Computing high frequency solutions of symmetric hyperbolic systems with polarized waves*

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December 25, 2012

Abstract

We develop computational methods for high frequency solutions of general symmetric hyperbolic systems with eigenvalue degeneracies (multiple eigenvalues with constant multiplicities) in the dispersion matrices that correspond to polarized waves. Physical examples of such systems include the three dimensional elastic waves and Maxwell equations. The computational methods are based on solving a coupled system of inhomogeneous Liouville equations which is the high frequency limit of the underlying hyperbolic systems by using the Wigner transform [12]. We first extend the level set methods developed in [5] for the homogeneous Liouville equation to the coupled inhomogeneous system, and find an efficient simplification in one space dimension for the Eulerian formulation which reduces the computational cost of two-dimesnional phase space Liouville equations into that of two one-dimensional equations. For the Lagrangian formulation, we introduce a geometric method which allows a significant simplification in the numerical evaluation of the energy density and flux. Numerical examples are presented in both one and two space dimensions to demonstrate the validity of the methods in the high frequency regime.

1 Introduction

We will study the general symmetric hyperbolic system of the form[1]

$$\begin{cases} A(\mathbf{x})\frac{\partial \mathbf{u}_\varepsilon}{\partial t} + D^j \frac{\partial \mathbf{u}_\varepsilon}{\partial x_j} = 0 \\ \mathbf{u}_\varepsilon(\mathbf{x},0) = \mathbf{u}_0(\mathbf{x}) e^{iS_0(\mathbf{x})/\varepsilon}, \end{cases} \tag{1.1}$$

where $\mathbf{u} \in \mathbb{C}^n$, $\mathbf{x} \in \mathbb{R}^d$, $A(\mathbf{x})$ is a $n \times n$ symmetric positive definite matrix, and the D^j are $n \times n$ symmetric constant matrices. Many physical systems such as Maxwell's equations, the elastic wave equations and the acoustic equations all may be put into the symmetric hyperbolic form with the correct choices of $A(\mathbf{x})$ and D^j. Here we are interested in high frequency solutions, where the high frequency is introduced by the wave length ε in the initial data in (1.1). In many physical applications ε is very small compared to the scale of the computational domain, and the numerical meshes and time steps need to resolve this small scale, thus computing the high frequency solutions, in particular in high dimensions, is prohibitively expensive.

One efficient way to deal with high frequency wave problems is to solve the limiting equation by finding the asymptotic equation when $\varepsilon \to 0$. The Wigner transform, introduced in [16], is a powerful mathematical tool to study this limit [3], since it is valid global in time, even beyond caustic formation. The limiting equation is the Liouville equation which does not depend on ε, permitting large time steps and mesh sizes. However, it encounters two major difficulties. First, the Liouville equation is defined in the phase space,

*This work was partially supported by NSF grants DMS-1114546 and DMS-1107291: NSF Research Network in Mathematical Sciences "KI-Net: Kinetic description of emerging challenges in multiscale problems of natural sciences".

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[1]Assume the following summation convention: repeated Latin indices are summed whereas repeated Greek indices are not summed.

thus doubling the computational dimension. Second, for the WKB kind of initial data given in (1.1), the solution is a superposition of Dirac Delta functions [4, 13] which are difficult to resolve numerically with a high order accuracy. The first difficulty can be dealt with by local level set methods [10, 11] in the Eulerian formulation, or using Lagrangian formulation which is just the particle method. The second difficulty, the numerical resolution of Delta function, was elegantly handled by a singularity decomposition method, first introduced in [6] for the semiclassical limit of the Schrödinger equation, and then extended to symmetric hyperbolic systems in [5]. The method is based on the observation that the solution to the linear Liouville equation of the form of the Delta functions can be decomposed into two solutions of the Liouville equations which are both bounded, one, roughly speaking, corresponding to strength (or amplitude of the wave) while the other one the kernel of the Delta function. The final solution is the combination of these two quantities involving the Delta function, but the Delta function needs to be computed only at the final output time, not during the time evolution! This significantly enhances the numerical resolution of the singular solutions to the Liouville equation. See [2, 7] for reviews of computational high frequency waves or semiclassical limit of quantum waves.

In this paper, we extend the singular decomposition method of [6, 5] to (1.1). Different from the problem studied in [5], here the dispersion matrix will have multiple eigenvalues while in [5] only simple eigenvalues are allowed. By assuming constant multiplicities of the multiple eigenvalues, the high frequency limit of (1.1), using the Wigner transform, becomes coupled systems of inhomogeneous Liouville equations (while in [5] they are decoupled homogeneous Liouville equations for different eigenvalues) [12]. The inhomogeneities arise due to the degeneracy of the eigenvalues, which describe the cross-polarization effects. We first show that the singular decomposition method developed in [6, 5] still applies here except that one needs to solve inhomogeneous Liouville system. We also found an efficient simplification in one space dimension for the Eulerian formulation which reduces the computational cost of two-dimensional phase space Liouville equations into that of two one-dimensional equations. For the Lagrangian formulation, we introduce a geometric method which allows a significant simplification in the numerical evaluation of the energy density and flux.

