \tag{2.5}$$

where

$$G := \nabla_{\mathbf{x}}\cdot\nabla_{\mathbf{k}}H(\mathbf{x},\mathbf{k}), \quad \mathbf{k} = \nabla_{\mathbf{x}}S(t,\mathbf{x}) = \mathbf{v}(t,\mathbf{x}). \tag{2.6}$$

In order to obtain the evolution equation for density in the phase space, we need to use the bi-characteristic field as shown in the following

Lemma 2.1. *Let $\tilde{v}(t,\mathbf{x},\mathbf{k})$ be a representative of $v(t,\mathbf{x})$ in the phase space such that $\tilde{v}(t,\mathbf{x},\mathbf{v}(t,\mathbf{x})) = v(t,\mathbf{x})$. Then*

$$\partial_t v + \nabla_{\mathbf{k}}H\cdot\nabla_{\mathbf{x}}v = L\tilde{v}(t,\mathbf{x},\mathbf{k}),$$

where

$$L := \partial_t + \nabla_{\mathbf{k}}\cdot\nabla_{\mathbf{x}} - \nabla_{\mathbf{x}}\cdot\nabla_{\mathbf{k}}$$

denotes the Liouville operator.

Proof. Using the fact that $\tilde{v}(t,x,\mathbf{v}(t,\mathbf{x})) = v(t,\mathbf{x})$, we have:

$$\partial_t v = \partial_t\tilde{v} + \nabla_{\mathbf{k}}\tilde{v}(t,\mathbf{x},\mathbf{k})\cdot\partial_t\mathbf{v},$$
$$\partial_{x_j}v = \partial_{x_j}\tilde{v} + \nabla_p\tilde{v}\cdot\partial_{x_j}\mathbf{v}, \quad i = 1,\ldots,n.$$

Thus, a straightforward calculation yields

$$\partial_t v + \nabla_{\mathbf{k}}H\cdot\nabla_{\mathbf{x}}v = \partial_t\tilde{v} + \nabla_{\mathbf{k}}H\cdot\nabla_{\mathbf{x}}\tilde{v} + (\partial_t\mathbf{v} + \nabla_{\mathbf{k}}H\cdot\nabla_{\mathbf{x}}\mathbf{v})\cdot\nabla_{\mathbf{k}}\tilde{v},$$

which when combined with the velocity equation (1.5) leads the RHS to $L\tilde{v}$ as asserted. □

Based on this lemma and (2.5) we have

$$L\tilde{\rho} = -\tilde{\rho}G. \tag{2.7}$$

We still need to evaluate G, given in (2.6), in the phase space via the level set function ϕ. Let $Q := \nabla_{\mathbf{k}}\phi(t,\mathbf{x},\mathbf{k})$, the invertibility of Q is assumed in our formal derivation. The differentiation of $\phi(t,\mathbf{x},\mathbf{v}(t,\mathbf{x})) = 0$ gives

$$\partial_t\mathbf{v} = -Q^{-1}\partial_t\phi, \quad \partial_{x_j}\mathbf{v} = -Q^{-1}\partial_{x_j}\phi, \quad j = 1,\ldots,n,$$

which used in (2.6) leads to

$$G = \sum_{j=1}^{n} H_{x_j k_j} - \sum_{j,l=1}^{n} H_{k_j k_l} (Q^{-1}\phi_{x_j})^l. \tag{2.8}$$

Following [22], we evaluate the multi-valued density in the physical space by projecting its value in phase space $(\mathbf{x},\mathbf{k})$ onto the manifold $\phi = 0$, i.e., for any x we compute

$$\bar{\rho}(\mathbf{x}, t) = \int \rho(t, \mathbf{x}, \mathbf{k}) |J(t, \mathbf{x}, \mathbf{k})| \delta(\phi)\, \mathrm{d}\mathbf{k},$$

where

$$J := \det(\nabla_{\mathbf{k}}\phi) = \det(Q).$$

Such a Jacobian matrix actually solves

$$L(J) = JG. \tag{2.9}$$

We shall prove this below. Combining this result with the density equation (2.7) gives us

$$L(\tilde{\rho}(t, \mathbf{x}, \mathbf{k})|J(t, \mathbf{x}, \mathbf{k})|) = 0.$$

This equation suggests that we just need to compute the quantity

$$f(t, \mathbf{x}, \mathbf{k}) := \tilde{\rho}(t, \mathbf{x}, \mathbf{k})|J(t, \mathbf{x}, \mathbf{k})|, \tag{2.10}$$

by solving the Liouville equation

$$\partial_t f + \nabla_{\mathbf{k}} H \cdot \nabla_{\mathbf{x}} f - \nabla_{\mathbf{x}} H \cdot \nabla_{\mathbf{k}} f = 0, \tag{2.11}$$

subject to the initial condition

$$f_0 = \rho_0(\mathbf{x}) J_0(\mathbf{x}, \mathbf{k}),$$

where $J_0 = 1$ if $\phi_0 = \mathbf{k} - \nabla_{\mathbf{x}} S_0$ is smooth and $J_0 = |\det(Q_0(\mathbf{x},\mathbf{k}))|$ for ϕ_0 chosen otherwise.

With this quantity f the singularities in density ρ are cancelled out by the zeros of $J(\phi)$! Thus, we can locally compute the density and flux by integration of f and $\mathbf{k}f$ along $\{\mathbf{k} \in \mathbb{R}^n : \phi(\mathbf{x}, \mathbf{k}) = 0\}$

$$\bar{\rho}(\mathbf{x}) = \int_{\mathbb{R}^d} f(\mathbf{x}, \mathbf{k}, t) \delta(\phi(\mathbf{x}, \mathbf{k}))\, \mathrm{d}\mathbf{k} \tag{2.12}$$

and the momentum is determined by

$$\overline{\rho u}(\mathbf{x}) = \int_{\mathbb{R}^d} \mathbf{k} f(\mathbf{x}, \mathbf{k}) \delta(\phi(\mathbf{x}, \mathbf{k}))\, \mathrm{d}\mathbf{k}, \tag{2.13}$$

where $\delta(\phi) := \prod_{i=1}^{n} \delta(\phi_i)$ with ϕ_i being the ith component of ϕ.

We now turn to justify the claim (2.9). By taking the gradient of the Liouville equation (2.3) with respect to k we obtain the following equation for $Q = \nabla_{\mathbf{k}}\phi$

$$L(Q) = \nabla_{\mathbf{k}}(L\phi) + Q\nabla_{\mathbf{k}}\nabla_{\mathbf{x}} H - \nabla_{\mathbf{x}}\phi D_{\mathbf{k}}^2 H = Q\nabla_{\mathbf{k}}\nabla_{\mathbf{x}} H - \nabla_{\mathbf{x}}\phi D_{\mathbf{k}}^2 H,$$

where the matrices $\nabla_{\mathbf{k}}\nabla_{\mathbf{x}} H := (H_{x_j k_l})$ and $D_{\mathbf{k}}^2 H := (H_{k_j k_l})$. Using the fact that for $J = \det(Q)$ the following holds [22]:

$$\{\partial_t, \nabla_{\mathbf{x},\mathbf{k}}\} J = J\,\mathrm{Tr}(Q^{-1}\{\partial_t, \nabla_{\mathbf{x},\mathbf{k}}\} Q), \tag{2.14}$$

we have

$$L(J) = J\,\mathrm{Tr}(Q^{-1} L(Q)),$$

where Tr is the usual trace map. This implies that

$$L(J) = J\mathrm{Tr}(Q^{-1}Q\nabla_{\mathbf{k}}\nabla_{\mathbf{x}}H - Q^{-1}\nabla_{\mathbf{x}}\phi D^2_{\mathbf{k}}H) = J\left[\mathrm{Tr}(\nabla_{\mathbf{k}}\nabla_{\mathbf{x}}H) - \mathrm{Tr}(Q^{-1}\nabla_{\mathbf{x}}\phi D^2_{\mathbf{k}}H)\right]$$
$$= J\left[\sum_{j=1}^{n} H_{x_jk_j} - \sum_{j,l=1}^{n}(Q^{-1}\phi_{x_j})^l H_{k_lk_j}\right] = JG,$$

as claimed in (2.9). For reader's convenience, an alternative direct proof is provided in Appendix A.

3. Applications

As mentioned in Section 1 our approach can, in principle, be applied to a large class of wave propagation problems provided that their WKB approximations can be described by the system of the form (1.3). In addition to the Schrödinger equation treated in [22], we now discuss possible applications to optical waves and the acoustic waves, among others.

3.1. Optical waves

We begin with the linear scalar wave equation

$$\partial_t^2 u - c^2(\mathbf{x})\Delta u = 0, \quad (t,\mathbf{x}) \in \mathbb{R}^+ \times \mathbb{R}^n, \tag{3.1}$$

where $c(\mathbf{x})$ is the local speed of wave propagation of the medium. We complement (3.1) with highly oscillatory initial data that generate high frequency solutions. The derivation of the geometrical optics equations in the linear case is classical and performed based on the usual asymptotic WKB expansion [20],

$$u(t,\mathbf{x}) = A(t,\mathbf{x})\mathrm{e}^{\mathrm{i}\frac{S(t,\mathbf{x})}{\varepsilon}}, \tag{3.2}$$

with

$$A(t,\mathbf{x}) = \sum_{l=0}^{\infty} \varepsilon^l A_l(t,\mathbf{x})\mathrm{i}^{-l}.$$

We now substitute the expression (3.2) into (3.1) and equate coefficients of powers of ε to zero. For ε^2, this, due to the sign ambiguity, gives two eikonal equations

$$\partial_t S \pm c(\mathbf{x})|\nabla_{\mathbf{x}}S| = 0. \tag{3.3}$$

Without loss of generality we will henceforth consider the one with a plus sign. For ε^1, we get the *transport equation* for the first amplitude term,

$$\partial_t A_0 + c(\mathbf{x})\frac{\nabla_{\mathbf{x}}S\cdot\nabla_{\mathbf{x}}A_0}{|\nabla_{\mathbf{x}}S|} + \frac{c^2\Delta S - \partial_t^2 S}{2c|\nabla_{\mathbf{x}}S|}A_0 = 0. \tag{3.4}$$

In order to use the approach introduced in Section 2, we need to further simplify this transport equation and find a quantity ρ so that both S and ρ solve the system (1.3) with $H(\mathbf{x},\mathbf{k}) = c(\mathbf{x})|\mathbf{k}|$.

To this end, we apply the differential operator ∂_t to the eikonal equation $\partial_t S + c(\mathbf{x})|\nabla_{\mathbf{x}}S| = 0$,

$$\partial_t^2 S = -c(\mathbf{x})\partial_t|\nabla_{\mathbf{x}}S| = -c(\mathbf{x})\frac{\nabla_{\mathbf{x}}S}{|\nabla_{\mathbf{x}}S|}\cdot\nabla_{\mathbf{x}}\partial_t S = c(\mathbf{x})\frac{\nabla_{\mathbf{x}}S}{|\nabla_{\mathbf{x}}S|}\cdot\nabla_{\mathbf{x}}(c(\mathbf{x})|\nabla_{\mathbf{x}}S|).$$

This enables us to simplify the coefficient of $A_0/2$ in (3.4) as

$$\frac{c^2\Delta S - \partial_t^2 S}{c|\nabla_{\mathbf{x}}S|} = c\frac{\Delta S}{|\nabla_{\mathbf{x}}S|} - \frac{\nabla_{\mathbf{x}}S}{|\nabla_{\mathbf{x}}S|^2}\cdot\nabla_{\mathbf{x}}(c(\mathbf{x})|\nabla_{\mathbf{x}}S|) = \nabla_{\mathbf{x}}\cdot\left(c(\mathbf{x})\frac{\nabla_{\mathbf{x}}S}{|\nabla_{\mathbf{x}}S|}\right) - 2\nabla_{\mathbf{x}}c\cdot\frac{\nabla_{\mathbf{x}}S}{|\nabla_{\mathbf{x}}S|}.$$

Thereby (3.4) can be rewritten as

$$\partial_t A_0^2 + c\frac{\nabla_{\mathbf{x}} S}{|\nabla_{\mathbf{x}} S|}\cdot\nabla_{\mathbf{x}} A_0^2 + \left(\nabla_{\mathbf{x}}\cdot\left(c(\mathbf{x})\frac{\nabla_{\mathbf{x}} S}{|\nabla_{\mathbf{x}} S|}\right) - 2\nabla_{\mathbf{x}} c\cdot\frac{\nabla_{\mathbf{x}} S}{|\nabla_{\mathbf{x}} S|}\right)A_0^2 = 0,$$

that is

$$\partial_t A_0^2 + c^2\nabla_{\mathbf{x}}\cdot\left(A_0^2\frac{\nabla_{\mathbf{x}} S}{c(\mathbf{x})|\nabla_{\mathbf{x}} S|}\right) = 0.$$

This suggests that $\rho = A_0^2/c^2$ satisfies the conservative transport equation

$$\partial_t\rho + \nabla_{\mathbf{x}}\cdot(\rho\nabla_{\mathbf{x}} H(\mathbf{x},\nabla_{\mathbf{x}} S)) = 0$$

with $H(\mathbf{x},\mathbf{k}) = c(\mathbf{x})|\mathbf{k}|$. We also note that for the eikonal equation with negative sign the weighted density A_0^2/c^2 still satisfies the above conservative transport equation except for $H(\mathbf{x},\mathbf{k}) = -c|\mathbf{k}|$.

3.2. Acoustic waves

We will now examine the possible applications to acoustic wave equations. Consider the acoustic equations for the velocity and pressure disturbances $\mathbf{v}$ and p:

$$\rho(\mathbf{x})\partial_t\mathbf{v} + \nabla_{\mathbf{x}} p = 0, \tag{3.5}$$

$$\kappa(\mathbf{x})\partial_t p + \nabla_{\mathbf{x}}\cdot\mathbf{v} = 0. \tag{3.6}$$

Here, ρ is the density and κ is the compressibility. With oscillatory initial data of the form

$$\mathbf{u}(0,\mathbf{x}) = \mathbf{u}_0(\mathbf{x})\exp(\mathrm{i}S_0(\mathbf{x})/\varepsilon),$$

where $\mathbf{u} = (\mathbf{v},p)$ and S_0 is the initial phase function, we can look for the WKB asymptotic solution

$$\mathbf{u}(t,\mathbf{x}) = A(t,\mathbf{x},\varepsilon)\exp(\mathrm{i}S(t,\mathbf{x})/\varepsilon).$$

Note that (3.5) is a symmetric hyperbolic system and the result in [29] can be directly applied. For acoustic waves there are four wave modes, two transverse ones are non-propagating, and two longitudinal waves are propagating with speed $\pm v(x)$, $v(x) = 1/\sqrt{\rho(\mathbf{x})\kappa(\mathbf{x})}$.

Let $\hat{k} = (\sin\theta\cos\phi, \sin\theta\sin\phi, \cos\theta)$, the vector

$$\mathbf{b}^+(\mathbf{x},\hat{k}) := \left(\frac{\hat{k}}{\sqrt{2\rho}}, \frac{1}{\sqrt{2\kappa}}\right)$$

and define an amplitude function $\mathscr{A}$ in the direction of $\mathbf{b}^+$ as

$$A(t,\mathbf{x},0) = \mathscr{A}(\mathbf{x})\mathbf{b}^+(\mathbf{x},\nabla_{\mathbf{x}} S).$$

According to those justified in [29], the non-negative function $\eta = |\mathscr{A}|^2$ satisfies

$$\partial_t\eta + \nabla_{\mathbf{x}}\cdot(\eta\nabla_p H(\mathbf{x},\nabla_{\mathbf{x}} S)) = 0$$

coupled with the eikonal equation

$$\partial_t S + H(\mathbf{x},\nabla_{\mathbf{x}} S) = 0,$$

where $H(\mathbf{x},\mathbf{k}) = v(x)|\mathbf{k}|$ is a single eigenvalue of the so called dispersive matrix given in [29]. The other longitudinal wave mode is simply identified by taking $H(\mathbf{x},\mathbf{k}) = -v(x)|\mathbf{k}|$. This again falls into our framework outlined in Section 2.

4. General symmetric hyperbolic systems

In this section, we formulate the level set approach for the general symmetric hyperbolic systems. The formulation is based on the derivation of the high frequency approximation using the Wigner transformation carried out in [29]. For rigorous justification of such limits see for example [16]. It enables one to compute the higher order physical observables or moments, such as the energy and energy flux.

Consider symmetric hyperbolic systems of the form:

$$A(x)\frac{\partial \mathbf{u}_\varepsilon}{\partial t}+\sum_{j=1}^{n}D^j\frac{\partial \mathbf{u}_\varepsilon}{\partial x^j}=0, \tag{4.1}$$

$$\mathbf{u}_\varepsilon(0,\mathbf{x})=\mathbf{B}(\mathbf{x})\mathrm{e}^{\frac{\mathrm{i}S_0(\mathbf{x})}{\varepsilon}}, \tag{4.2}$$

where $\mathbf{u}_\varepsilon \in C^M$ is a complex-valued vector and $\mathbf{x}\in\mathbb{R}^n$. Assume that the matrix $A(x)$ is symmetric and positive definite and that the matrices D^j are symmetric and independent of $\mathbf{x}$ and t.