While the polarization effects usually appear in three dimensional space for elastic waves and electromagnetic waves, our method, developed for one and two dimensional hyperbolic systems, is the first of its kind to deal with polarized waves thus provides a foundation for three dimensional simulation which will be developed in the near future. Furthermore, similar effects also appear in molecular dynamics with quantum transitions [15] and mixing of Bloch bands in solid state physics [14] where the multiplicity is a variable thus more elaborate numerical methods along the line of this paper are desirable.

This paper is organized as follows. In Section 2, we will introduce and then use the Wigner transform to obtain, in the limit that $\varepsilon \to 0$, a coupled system of Liouville equations which govern the evolution of this high frequency limit, as shown in [12]. In Section 3 we will prove the singularity decomposition result. In Section 4 we will discuss simplifications which occur in the one space dimension case. In Section 5 we will discuss d-dimensional implementation of our method in the Eulerian and Lagrangian frames as well as introduce a geometric reduction of computational complexity for the evaluation of energy and energy flux in the Lagrangian framework. In Section 6 we will show some illustrative numerical examples in one and two dimensions. Finally, Section 7 will contain our conclusions.

2 The Wigner Transform of Hyperbolic Systems

This section is based primarily on the derivation which appears in [12].

The energy density and d components of flux for a solution of (1.1) are given by

$$\mathcal{E}(t,\mathrm{x}) = \frac{1}{2}\langle A(\mathbf{x})\mathbf{u}_\varepsilon(t,\mathbf{x}), \mathbf{u}_\varepsilon(t,\mathbf{x})\rangle \tag{2.1}$$

$$\mathcal{F}_i(t,\mathbf{x}) = \frac{1}{2}\langle D^i\mathbf{u}_\varepsilon(t,\mathbf{x}), \mathbf{u}_\varepsilon(t,\mathbf{x})\rangle \tag{2.2}$$

respectively where $\langle\cdot,\cdot\rangle$ is the standard Euclidian inner product on $\mathbb{C}^n$. By taking an inner product of (1.1)

with $\mathbf{u}_\varepsilon(t,\mathbf{x})$ one gets the energy conservation law

$$\frac{\partial \mathcal{E}}{\partial t} + \nabla \cdot \mathcal{F} = 0. \tag{2.3}$$

Integration of (2.3) shows conservation of total energy:

$$\frac{d}{dt}\int \mathcal{E}(t,\mathbf{x})d\mathbf{x} = 0. \tag{2.4}$$

Next define the scaled Wigner transform

$$W^\varepsilon(t,\mathbf{x},\mathbf{k})d\mathbf{k} = \left(\frac{1}{2\pi}\right)^d \int e^{i\mathbf{k}\cdot\mathbf{y}}\mathbf{u}_\varepsilon(t,\mathbf{x}-\varepsilon\mathbf{y}/2)\mathbf{u}_\varepsilon^*(t,\mathbf{x}+\varepsilon\mathbf{y}/2)d\mathbf{y} \tag{2.5}$$

where $\mathbf{u}^* = \overline{\mathbf{u}}^T$ is the conjugate transpose of $\mathbf{u}$. The matrix $W(t,\mathbf{x},\mathbf{k})$ is Hermitian but only becomes positive definite in the limit as $\varepsilon \to 0$ [12]. It has the useful property that

$$\int W^\varepsilon(t,\mathbf{x},\mathbf{k})d\mathbf{k} = \mathbf{u}_\varepsilon(t,\mathbf{x})\mathbf{u}_\varepsilon^*(t,\mathbf{x}). \tag{2.6}$$

The energy density and flux may be recovered from $W(t,\mathbf{x},\mathbf{k})$ via

$$\mathcal{E}(t,\mathbf{x}) = \frac{1}{2}\int \mathrm{Tr}(A(\mathbf{x})W^\varepsilon(t,\mathbf{x},\mathbf{k}))d\mathbf{k}, \tag{2.7}$$

$$\mathcal{F}_j(t,\mathbf{x}) = \frac{1}{2}\int \mathrm{Tr}(D^j W^\varepsilon(t,\mathbf{x},\mathbf{k}))d\mathbf{k}. \tag{2.8}$$

Introduce a natural inner product for the system (1.1) as

$$\langle \mathbf{u},\mathbf{v}\rangle_A = \langle A\mathbf{u},\mathbf{v}\rangle \tag{2.9}$$

and note that with this definition the energy (2.1) may be written as $\mathcal{E} = \frac{1}{2}\langle \mathbf{u},\mathbf{u}\rangle_A$. Define the *dispersion matrix* as the sum

$$L(\mathbf{x},\mathbf{k}) = A^{-1}(\mathbf{x})k_i D^i \tag{2.10}$$

and note that $L(\mathbf{x},\mathbf{k})$ is self-adjoint with respect to (2.9):

$$\langle L\mathbf{u},\mathbf{v}\rangle_A = \langle \mathbf{u},L\mathbf{v}\rangle_A. \tag{2.11}$$

Therefore, all eigenvalues ω_τ of $L(\mathbf{x},\mathbf{k})$ are real and the corresponding eigenvectors $\mathbf{b}^\tau$ can be chosen to be orthogonal with respect to $\langle\cdot,\cdot\rangle_A$:

$$L(\mathbf{x},\mathbf{k})\mathbf{b}^\tau(\mathbf{x},\mathbf{k}) = \omega_\tau(\mathbf{x},\mathbf{k})\mathbf{b}^\tau(\mathbf{x},\mathbf{k}), \quad \langle \mathbf{b}^\tau,\mathbf{b}^\beta\rangle_A = \delta_{\tau\beta}. \tag{2.12}$$

We assume that the eigenvalues have constant multiplicity independent of $\mathbf{x},\mathbf{k}$. This assumption is valid for many physical examples including all those studied in this paper.