The energy density $\mathscr{E}$ for solution of (4.1) is given by the inner product

$$\mathscr{E}(t,\mathbf{x})=\frac{1}{2}(A(\mathbf{x})\mathbf{u}_\varepsilon(t,\mathbf{x}),\quad \mathbf{u}_\varepsilon(t,x))=\frac{1}{2}\sum_{j,l=1}^{n}A_{jl}(\mathbf{x})u_{\varepsilon,j}(t,\mathbf{x})\overline{u}_{\varepsilon,l}(t,\mathbf{x}) \tag{4.3}$$

and the energy flux $\mathscr{F}(\mathbf{x})$ by

$$\mathscr{F}_j(t,\mathbf{x})=\tfrac{1}{2}(D^j\mathbf{u}_\varepsilon(t,\mathbf{x}),\mathbf{u}_\varepsilon(t,\mathbf{x})). \tag{4.4}$$

Taking the inner product of (4.1) with $\mathbf{u}(t,\mathbf{x})$ yields the energy conservation law

$$\frac{\partial \mathscr{E}}{\partial t}+\nabla\cdot\mathscr{F}=0. \tag{4.5}$$

Integration of (4.5) shows that the total energy is conserved:

$$\frac{\partial}{\partial t}\int \mathscr{E}(t,\mathbf{x})\,\mathrm{d}\mathbf{x}=0. \tag{4.6}$$

Introduce the new inner product

$$\langle \mathbf{u},\mathbf{v}\rangle_A=(A\mathbf{u},\mathbf{v}). \tag{4.7}$$

Then the energy density is $\mathscr{E}=\frac{1}{2}\langle\mathbf{u},\mathbf{u}\rangle_A$. Define the scaled Wigner transformation

$$W^\varepsilon(t,\mathbf{x},\mathbf{k})=\left(\frac{1}{2\pi}\right)^d\int \mathrm{e}^{\mathrm{i}\mathbf{k}\cdot\mathbf{y}}\mathbf{u}_\varepsilon(t,\mathbf{x}-\varepsilon\mathbf{y}/2)\mathbf{u}_\varepsilon^*(\mathbf{x}+\varepsilon\mathbf{y}/2)\,\mathrm{d}\mathbf{y}, \tag{4.8}$$

where $\mathbf{u}^*=\bar{\mathbf{u}}^{\mathrm{T}}$ is the conjugate transpose of u. The matrix $W(t,\mathbf{x},\mathbf{k})$ is Hermitian but not necessarily positive definite. It becomes positive definite in the limit $\varepsilon\to 0$. It has the properties

$$\int W^\varepsilon(t,\mathbf{x},\mathbf{k})\,\mathrm{d}\mathbf{k}=\mathbf{u}_\varepsilon(t,\mathbf{x})\mathbf{u}_\varepsilon^*(t,\mathbf{x}). \tag{4.9}$$

The energy density can be expressed in terms of $W(t,\mathbf{x},k)$ by

$$\mathscr{E}(t,\mathbf{x})=\frac{1}{2}\int \mathrm{Tr}(A(\mathbf{x})W^\varepsilon(t,\mathbf{x},\mathbf{k}))\,\mathrm{d}\mathbf{k}, \tag{4.10}$$

while the energy flux $\mathscr{F}(t,\mathbf{x})$ can be recovered from

$$\mathscr{F}_j(t,\mathbf{x},\mathbf{k}) = \frac{1}{2}\int \mathrm{Tr}(D^j W^\varepsilon(t,\mathbf{x},\mathbf{k}))\,\mathrm{d}\mathbf{k}. \tag{4.11}$$

Introduce the *dispersion matrix* $L(\mathbf{x},\mathbf{k})$

$$L(\mathbf{x},\mathbf{k}) = A^{-1}(\mathbf{x})k_i D^i. \tag{4.12}$$

It is self-adjoint with respect to the inner product $\langle,\rangle_A$:

$$\langle L\mathbf{u},\mathbf{v}\rangle_A = \langle \mathbf{u}, L\mathbf{v}\rangle_A. \tag{4.13}$$

Therefore, all its eigenvalues ω_τ are real and the corresponding eigenvectors $\mathbf{b}^\tau$ can be chosen to be orthogonal with respect to $\langle,\rangle_A$:

$$L(\mathbf{x},\mathbf{k})\mathbf{b}^\tau(\mathbf{x},\mathbf{k}) = \omega_\tau(\mathbf{x},\mathbf{k})\mathbf{b}^\tau(\mathbf{x},\mathbf{k}), \quad \langle \mathbf{b}^\tau, \mathbf{b}^\beta\rangle_A = \delta_{\tau\beta}. \tag{4.14}$$

We assume that the eigenvalues have constant multiplicity independent of $\mathbf{x}$,$\mathbf{k}$. This hypothesis is satisfied by many physical examples including those under study in this paper.

4.1. Case I: the dispersion matrix has only simple eigenvalues

We first assume that all the eigenvalues $\omega_\tau(\mathbf{x},\mathbf{k})$ are simple. Define the matrices $B^\tau(\mathbf{x},\mathbf{k})$ by

$$B^\tau(\mathbf{x},\mathbf{k}) = \mathbf{b}^\tau(\mathbf{x},\mathbf{k})\mathbf{b}^{\tau*}(\mathbf{x},\mathbf{k}). \tag{4.15}$$

In the limit $\varepsilon \to 0$, the Wigner matrix $W^\varepsilon(t,\mathbf{x},\mathbf{k})$ is approximated by $W^{(0)}(t,\mathbf{x},\mathbf{k})$

$$W^{(0)}(t,\mathbf{x},\mathbf{k}) = \sum_{\tau=1}^{n} a^\tau(t,\mathbf{x},\mathbf{k})B^\tau(\mathbf{x},\mathbf{k}). \tag{4.16}$$

The scalar function $a^\tau(t,\mathbf{x},\mathbf{k})$, determined by the projection

$$a^\tau = \mathrm{Tr}(AW^{(0)*}AB^\tau) \tag{4.17}$$

solves the Liouville equation

$$\frac{\partial a^\tau}{\partial t} + \nabla_\mathbf{k}\omega_\tau \cdot \nabla_\mathbf{x} a^\tau - \nabla_\mathbf{x}\omega_\tau \cdot \nabla_\mathbf{k} a^\tau = 0. \tag{4.18}$$

See [29]. To find the initial data for a^τ, applying (4.2) in (4.8)

$$W^\varepsilon(0,\mathbf{x},\mathbf{k}) = \left(\frac{1}{2\pi}\right)^n \int \mathrm{e}^{\mathrm{i}\mathbf{k}\cdot\mathbf{y}}\mathbf{B}_0(\mathbf{x}-\varepsilon\mathbf{y}/2)\mathbf{B}_0^*(\mathbf{x}+\varepsilon\mathbf{y}/2)\mathrm{e}^{\mathrm{i}(S_0(\mathbf{x}-\varepsilon\mathbf{y}/2)-S_0(\mathbf{x}+\varepsilon\mathbf{y}/2))/\varepsilon}\,\mathrm{d}\mathbf{y}. \tag{4.19}$$

The weak limit of $W^\varepsilon(0,x,\mathbf{k})$, in the sense of distribution, is

$$W^{(0)}(0,\mathbf{x},\mathbf{k}) = \mathbf{B}_0(\mathbf{x})\mathbf{B}_0^*(\mathbf{x})\delta(\mathbf{k}-\nabla S_0(\mathbf{x})). \tag{4.20}$$

Using (4.17), one gets

$$a^\tau(0,\mathbf{x},\mathbf{k}) = \mathrm{Tr}(A\mathbf{B}_0\mathbf{B}_0^*AB^\tau)\delta(\mathbf{k}-\nabla S_0(\mathbf{x})). \tag{4.21}$$

Once a^τ is computed, one can obtain $W^{(0)}$ via (4.16), and consequently the energy density using (4.10) and the flux using (4.11).

Our level set method for (4.18) and (4.21), similar to what was done for the Schrödinger equation in our previous work [22], consists of solving the following two initial value problems of the Liouville equation with bounded – rather than measure valued – initial data:

$$\frac{\partial \phi^\tau}{\partial t} + \nabla_{\mathbf{k}}\omega_\tau \cdot \nabla_{\mathbf{x}}\phi^\tau - \nabla_{\mathbf{x}}\omega_\tau \cdot \nabla_{\mathbf{k}}\phi^\tau = 0, \tag{4.22}$$

$$\phi^\tau(0,\mathbf{x},\mathbf{k}) = \phi_0^\tau(\mathbf{x}), \quad \tau = 1,\ldots,n; \tag{4.23}$$

$$\frac{\partial f^\tau}{\partial t} + \nabla_{\mathbf{k}}\omega_\tau \cdot \nabla_{\mathbf{x}}f^\tau - \nabla_{\mathbf{x}}\omega_\tau \cdot \nabla_{\mathbf{k}}f^\tau = 0, \tag{4.24}$$

$$f^\tau(0,\mathbf{x},\mathbf{k}) = \mathrm{Tr}(A\mathbf{B}_0\mathbf{B}_0^*AB^\tau)|\nabla_{\mathbf{k}}\phi_0^\tau|, \quad \tau = 1,\ldots,n, \tag{4.25}$$

where $\phi_0^\tau = \mathbf{k}_\tau - \partial_{x_\tau}S_0$ for $S_0 \in C^1$, or the signed distance function otherwise.

Remark. If ∇S_0 is not continuous, then $\delta(\mathbf{k} - \nabla S_0)$ in (4.20), and in (4.21), is not well defined. It is still an open question what the high frequency limit is under this circumstance. Here, assuming that ∇S_0 has simple jumps along piecewise smooth curves, we can regularize the initial data by embedding the completion of the subgraph of each component of ∇S_0 in phase space by the signed distance functions ϕ_0^τ. A similar approach to Hamilton–Jacobi equations was proposed by Giga and Sato [17]. See also [31]. It remains a question that how to regularize the WKB initial data (4.2) so that in the high frequency limit this regularized initial data (via the signed distance function) is obtained.

We have the following theorem.

Theorem 4.1. *Let* $\phi = (\phi^1,\ldots,\phi^n)^{\mathrm{T}}$. *If* ω_τ *is smooth, then solution to* (4.18), *with initial data*

$$a^\tau(0,\mathbf{x},\mathbf{k}) = Tr(A\mathbf{B}_0\mathbf{B}_0^*AB^\tau)|\nabla_{\mathbf{k}}\phi_0^\tau|\delta(\phi_0^\tau) \tag{4.26}$$

is given by

$$a^\tau(t,\mathbf{x},\mathbf{k}) = f^\tau(t,\mathbf{x},\mathbf{k})\delta(\boldsymbol{\phi}(t,\mathbf{x},\mathbf{k})). \tag{4.27}$$

Proof. The proof uses simply the method of characteristics. It is the same as the analogous result for the Schrödinger equation we did in [22]. □

4.2. Case II: the dispersion matrix has multiple eigenvalues

We now consider the case when the dispersion matrix $L(\mathbf{x},\mathbf{k})$ has multiple eigenvalues. Let $\omega_\tau(\mathbf{x},\mathbf{k})$ be an eigenvalue of multiplicity r and let the corresponding eigenvectors $b^{\tau,j}$, $j = 1,\ldots,r$ be orthonormal with respect to $\langle,\rangle_A$. Given a pair of eigenvectors $\mathbf{b}^{\tau,j},\mathbf{b}^{\tau,l}$ we define the $N \times N$ matrix

$$B^{\tau,jl} = \mathbf{b}^{\tau,j}\mathbf{b}^{\tau,l*}, \quad j,l = 1,\ldots,r. \tag{4.28}$$

The limiting Wigner matrix $W^{(0)}(t,\mathbf{x},\mathbf{k})$ has the representation

$$W^{(0)}(t,\mathbf{x},\mathbf{k}) = \sum_{\tau,j,l} a_{jl}^\tau B^{\tau,jl}(\mathbf{x},\mathbf{k}), \tag{4.29}$$

where a_{jl}^τ are scalar functions. Define the $r \times r$ *coherence matrices* $W^\tau(t,\mathbf{x},\mathbf{k})$ by

$$W_{ij}^\tau(t,\mathbf{x},\mathbf{k}) = a_{jl}^\tau(t,\mathbf{x},\mathbf{k}), \quad j,l = 1,\ldots,r. \tag{4.30}$$

The coherence matrices $W^\tau(t,\mathbf{x},\mathbf{k})$ are Hermitian and positive definite because they are projections of the limiting Wigner matrix $W^{(0)}(t,\mathbf{x},\mathbf{k})$ which is Hermitian and positive definite. The functions a_{jl}^τ are given by

$$a_{jl}^\tau(t,\mathbf{x},\mathbf{k}) = \mathrm{Tr}(AW^{(0)}(t,\mathbf{x},\mathbf{k})AB^{\tau,jl}(\mathbf{x},\mathbf{k})). \tag{4.31}$$

Then each of the coherence matrices $W^\tau(t,\mathbf{x},\mathbf{k})$ satisfies the transport equation [29]

$$\frac{\partial W^\tau}{\partial t} + \nabla_{\mathbf{k}}\omega_\tau \cdot \nabla_{\mathbf{x}}W^\tau - \nabla_{\mathbf{x}}\omega_\tau \cdot \nabla_{\mathbf{k}}W^\tau + W^\tau N^\tau - N^\tau W^\tau = 0, \tag{4.32}$$

where the skew-symmetric coupling matrices $N^\tau(\mathbf{x},\mathbf{k})$ are given by

$$N^\tau_{mn}(\mathbf{x},\mathbf{k}) = \sum_{j=1}^{n}\left[\left(\mathbf{b}^{\tau,n}, D^j\frac{\partial \mathbf{b}^{\tau,m}}{\partial x^j}\right) - \frac{\partial\omega_\tau}{\partial x^j}\left(A\mathbf{b}^{\tau,n},\frac{\partial \mathbf{b}^{\tau,m}}{\partial k_j}\right) - \frac{1}{2}\frac{\partial^2\omega_\tau}{\partial x^j\partial k_j}\delta_{nm}\right]. \tag{4.33}$$

The level set method, described for the simple eigenvalue case, applies now to the case when W^τ and N^τ commute. In this case, the matrix Liouville equation (4.32) becomes a homogeneous decoupled scalar Liouville equation for each W^τ_{jl}.

4.3. Acoustic waves

Consider the acoustic equations for the velocity and pressure disturbances $\mathbf{v}$ and p:

$$\rho(\mathbf{x})\partial_t\mathbf{v} + \nabla_\mathbf{x} p = 0, \tag{4.34}$$

$$\kappa(\mathbf{x})\partial_t p + \nabla_\mathbf{x}\cdot\mathbf{v} = 0, \tag{4.35}$$

with oscillatory initial data of the form

$$\mathbf{u}(0,\mathbf{x}) = \mathbf{u}_0(\mathbf{x})\exp(\mathrm{i}S_0(\mathbf{x})/\varepsilon),$$

where $\mathbf{u} = (\mathbf{v},p)$ and S_0 is the initial phase function. This is a symmetric hyperbolic system and the result in [29] can be directly applied. We Look for the WKB asymptotic solution

$$\mathbf{u}(t,\mathbf{x}) = A(t,\mathbf{x},\varepsilon)\exp(\mathrm{i}S(t,\mathbf{x})/\varepsilon).$$

Let $\hat{\mathbf{k}} = (\sin\theta\cos\phi, \sin\theta\sin\phi, \cos\theta)$,

$$\mathbf{b}^+(\mathbf{x},\hat{\mathbf{k}}) := \left(\frac{\hat{p}}{\sqrt{2\rho}}, \frac{1}{\sqrt{2\kappa}}\right),$$

and define an amplitude function $\mathscr{A}$ in the direction of $\mathbf{b}^+$ as

$$A(0,\mathbf{x},0) = \mathscr{A}_0(\mathbf{x})\mathbf{b}^+(\mathbf{x},\nabla_\mathbf{x}S_0).$$

The energy density is

$$\mathscr{E} = \tfrac{1}{2}\rho(\mathbf{x})|\mathbf{v}|^2 + \tfrac{1}{2}\kappa(\mathbf{x})p^2, \tag{4.36}$$

while the energy flux is

$$\mathscr{F} = p(t,\mathbf{x})\mathbf{v}(t,\mathbf{x}). \tag{4.37}$$

Let $v(\mathbf{x}) = 1/\sqrt{\kappa(\mathbf{x})\rho(\mathbf{x})}$. Using the Wigner analysis similar to that in [29], the high frequency approximation, as $\varepsilon\to 0$, is given by:

$$\partial_t a^+ + v(\mathbf{x})\hat{\mathbf{k}}\cdot\nabla_\mathbf{x}a^+ - |\mathbf{k}|\nabla_\mathbf{x}v(\mathbf{x})\cdot\nabla_\mathbf{k}a^+ = 0, \tag{4.38}$$

$$a^+(0,\mathbf{x},\mathbf{k}) = \mathscr{A}_0(\mathbf{x})\delta(\mathbf{k}-\nabla S_0(\mathbf{x})). \tag{4.39}$$

Now this problem is a particular case of the more general form (4.18) and (4.21). To evaluate the energy and energy flux one uses:

$$\mathscr{E}(t,\mathbf{x}) = \int a^+(t,\mathbf{x},\mathbf{k})\,\mathrm{d}\mathbf{k}, \tag{4.40}$$

$$\mathscr{F}(t,\mathbf{x}) = \int \hat{\mathbf{k}}v(\mathbf{x})a^+(t,\mathbf{x},\mathbf{k})\,\mathrm{d}\mathbf{k}. \tag{4.41}$$

Remark 1. In the level set method for general symmetric hyperbolic systems, the Hamiltonian is assumed to be smooth. For the acoustic waves, the Hamiltonian has a singularity at $\mathbf{k} = 0$. Thus, the level set method can only be used when the space gradient $\nabla S(t,\mathbf{x})$ stays away from zero.