In general the eigenvalues of $L(\mathbf{x},\mathbf{k})$ are multiple eigenvalues so let $\omega_\tau(\mathbf{x},\mathbf{k})$ be an eigenvalue of multiplicity r and let the corresponding eigenvectors $\mathbf{b}^{\tau,i}$, $i = 1,...,r$ be orthonormal with respect to $\langle\cdot,\cdot\rangle_A$. Define the $n\times n$ matrices

$$B^{\tau,ij} = \mathbf{b}^{\tau,i}\mathbf{b}^{\tau,j*}, \tag{2.13}$$

with $i,j = 1,...,r$. In the limit that $\varepsilon \to 0$, the Wigner matrix $W^\varepsilon(t,\mathbf{x},\mathbf{k})$ is approximated by $W^{(0)}(t,\mathbf{x},\mathbf{k})$ which may be written as

$$W^{(0)}(t,\mathbf{x},\mathbf{k}) = \sum_{\tau,i,j} w_{ij}^\tau(t,\mathbf{x},\mathbf{k})B^{\tau,ij}(\mathbf{x},\mathbf{k}). \tag{2.14}$$

We define the $r\times r$ *coherence matrices* as

$$W^\tau(t,\mathbf{x},\mathbf{k}) = \left(w_{ij}^\tau(t,\mathbf{x},\mathbf{k})\right)_{r\times r}. \tag{2.15}$$

Note that the multiplicity r of the eigenvalues ω_τ depends on τ but this is not indicated explicitly. The entries of the coherence matrix W_{ij}^τ can be recovered via

$$W_{ij}^\tau(t,\mathbf{x},\mathbf{k}) = \langle\langle W^{(0)}(t,\mathbf{x},\mathbf{k}), B^{\tau,ij}(\mathbf{x},\mathbf{k})\rangle\rangle \tag{2.16}$$

where $\langle\langle X, Y\rangle\rangle = \mathrm{Tr}(AX^*AY)$ is a matrix inner product. From here we can deduce that each of the coherence matrices (2.16) satisfies the coupled system of Liouville equations

$$\partial_t W^\tau + \nabla_{\mathbf{k}}\omega_\tau \cdot \nabla_{\mathbf{x}} W^\tau - \nabla_{\mathbf{x}}\omega_\tau \cdot \nabla_{\mathbf{k}} W^\tau = N^\tau W^\tau - W^\tau N^\tau \tag{2.17}$$

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

$$N_{mn}^\tau(\mathbf{x},\mathbf{k}) = \left\langle \mathbf{b}^{\tau,n}, D^i \frac{\partial \mathbf{b}^{\tau,m}}{\partial x_i} \right\rangle - \frac{\partial \omega_\tau}{\partial x_i}\left\langle \mathbf{b}^{\tau,n}, \frac{\partial \mathbf{b}^{\tau,m}}{\partial k_i}\right\rangle_A - \frac{1}{2}\frac{\partial^2 \omega_\tau}{\partial_{x_i}\partial_{k_i}}\delta_{nm}. \tag{2.18}$$

In the sense of distributions, the weak limit of $W^\varepsilon(0,\mathbf{x},\mathbf{k})$ as $\varepsilon \to 0$ gives the initial condition

$$W^{(0)}(0,\mathbf{x},\mathbf{k}) = \mathbf{u}_0(\mathbf{x})\mathbf{u}_0^*(\mathbf{x})\delta(\mathbf{k} - \nabla S_0(\mathbf{x})). \tag{2.19}$$

Using (2.16) this implies that

$$W_{ij}^\tau(0,\mathbf{x},\mathbf{k}) = \mathrm{Tr}(A\mathbf{u}_0\mathbf{u}_0^* A B^{\tau,ij})\delta(\mathbf{k} - \nabla S_0(\mathbf{x})). \tag{2.20}$$

In summary, W^τ is computed via (2.17) with initial condition given by (2.20). Next $W^{(0)}$ follows from W^τ via (2.14) from which one may compute the approximate energy density and flux using

$$\mathcal{E}^{(0)}(t,\mathbf{x}) = \frac{1}{2}\int \mathrm{Tr}(A(\mathbf{x})W^{(0)}(t,\mathbf{x},\mathbf{k}))d\mathbf{k}, \tag{2.21}$$

$$\mathcal{F}_j^{(0)}(t,\mathbf{x}) = \frac{1}{2}\int \mathrm{Tr}(D^j W^{(0)}(t,\mathbf{x},\mathbf{k}))d\mathbf{k} \tag{2.22}$$

respectively. In the next section we show how to solve (2.17) with singular initial conditions of the form (2.20).