Remark 2. The linear scalar wave equation,

$$\partial_t^2 u - c^2(\mathbf{x})\Delta u = 0, \quad (t,\mathbf{x}) \in \mathbb{R}^+ \times \mathbb{R}^3, \tag{4.42}$$

can be reformulated into the form of acoustic equations via the change of variables

$$p = -\partial_t u, \quad \mathbf{v} = \nabla u. \tag{4.43}$$

The corresponding first order system becomes

$$\partial_t \mathbf{v} + \nabla p = 0, \tag{4.44}$$

$$\partial_t p + c^2(\mathbf{x})\nabla \cdot \mathbf{v} = 0, \tag{4.45}$$

which is a special case of (4.34) with

$$\rho(x) = 1, \quad \kappa(x) = 1/c^2(\mathbf{x}).$$

This procedure gives an alterative way to compute energy flux and high-order observables for waves governed by the single wave equation.

5. Numerical implementation and examples

We implement the level set method for the optical wave equation, as discussed in Section 3. We are interested in computing the amplitude $\bar{A}^2$. Our algorithm can be summarized as follows.

(1) Initialize: construct the level set functions $\Phi_0 = (\phi_j^{(0)})$ that embed the initial data $\nabla_{\mathbf{x}} S_0$,

$$\phi_j^{(0)}(\mathbf{x},\mathbf{k}) = k_j - \frac{\partial}{\partial x_j} S_0(\mathbf{x}), \quad j = 1,\ldots,d,$$

and the phase space modified amplitude function

$$f_0(x,\mathbf{k}) = \begin{cases} \frac{\bar{A}_0^2(x)}{c^2(x)}, & 0 < \tilde{k} < k_j, \quad j = 1,2,\ldots,d, \\ 0, & \text{otherwise.} \end{cases}$$

Here, $\mathbf{k} = (k_1,k_2,\ldots,k_d)$ and $\tilde{k} < \min_{1\leqslant j\leqslant d} \left\| \partial S_0(\mathbf{x})/\partial x_j \right\|_\infty$ is a predetermined constant.

(2) Evolve the Liouville equation in phase space using $\phi_j^{(0)}$ and f_0 constructed above as initial conditions:

$$w_t + c(\mathbf{x})\frac{\mathbf{k}}{|\mathbf{k}|} \cdot \nabla_{\mathbf{x}} w - \nabla_{\mathbf{x}} c(x)|\mathbf{k}| \cdot \nabla_{\mathbf{k}} w = 0$$

with $w(\mathbf{x},\mathbf{k},t=0) = \phi_j^{(0)},\ j = 1,\ldots,d$ and f_0, respectively. We shall use $\phi_j(\mathbf{x},\mathbf{k},t)$ and $f(\mathbf{x},\mathbf{k},t)$ to denote the corresponding solutions.

(3) Evaluate $\bar{A}^2(\mathbf{x},t)$ by integrating f along $\{\mathbf{k} \in \mathbb{R}^d \setminus \{\mathbf{0}\} : \Phi(\mathbf{x},\mathbf{k}) = 0\}$:

$$\bar{A}^2(\mathbf{x},t) = c^2(\mathbf{x}) \int_{\mathbb{R}^d \setminus \{\mathbf{o}\}} f(\mathbf{x},\mathbf{k},t)\delta(\Phi(\mathbf{x},\mathbf{k},t))\, \mathrm{d}\mathbf{k},$$

where $\delta(\Phi) := \prod_{j=1}^n \delta(\phi_j)$ with ϕ_j being the jth component of Φ.

The numerical techniques related to the simulations below have been documented in our previous papers as well as many other related works. For advancing the solutions for the Liouville equations, we refer the readers to [26,22] and also [7]. The papers by Min [25] is particularly useful for efficiency. A good numerical treatment of delta functions in the level set context was developed in the work of Engquist et al. [13].

There is, however, a minor numerical issue in our current approach to the wave equations that is outside of the scope of the references listed above. Consider the Hamiltonian $H(\mathbf{x},\mathbf{p}) = c(x)|\mathbf{p}|$ defined with a smooth, positive function $c(x)$. The corresponding wave front velocity $\vec{v}(\mathbf{x},\mathbf{p}) = (c(\mathbf{x})\mathbf{p}/|\mathbf{p}|, -\nabla c(x)|\mathbf{p}|)$ is not defined in the set $O_p = \{(\mathbf{x},\mathbf{p}) \in \mathbb{R}^{2d} : |\mathbf{p}| = 0\}$. We point out that in the papers [12,26], for example, the location of a single wave front is tracked by the reduced Liouville equation with $\mathbf{p}$ constrained to lie on the sphere S^d and $|\mathbf{p}|$ replaced by $1/c(\mathbf{x})$. Thus, one does not encounter this singularity. However, wave fronts in the entire computational domains are tracked simultaneously by our formalism. The singularity in the velocity field suggests that O_p should not be part of the domain and that suitable boundary conditions may have to be prescribed at $\partial O_p \subset \mathbb{R}^{2d}$. In the full phase space, the trajectory of a particle under this velocity field $\vec{v}$, starting from $(x_0,\mathbf{p}_0) \notin O_p$, will never cross O_p for all time. This is due to the energy preserving property of Hamiltonian flows. Thus, the computational domain $\Omega \subset \mathbb{R}^{2d}$ may safely exclude O_p. In the following calculations, we simply place a grid in $\mathbb{R}^{2d}$ that does not intersect with O_p, and modified our discretizations for the grid points near the set O_p. The exclusion of O_p from the domain is a standard idea used to solve spherically or cylindrically symmetric problems using a spherical or cylindrical coordinate system. At the regions of ∂O_p where the characteristics are flowing into $\mathbb{R}^{2d} \setminus O_p$, we prescribe a dimension-by-dimension extension boundary condition. Let h denote the mesh size in $\mathbf{k}$. Near O_p, i.e. at points $(x',\mathbf{k}')$ where $|\mathbf{k}'| \leqslant h$, if $\partial_{x_j} c(\mathbf{x}') \geqslant 0$, for some j, we replace backward differencing along the k_j-axis (or the corresponding WENO discretization) by forward differencing, and vice versa for the case $\partial_{x_j} c(\mathbf{x}') < 0$. This is equivalent to an extrapolation along the k_j-axis, and it somewhat resembles the Ghost Fluid method [14].

Consider the simple 1d example, in which $c(x)$ is increasing. In the upper half-plane of the $x - k$ space, the velocity is pointing in the positive x-direction and in the negative k-direction. Thus, the level sets of ϕ or f will bundle up near $k = 0^+$, and the support of f may come exponentially close to the x-axis. On the other hand, in the lower half-plane, the characteristics are diverging from the x-axis. Fig. 2 illustrates this scenario. Therefore, without enforcing the boundary conditions at ∂O_p, which is the x-axis, an upwind discretization at grid points may eventually propagate portions of the energy (carried by the support of f) across the x-axis and translate it to the left! Fig. 1 shows such a situation. We point out that if $\tilde{k}$ in Step 1 above is

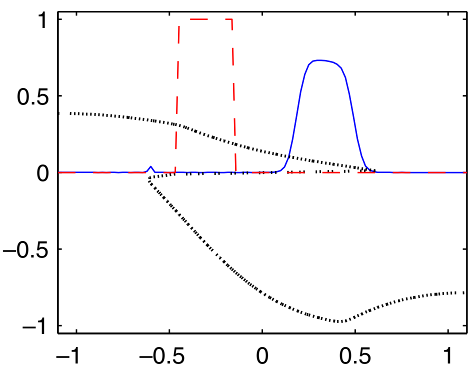

Fig. 1. Inappropriate upwinding scheme incorrectly propagates an energy packet across the singularity of the velocity field in phase space. In this case, $c'(x) > 0$ and the initial phase function $S_0(x)$ is $-x^2/4$. The dashed curve represents the initial amplitude location. It is transported to the right along in the x-direction. The "ghost" energy is created and transported to the left. The dotted curve represents the computed multi-valued $\nabla_x S$.

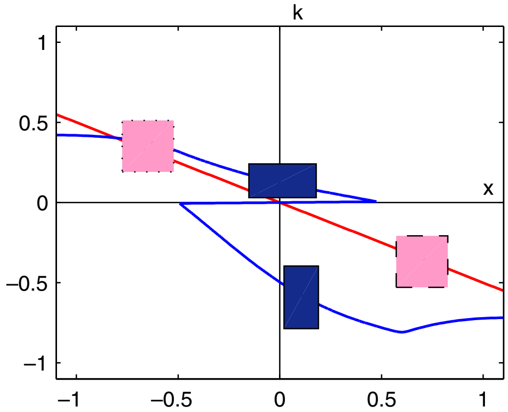

Fig. 2. Illustration of the Hamiltonian flow of the optical wave equation and the transport of energy in phase space. In this case, $c'(x) > 0$ and the initial phase function $S_0(x)$ is $-x^2/4$.

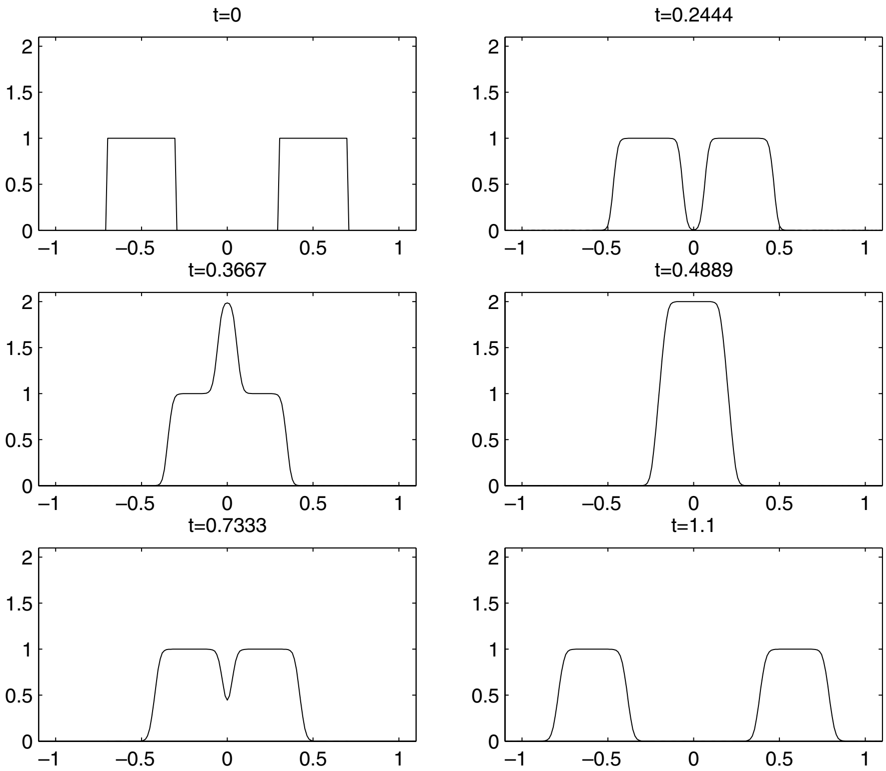

Fig. 3. Self-crossing wavefronts in one dimensions.

big enough compared to the grid and to the time interval of interest, we may not see the stated incorrect propagation of energy. Furthermore, the solution may develop a large jump across O_p and differencing across a large jump of the level set function may introduce numerical instability and may propagate portions of the energy across O, the singularity in the velocity. This potential large jump in ϕ_j and f across O_p also suggests the use of a ''one-sided'' approximate Dirac-δ function near O_p for better resolution of the amplitude.

Example 5.1. (1D self-crossing wavefronts) $c(x) = 1.0$, $S_0(x) = -(x^2 - 0.25)/4$, and $\bar{A}_0(x) = \chi_{[-0.7,-0.3]\cup[0.3,0.7]}(x)$, where $\chi_\Omega(x)$ is the characteristic function of the set Ω. See Fig. 3.

Example 5.2. (1D with variable speed) $c(x) = (3 + 1.5\tanh(x))$. We ran two simulations using $S_0(x) = -x^2/4$, $A_0(x) = \chi_{[-0.65,-0.35]\cup[0.35,0.65]}(x)$, where $\chi_\Omega(x)$ is the characteristic function of the set Ω. The results are shown in Fig. 4.

Example 5.3. (Wave guide) We are interested in a plane wave parallel to the x-axis, travelling in the positive direction in the z-axis. The index of refraction $\eta(x,y,z) = c^{-1}(x,y,z) = 1 + \exp(-x^2)$, is independent of z. In this case, we can use z as time axis and reduce the problem by one more dimension. The convection in this reduced phase space, x–θ–z space, is

$$\frac{\partial}{\partial z}u + \tan\theta u_x + \frac{\eta_x}{\eta}u_\theta = 0.$$

We initialize $u(x,\theta) = \theta$, $\theta \in [-\pi/2 + \theta_0, \pi/2 - \theta_0]$, $x \in [-3,3]$ and $f(x,\theta,z=0) = A_0^2(x)\eta^2(x)$.

Fig. 5 shows the multi-valued wavefront plotted in $x - \theta$ space (left), and $A^2(x,z_1) = \eta^2(x)\int f(x,\theta,z_1)\delta(\phi(x,\theta,z_1))\,d\theta$ plotted as a function of x (right).

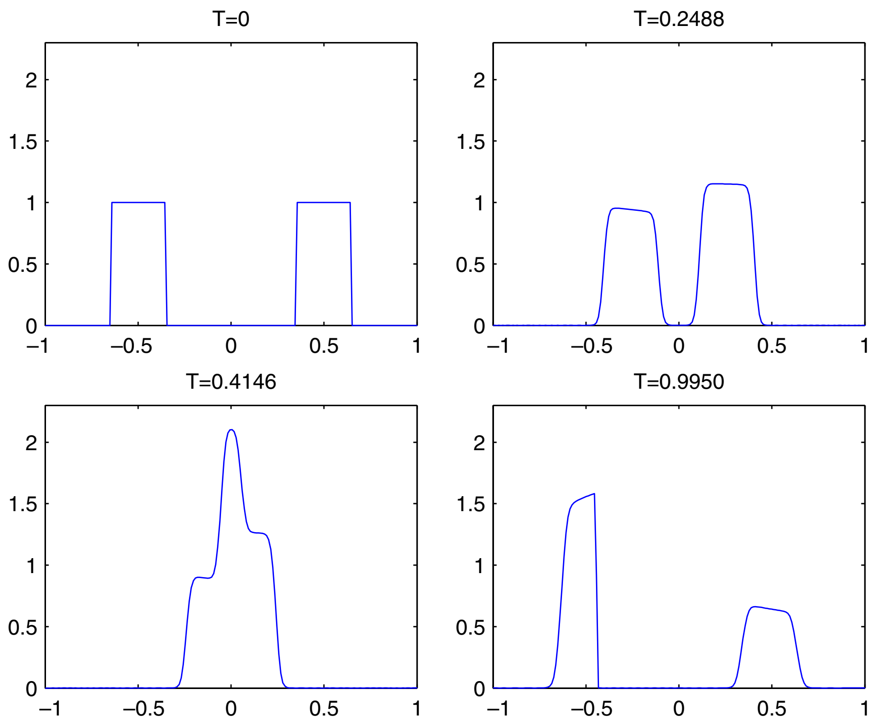

Fig. 4. Energy transport with variable coefficients.

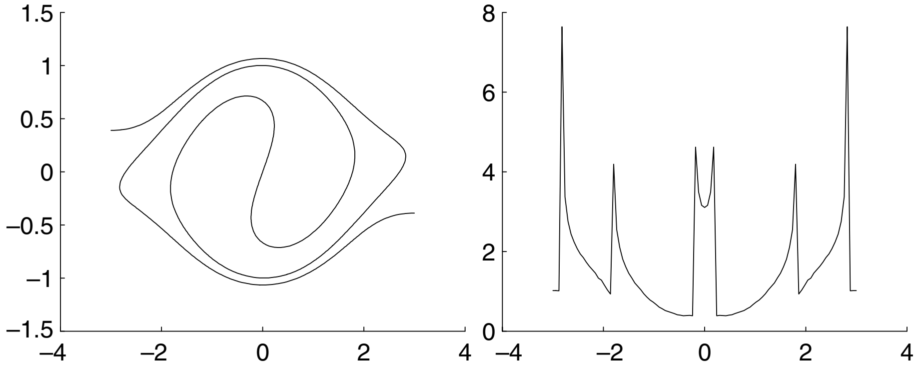

Fig. 5. The multi-valued wavefronts and the averaged amplitude $\bar{A}^2$ from Example 5.3 are shown, respectively, on the left and right subfigures.