3 A Singularity Decomposition Method

From the previous section we wish to solve the Liouville equation (2.17) together with the initial condition (2.20). Since accuracy is reduced when an initial condition containing a delta function is evolved numerically, it is desirable to decompose the original Liouville equation into two separate equations which have bounded initial conditions [5, 6]. To this end we have the following theorem.

Theorem 3.1. *Define the Liouville operator*

$$\mathcal{L} = \partial_t + \nabla_{\mathbf{k}}\omega_\tau \cdot \nabla_{\mathbf{x}} - \nabla_{\mathbf{x}}\omega_\tau \cdot \nabla_{\mathbf{k}} \tag{3.1}$$

and the coupling matrix N^τ as in (2.18). Then the solution $W^\tau(t,\mathbf{x},\mathbf{k})$ to the system

$$\begin{cases} \mathcal{L}W^\tau = N^\tau W^\tau - W^\tau N^\tau \\ W^\tau(0,\mathbf{x},\mathbf{k}) = U_0^\tau(\mathbf{x},\mathbf{k})\delta(\mathbf{g}_0^\tau(\mathbf{x},\mathbf{k})) \end{cases} \tag{3.2}$$

for a smooth function $\mathbf{g}_0^\tau(\mathbf{x},\mathbf{k})$ may be written as $U^\tau(t,\mathbf{x},\mathbf{k})\delta(\mathbf{g}^\tau(t,\mathbf{x},\mathbf{k}))$ where the matrix function U^τ and vector function $\mathbf{g}^\tau$ are governed by

$$\begin{cases} \mathcal{L}U^\tau = N^\tau U^\tau - U^\tau N^\tau \\ U^\tau(0,\mathbf{x},\mathbf{k}) = U_0^\tau(\mathbf{x},\mathbf{k}) \end{cases} \tag{3.3}$$

and

$$\begin{cases} \mathcal{L}\mathbf{g}^\tau = 0 \\ \mathbf{g}^\tau(0,\mathbf{x},\mathbf{k}) = \mathbf{g}_0^\tau(\mathbf{x},\mathbf{k}) \end{cases} \tag{3.4}$$

respectively.

Proof. (We drop the τ superscript notation for the duration of the proof) We begin by defining the weak equivalent to

$$\begin{cases} \mathcal{L}W = NW - WN \\ W(0, \mathbf{x}, \mathbf{k}) = W_0(\mathbf{x}, \mathbf{k}) \end{cases} \tag{3.5}$$

as requiring that for any $d \times d$ matrix $\phi(t, \mathbf{x}, \mathbf{k})$ where $\phi_{i,j} \in C_0^\infty(\mathbb{R}^+ \times \mathbb{R}^n \times \mathbb{R}^n)$, the following holds

$$\int_{\mathbb{R}^{2n}} \mathrm{Tr}(W_0 \phi|_{t=0}) d\mathbf{x} d\mathbf{k} - \int_0^\infty \int_{\mathbb{R}^{2n}} \mathrm{Tr}(W \mathcal{L}\phi) d\mathbf{x} d\mathbf{k} dt = \int_0^\infty \int_{\mathbb{R}^{2n}} \mathrm{Tr}((NW - WN)\phi) d\mathbf{x} d\mathbf{k} dt. \tag{3.6}$$

Note that we use the trace of the matrix product here to represent $\sum_{i,j} \phi_{j,i} W_{i,j}$ for ease of notation. Simple integration by parts shows that for smooth W, (3.5) and (3.6) are equivalent. Define the Hamiltonian flow $H_t(\mathbf{x}_0, \mathbf{k}_0)$ which evolves any point $(\mathbf{x}_0, \mathbf{k}_0)$ in phase space forward to time t according the Hamiltonian system

$$\begin{cases} \frac{d}{dt}\mathbf{x}(t) = \nabla_{\mathbf{k}} \omega_\tau \\ \frac{d}{dt}\mathbf{k}(t) = -\nabla_{\mathbf{x}} \omega_\tau \end{cases} . \tag{3.7}$$

We change coordinates to $(t, \mathbf{x}_0, \mathbf{k}_0)$ defined by $(t, \mathbf{x}, \mathbf{k}) = (t, H_t(\mathbf{x}_0, \mathbf{k}_0))$. Since the determinant of the Jacobian of this transform is 1 we rewrite (3.6) as

$$\int_{\mathbb{R}^{2n}} \mathrm{Tr}(W_0 \phi|_{t=0}) d\mathbf{x}_0 d\mathbf{k}_0 - \int_0^\infty \int_{\mathbb{R}^{2n}} \mathrm{Tr}(W \frac{d}{dt}\phi) d\mathbf{x}_0 d\mathbf{k}_0 dt = \int_0^\infty \int_{\mathbb{R}^{2n}} \mathrm{Tr}((NW - WN)\phi) d\mathbf{x}_0 d\mathbf{k}_0 dt \tag{3.8}$$