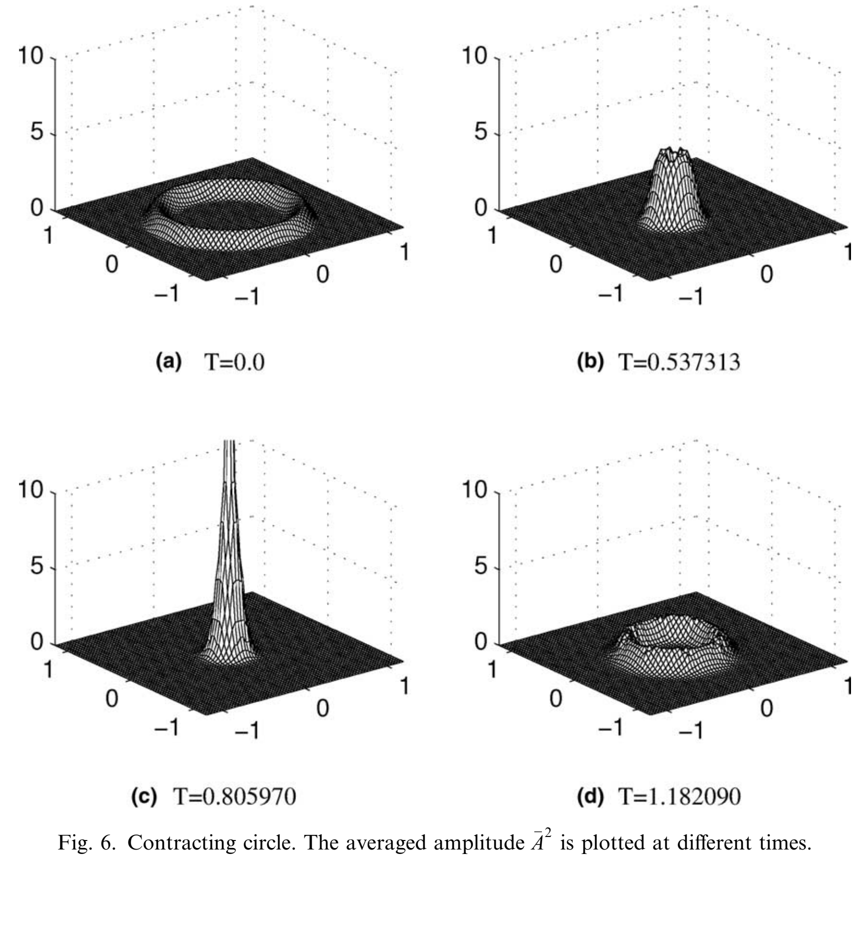

Fig. 6. Contracting circle. The averaged amplitude $\bar{A}^2$ is plotted at different times.

Example 5.4. (Contracting circle and ellipse in 2D)

$$\text{Circle}: \ S_0(x,y) = -(x^2+y^2-0.5)/2, \ c(x) \equiv 1.A_0(x,y) = 0.3 * \delta^{\cos}_{0.3}(-S(x,y)).$$
$$\text{Ellipse}: \ S_0(x,y) = -(x^2+9y^2-0.6), \ c(x) \equiv 1.A_0(x,y) = 0.3 * \delta^{\cos}_{0.3}(-S(x,y)).$$

$$\delta^{\cos}_{\alpha}(x) = \begin{cases} \frac{1}{2\alpha}(1+\cos(\frac{\pi x}{\alpha})), & |x| \leqslant \eta, \\ 0, & |x| > \eta. \end{cases}$$

Figs. 6 and 7 show the respective $\bar{A}^2$ at different times. In addition, in Fig. 8, we plotted three wave fronts computed using ray tracing on the ellipses that are initially defined by $x^2+9y^2-r=0$ with $r=0.45$, 0.6, and 0.7.

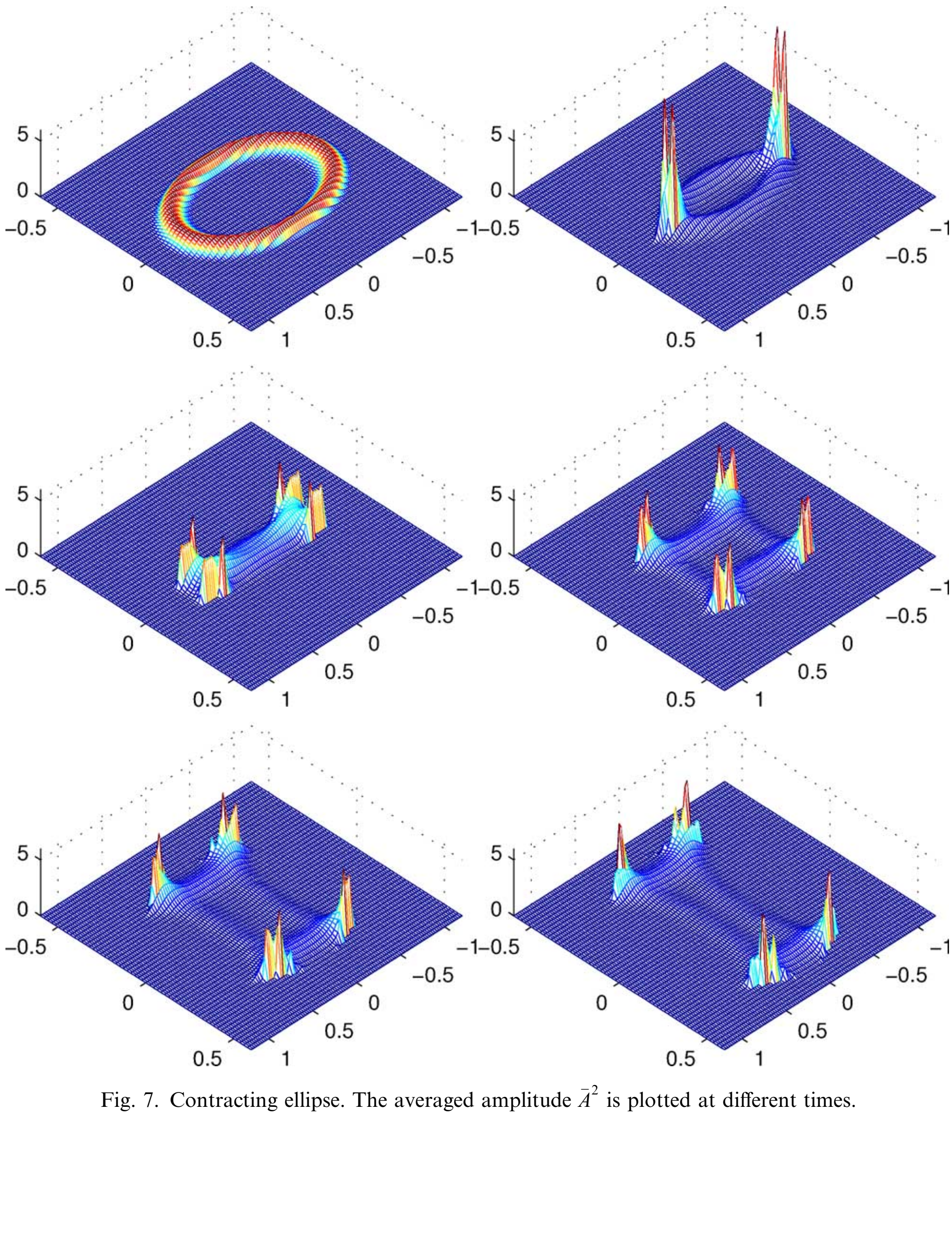

Fig. 7. Contracting ellipse. The averaged amplitude $\bar{A}^2$ is plotted at different times.

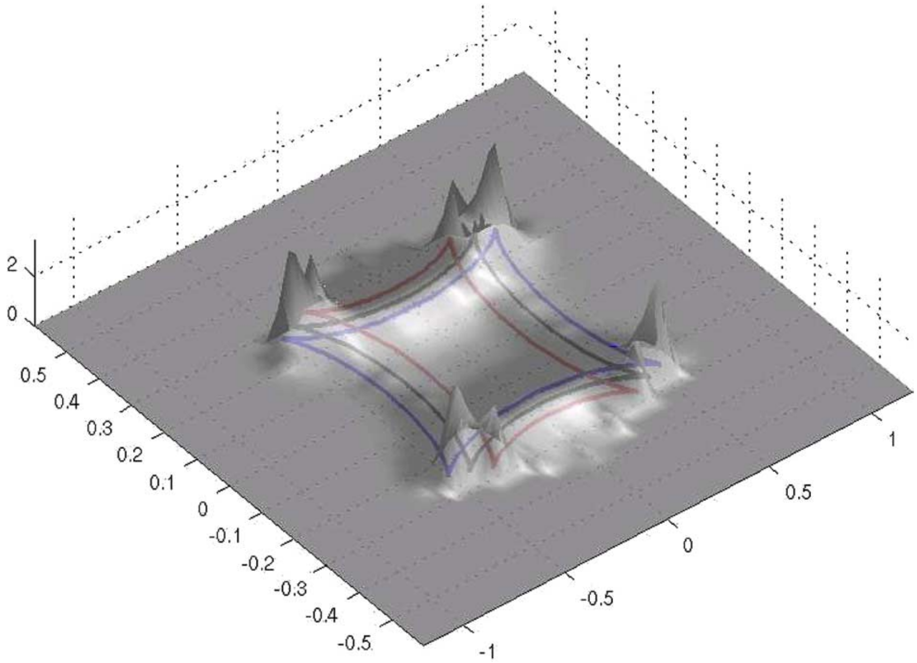

Fig. 8. Contracting ellipse at $T = 0.460526$. We plotted a three wave fronts underneath the graph of $\bar{A}^2$; these wave fronts correspond to the ellipse defined, at $T = 0$, by the zeros of $x^2 + 9y^2 - r = 0$ with $r = 0.45$, 0.6, and 0.75.

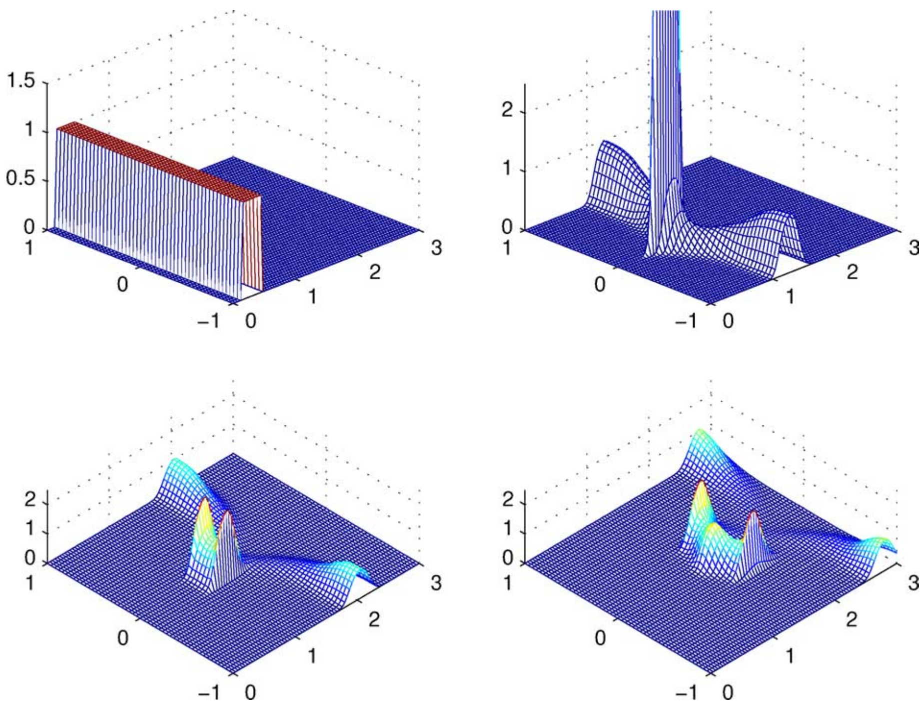

Fig. 9. Contracting circle. The averaged amplitude $\bar{A}^2$ is plotted at different times.

Example 5.5. (Waveguide) $c(x,y) = 2 - \exp(-9y^2)$, and $S_0(x,y) = x$,

$$\bar{A}_0^2(x,y) = \begin{cases} 1, & |x-0.3| \leqslant 0.15, \\ 0, & \text{otherwise.} \end{cases}$$

Fig. 9 shows four snapshots of the transport of the amplitude $\bar{A}^2(x,y,t)$.

6. Conclusion

We have introduced a systematic level set method for computing the energy transport for high frequency wave propagation problems, including a large class of physically important symmetric hyperbolic systems. In our approach, the distribution of energy on the lower dimensional Lagrangian manifold is implicitly located in phase space by a system of level set functions that solve the Liouville equation. The evaluation of the observable energy can be performed, at any time needed, by a simple integration step.

Our method can be applied to a class of problems arising in geometrical optics, seismic imaging and multiple arrivals where the computation of multi-valued solutions are essential. Recently, there has been an increasing interest in designing efficient methods with the ability to capture multi-valued physical variables instead of the viscosity solution, see, e.g. [5,11,12,26–28]. The techniques discussed in this paper are naturally geometrical and very well suited for handling multi-valued solutions.

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Appendix A

In this appendix, we provide an alterative proof of (2.9), which plays a key role in our analysis of Section 2.

First we have

$$L(J) = L(\det(\nabla_{\mathbf{k}}\phi)) = \sum_{r=1}^{n} \det \begin{pmatrix} \phi^1_{k_1} & \cdots & \phi^1_{k_{r-1}} & L(\phi^1_{k_r}) & \cdots & \phi^1_{k_n} \\ \vdots & \ddots & \vdots & \vdots & \ddots & \vdots \\ \phi^n_{k_1} & \cdots & \phi^n_{k_{r-1}} & L(\phi^n_{k_r}) & \cdots & \phi^n_{k_n} \end{pmatrix}. \tag{7.1}$$

From $L\phi^i = 0$ it follows $\partial_{k_r} L\phi^i = 0$, which leads to

$$L\phi^i_{k_r} = \sum_j \phi^i_{k_j} H_{x_j k_r} - \sum_j H_{k_j k_r} \phi^i_{x_j}. \tag{7.2}$$

Substituting (7.2) into (7.1) we then obtain

$$L(J) = \sum_{r=1}^{n} \det \begin{pmatrix} \phi^1_{k_1} & \cdots & \sum_j \phi^1_{k_j} H_{x_j k_r} & \cdots & \phi^1_{k_n} \\ \vdots & \ddots & \vdots & \ddots & \vdots \\ \phi^n_{k_1} & \cdots & \sum_j \phi^n_{k_j} H_{x_j k_r} & \cdots & \phi^n_{k_n} \end{pmatrix} - \sum_{r=1}^{n} \det \begin{pmatrix} \phi^1_{k_1} & \cdots & \sum_j \phi^1_{k_j} H_{k_j k_r} & \cdots & \phi^1_{k_n} \\ \vdots & \ddots & \vdots & \ddots & \vdots \\ \phi^n_{k_1} & \cdots & \sum_j \phi^n_{k_j} H_{k_j k_r} & \cdots & \phi^n_{k_n} \end{pmatrix} = I + II. \tag{7.3}$$

Now

$$I = \sum_{r=1}^{n} H_{x_r k_r} \det \begin{pmatrix} \phi^1_{k_1} & \cdots & \phi^1_{k_r} & \cdots & \phi^1_{k_n} \\ \vdots & \ddots & \vdots & \ddots & \vdots \\ \phi^n_{k_1} & \cdots & \phi^n_{k_r} & \cdots & \phi^n_{k_n} \end{pmatrix} = \det(\nabla_{\mathbf{k}}\phi) \sum_{r=1}^{n} H_{x_r k_r} = J \sum_{i=1}^{n} H_{x_i k_i}.$$

Also, using Cramer's rule we can show that

$$((\nabla_{\mathbf{k}}\phi)^{-1}\phi_{x_i})^r = \frac{1}{\det(\nabla_{\mathbf{k}}\phi)} \det \begin{pmatrix} \phi^1_{k_1} & \cdots & \phi^1_{k_r} & \phi^1_{x_i} & \cdots & \phi^1_{k_n} \\ \vdots & \ddots & \vdots & \vdots & \ddots & \vdots \\ \phi^n_{k_1} & \cdots & \phi^n_{k_r} & \phi^n_{x_i} & \cdots & \phi^n_{k_n} \end{pmatrix}.$$

So

$$II = \det(\nabla_{\mathbf{k}}\phi)(-\sum_{j,r} H_{k_i k_r}((\nabla_{\mathbf{k}}\phi)^{-1}\phi_{x_i})^r) = -J \sum_{i,j=1}^{n} H_{k_i k_j}(Q^{-1}\phi_{x_i})^j.$$

Thus, a substitution of I and II into (7.3) leads to

$$L(J) = J\left(\sum_{i=1}^{n} H_{x_i k_i} - \sum_{i,j=1}^{n} H_{k_i k_j}(Q^{-1}\phi_{x_i})^j\right),$$

which by (2.8) is as claimed in (2.9).

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