where we have taken advantage of the fact that $\mathcal{L}\phi(t, \mathbf{x}, \mathbf{k}) = \frac{d}{dt}\phi(t, H_t(\mathbf{x}_0, \mathbf{k}_0))$. Note that in this paper $\frac{d}{dt}$ always represents the full derivative in time and that one also has

$$\mathcal{L}U(t, \mathbf{x}, \mathbf{k}) = \frac{d}{dt} U(t, H_t(\mathbf{x}_0, \mathbf{k}_0)) = N(H_t(\mathbf{x}_0, \mathbf{k}_0)) U(t, H_t(\mathbf{x}_0, \mathbf{k}_0)) - U(t, H_t(\mathbf{x}_0, \mathbf{k}_0)) N(H_t(\mathbf{x}_0, \mathbf{k}_0)) \tag{3.9}$$

and

$$\mathcal{L}\mathbf{g}(t, \mathbf{x}, \mathbf{k}) = \frac{d}{dt}\mathbf{g}(t, H_t(\mathbf{x}_0, \mathbf{k}_0)) = \mathbf{0}. \tag{3.10}$$

Substituting the anzats $U(t, \mathbf{x}, \mathbf{k})\delta(\mathbf{g}(t, \mathbf{x}, \mathbf{k}))$ into the left hand side of (3.8) we obtain

$$\int_{\mathbb{R}^{2n}} \mathrm{Tr}\left(U_0(\mathbf{x}_0, \mathbf{k}_0)\delta(\mathbf{g}_0(\mathbf{x}_0, \mathbf{k}_0))\phi|_{t=0}\right) d\mathbf{x}_0 d\mathbf{k}_0 - \int_0^\infty \int_{\mathbb{R}^{2n}} \mathrm{Tr}\left(U(t, H_t(\mathbf{x}_0, \mathbf{k}_0))\delta(\mathbf{g}(t, H_t(\mathbf{x}_0, \mathbf{k}_0))) \frac{d}{dt}\phi\right) d\mathbf{x}_0 d\mathbf{k}_0 dt. \tag{3.11}$$

Noting first that (3.10) implies $\mathbf{g}(t, H_t(\mathbf{x}_0, \mathbf{k}_0)) = \mathbf{g}(0, \mathbf{x}_0, \mathbf{k}_0)$, observe that the above space integrals are weighted surface integrals in $2d$-dimensional phase space over a d-dimensional sub-manifold defined by the zero set of $\mathbf{g}(0, \mathbf{x}_0, \mathbf{k}_0)$ and that the weight given in terms of the inverse volume of $\nabla\mathbf{g}(0, \mathbf{x}_0, \mathbf{k}_0)$. Denoting this zero-set manifold as $\mathcal{S}$, (3.11) may be written as

$$\int_{\mathcal{S}} \mathrm{Tr}(U\phi|_{t=0}) \frac{1}{\mathrm{vol}(\nabla\mathbf{g})} d\sigma - \int_0^\infty \int_S \mathrm{Tr}(U \frac{d}{dt}\phi) \frac{1}{\mathrm{vol}(\nabla\mathbf{g})} d\sigma dt \tag{3.12}$$

Where

$$\mathrm{vol}(\nabla\mathbf{g}) = \sqrt{\det(G)} \tag{3.13}$$

and G is the *Gramian matrix* defined as $G_{i,j} = \nabla\mathbf{g}_i \cdot \nabla\mathbf{g}_j$ with the gradients taken over the $2n$ space coordinates. (3.12) is an application of the smooth Coarea formula and $\mathrm{vol}(\mathbf{g}(0, \mathbf{x}_0, \mathbf{k}_0))$ is non-zero because the initial conditions given to $\mathbf{g}$. Further note that $\mathrm{vol}(\mathbf{g}(0, \mathbf{x}_0, \mathbf{k}_0))$ is independent of time as is the surface $\mathcal{S}$ over which the integrals are performed. Also since $\mathcal{S}$ is fixed in time, $\frac{d}{dt}\phi$ is still the full derivative in time. Thus integrate by parts in time so that (3.12) becomes

$$\int_0^\infty \int_S \mathrm{Tr}\left(\left[\frac{d}{dt}U\right]\phi\right) \frac{1}{\mathrm{vol}(\nabla\mathbf{g})} d\sigma dt. \tag{3.14}$$

Then using (3.9),

$$\int_0^\infty \int_S \mathrm{Tr}\left(\left[\frac{d}{dt}U\right]\phi\right)\frac{1}{\mathrm{vol}(\nabla \mathbf{g})}d\sigma dt = \int_0^\infty \int_S \mathrm{Tr}((NU-UN)\phi)\frac{1}{\mathrm{vol}(\nabla \mathbf{g})}d\sigma dt. \tag{3.15}$$

Finally,

$$\begin{aligned}\int_0^\infty \int_S \mathrm{Tr}((NU-UN)\phi)\frac{1}{\mathrm{vol}(\nabla \mathbf{g})}d\sigma dt &= \int_0^\infty \int_{\mathbb{R}^{2n}} \mathrm{Tr}((NU\delta(\mathbf{g})-U\delta(\mathbf{g})N)\phi)d\mathbf{x}_0 d\mathbf{k}_0 dt \\ &= \int_0^\infty \int_{\mathbb{R}^{2n}} \mathrm{Tr}((NW-WN)\phi)d\mathbf{x}_0 d\mathbf{k}_0 dt\end{aligned} \tag{3.16}$$

and this completes the proof. □

Remark. In our application of Theorem 3.1 to (2.17) and (2.19), the initial amplitude $U_0^\tau(\mathbf{x},\mathbf{k})$ for U is independent of $\mathbf{k}$ though the proof above does not require this to be the case. Also, when the eigenvalues of the dispersion matrix (2.10) are simple, the coupling matrix (2.18) is zero and the Theorem 3.1 reduces to ones proven in [5, 6] for homogeneous Liouville equations. For now, $\nabla S_0(\mathbf{x})$ is assumed to be differentiable. A discussion of some cases where $\nabla S_0(\mathbf{x})$ is discontinuous may be found in [5, 6].

Using Theorem 3.1, the computation of delta functions during time evolution is avoided and delta functions only appear in post processing steps when one wishes to evaluate energy density (2.21) and flux (2.22). In particular, our method uses the decomposition in Theorem 3.1 to replace solving

$$\begin{cases}\partial_t W^\tau + \nabla_{\mathbf{k}}\omega_\tau \cdot \nabla_{\mathbf{x}} W^\tau - \nabla_{\mathbf{x}}\omega_\tau \cdot \nabla_{\mathbf{k}} W^\tau = N^\tau W^\tau - W^\tau N^\tau \\ W^\tau_{ij}(0,\mathbf{x},\mathbf{k}) = \mathrm{Tr}(A\mathbf{u}_0\mathbf{u}_0^* A B^{\tau,ij})\delta(\mathbf{k}-\nabla S_0(\mathbf{x}))\end{cases} \tag{3.17}$$

with instead solving both

$$\begin{cases}\mathcal{L}U^\tau = N^\tau U^\tau - U^\tau N^\tau \\ U^\tau(0,\mathbf{x},\mathbf{k})_{ij} = \mathrm{Tr}(A\mathbf{u}_0\mathbf{u}_0^* A B^{\tau,ij})\end{cases} \tag{3.18}$$

and

$$\begin{cases}\mathcal{L}\mathbf{g}^\tau = 0 \\ \mathbf{g}^\tau(0,\mathbf{x},\mathbf{k}) = \mathbf{k}-\nabla S_0(\mathbf{x}).\end{cases} \tag{3.19}$$

Next one obtains $W^\tau(t,\mathbf{x},\mathbf{k})$ using

$$W^\tau(t,\mathbf{x},\mathbf{k}) = U^\tau(t,\mathbf{x},\mathbf{k})\delta(\mathbf{g}^\tau(t,\mathbf{x},\mathbf{k})), \tag{3.20}$$

obtains $W^{(0)}(t,\mathbf{x},\mathbf{k})$ using (2.14) and then finally obtains energy density and flux using (2.21) and (2.22) respectively. A method which solves the Liouville equations (3.18) and (3.19) directly is called *Eulerian* whereas a method which solves them along their respective characteristics is *Lagrangian*. Which approach is preferable, Eulerian or Lagrangian, depends greatly on the individual problem and in the following sections we discuss both.

4 The Eulerian Formulation

4.1 d Dimensions

The Eulerian formulation of our method starts by solving (3.18) and (3.19) in $2d$ dimensions. For a given ω_τ we denote the solutions to (3.18) and (3.19) by $U^\tau(t,\mathbf{x},\mathbf{k})$ and $\mathbf{g}^\tau(t,\mathbf{x},\mathbf{k})$ respectively. Once these solutions are obtained, we recover $W^\tau(t,\mathbf{x},\mathbf{k})$ via (3.20) and $W^{(0)}(t,\mathbf{x},\mathbf{k})$ via (2.14). After this, energy density and flux follow from (2.21) and (2.22) respectively which requires detecting the zero set of $\mathbf{g}^\tau$. At the initial time, the zero set of $\mathbf{g}^\tau$ is given by the initial condition in (3.19) and so for each $\mathbf{x}$ there is exactly one $\mathbf{k}$ where $\mathbf{g}^\tau = \mathbf{0}$. We call $\mathbf{g}^\tau$ is *single valued* when this property holds. At some later time, it may be the case that for some $\mathbf{x}$ there are multiple $\mathbf{k}$ where $\mathbf{g}^\tau = \mathbf{0}$ and we call $\mathbf{g}^\tau$ *multiple valued* in this case [4, 13] (see Figure 4.1 for an example of a multiple valued solution). A point $(\mathbf{x},\mathbf{k})$ where $\mathbf{g}^\tau(t,\mathbf{x},\mathbf{k}) = \mathbf{0}$ and

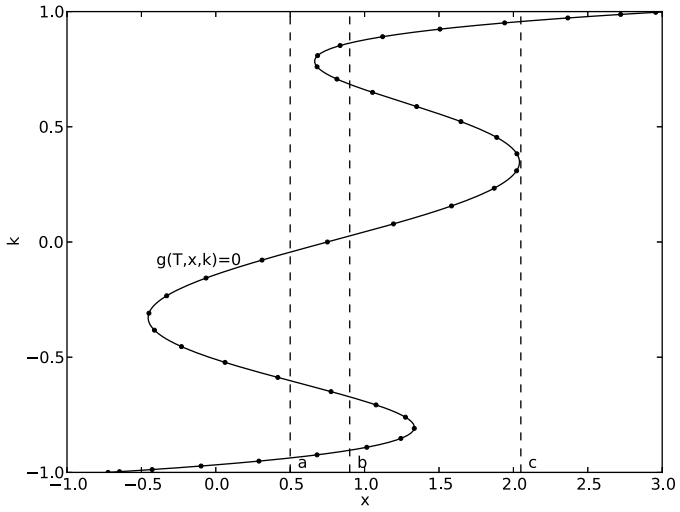

Figure 4.1: In reference to evaluating (5.10) and (5.11), if $x = a$ then $s_a = 3$ and if $x = b$ then $s_b = 5$ (note that τ notation has been dropped for simplicity). In reference to evaluating (5.20) and (5.21), the simplices here are simply the x intervals delineated by the dots along the curve $g(T, x, k) = 0$. If $x = a$ then x falls into 3 distinct intervals and if $x = b$ then x falls into 5 distinct intervals. $x = c$ is an example of a point where $g(T, x, k)$ has a caustic.

$\text{vol}\left(\nabla_{\mathbf{k}}\mathbf{g}^{\tau}(t, \mathbf{x}, \mathbf{k})\right) = 0$ is called a *caustic* and at these points, the energy density (2.21) and flux (2.22) are not well defined (the point $x = c$ in Figure 4.1 is an example of such a point). Away from caustics, however, if we define $K^{\tau}(t, \mathbf{x}) = \{\mathbf{k} : \mathbf{g}^{\tau}(t, \mathbf{x}, \mathbf{k}) = \mathbf{0}\}$ then the energy density and flux may be evaluated at final time $t = T$ as

$$\mathcal{E}^{(0)}(T, \mathbf{x}) = \sum_{\tau} \left[\sum_{\mathbf{k} \in K^{\tau}(T, \mathbf{x})} \frac{1}{2} \text{Tr} \left(A(\mathbf{x}) \frac{\tilde{U}^{\tau}(T, \mathbf{x}, \mathbf{k})}{\text{vol}\left[\nabla_{\mathbf{k}}\mathbf{g}^{\tau}(T, \mathbf{x}, \mathbf{k})\right]} \right) \right] \tag{4.1}$$

and

$$\mathcal{F}_j^{(0)}(T, \mathbf{x}) = \sum_{\tau} \left[\sum_{\mathbf{k} \in K^{\tau}(T, \mathbf{x})} \frac{1}{2} \text{Tr} \left(D^j \frac{\tilde{U}^{\tau}(T, \mathbf{x}, \mathbf{k})}{\text{vol}\left[\nabla_{\mathbf{k}}\mathbf{g}^{\tau}(T, \mathbf{x}, \mathbf{k})\right]} \right) \right] \tag{4.2}$$

respectively where

$$\tilde{U}^{\tau}(t, \mathbf{x}, \mathbf{k}) \equiv \sum_{ij} U_{ij}^{\tau}(t, \mathbf{x}, \mathbf{k}) B^{\tau, ij}(\mathbf{x}, \mathbf{k}) \tag{4.3}$$

is a partially summed version of (2.14).

K^{τ} could be approximated numerically in many ways one of which is the following. Define the fixed square grid in the phase variables by $\mathbf{k}_{\mathbf{z}} = h\mathbf{z}$ where $z_i \in \mathbb{Z}$ and $h > 0$ is the step size. Then for a given $\mathbf{x}$ and $\mathbf{g}^{\tau}(t, \mathbf{x}, \mathbf{k})$, define the sets S_i with $i = 1, ..., d$ by

$$S_i = \{\mathbf{k}_{\mathbf{z}} : g_i^{\tau}(t, \mathbf{x}, \mathbf{k}_{\mathbf{z}}) g_i^{\tau}(t, \mathbf{x}, \mathbf{k}_{\mathbf{z}+\mathbf{e}_i}) < 0\} \tag{4.4}$$

where $\mathbf{e}_i$ is i^{th} unit vector in $\mathbb{R}^d$. Then for sufficiently small h, we have

$$K^{\tau}(t, \mathbf{x}) \approx \cap_{i=1}^{d} S_i. \tag{4.5}$$

Alternately, one could evaluate (2.21) and (2.22) by introducing numerical delta function in (3.20) as is in [5, 6]. This alternate approach avoids the need to find $K^{\tau}(t, \mathbf{x}) = \{\mathbf{k} : \mathbf{g}^{\tau}(t, \mathbf{x}, \mathbf{k}) = \mathbf{0}\}$ explicitly but may introduce more error depending on the numerical delta function used.

To reduce the computational cost of solving the Liouville equations on $2d$ dimensions, one may take advantage of optimized techniques for solving Liouville equations found in, for example, [1, 5, 6, 8, 10, 11]. In particular, the local level set approach allows for computation only around the zero set of $\mathbf{g}^\tau(t, \mathbf{x}, \mathbf{k})$ [10]. Beyond this, in one dimension the computations on two-dimensional phase space can be reduced to just one dimension as seen in Section 4.2.

4.2 One Dimension

In one dimension, $\mathbf{x}, \mathbf{k}$ and $\mathbf{g}^\tau$ are all scalars so will be denoted x, k and g^τ respectively. Since in one dimension k appears as a scalar multiple in the dispersion matrix L given by (2.10), the eigenvalues of L will always be of the form $\omega^\tau(x, k) = k\lambda^\tau(x)$ and the corresponding eigenvectors $\mathbf{b}^\tau$ will always be k independent. Consequently, the coupling matrix N^τ given in (2.18) is also k independent. Finally, from (2.20) it follows that the initial conditions of (3.18) are k independent so that (3.18) reduces to

$$\begin{cases} [\partial_t + \lambda(x)\partial_x]U^\tau = N^\tau U^\tau - U^\tau N^\tau \\ U^\tau(0, x) = \mathcal{A}^\tau(x). \end{cases} \tag{4.6}$$

For g^τ of (3.4) we have the following simple Theorem:

Theorem 4.1. *The solution to*

$$\begin{cases} [\partial_t + \lambda(x)\partial_x - k\lambda'(x)\partial_k]g^\tau = 0 \\ g^\tau(x, k, 0) = k - \partial_x S_0(x) \end{cases} \tag{4.7}$$

may be written as $g^\tau(t, x, k) = k\Gamma_1(t, x) + \Gamma_0(t, x)$ *with* Γ_0 *and* Γ_1 *governed by*

$$\begin{cases} [\partial_t + \lambda(x)\partial_x]\Gamma_0 = 0 \\ \Gamma_0(x, 0) = -\partial_x S_0(x) \end{cases} \tag{4.8}$$

and

$$\begin{cases} [\partial_t + \lambda(x)\partial_x - \lambda'(x)]\Gamma_1 = 0 \\ \Gamma_1(x, 0) = 1 \end{cases} \tag{4.9}$$

respectively.

Proof. The proof is a simple substitution of the assumed form for g^τ into (4.7). □

Already, the computation has been reduced from one on two-dimensional phase space to one dimension but further simplification comes in the post processing steps for finding energy density or flux by noting that

$$\int_{\mathbb{R}} \delta(g^\tau(x, k, t))dk = \int_{\mathbb{R}} \delta(k\Gamma_1(x, t) + \Gamma_0(x, t))dk = \frac{1}{|\Gamma_1(x, t)|} \tag{4.10}$$

so that Γ_0 needs not be computed. Also note that the function $S_0(x)$ is no longer used in the computation. This suggests that in 1D at least, the high frequency limit ($\varepsilon \to 0$) of the energy density and flux is independent of $S_0(x)$. But higher moments of W^τ clearly depend on $S_0(\mathbf{x})$.

In summary, in one dimension, the equations (3.18) and (3.19) reduce to (4.6) and (4.7) respectively. Then (4.7) may be solved by instead solving both (4.8) and (4.9) and then using $g^\tau(t, x, k) = k\Gamma_1(t, x) + \Gamma_0(t, x)$. Thus all computations to acquire $U^\tau(t, x, k)$ and $g^\tau(t, x, k)$ are performed in one dimension.

Remark. The existence of an extension of the decomposition in Theorem 4.1 to higher dimensional space remains an open question.

5 The Lagrangian Formulation

For the Lagrangian formulation, we solve (3.18) and (3.19) by the method of characteristics. Since Theorem 3.1 implies that the only values of $\mathbf{g}^\tau(t, \mathbf{x}, \mathbf{k})$ and $\partial_{k_i}\mathbf{g}^\tau(t, \mathbf{x}, \mathbf{k})$ needed for computing energy density and flux are those along the zero level set of $\mathbf{g}^\tau(t, \mathbf{x}, \mathbf{k})$, we present two possible methods both of which reduce a computation on $2d$-dimensional phase space to d dimensions. Then we discuss the numerical treatment of caustics using the Lagrangian approach.

5.1 The Method of Characteristics

For a given eigenvalue ω_τ the Hamiltonian system defining the bicharacteristics of the Liouville equations (2.17) is (3.7) with initial conditions given by

$$(\mathbf{x}(0), \mathbf{k}(0)) = (\mathbf{x}_0, \nabla_{\mathbf{x}} S_0(\mathbf{x}_0)). \tag{5.1}$$

Note that even though the trajectory of $\mathbf{x}(t)$ and $\mathbf{k}(t)$ depends on the eigenvalue ω^τ, we don't indicate this explicitly. From (3.18), U^τ along the characteristics is governed by

$$\frac{d}{dt} U^\tau(t, \mathbf{x}(t), \mathbf{k}(t)) = N^\tau(t) U^\tau - U^\tau N^\tau(t) \tag{5.2}$$

with the initial conditions

$$U_0^\tau(0, \mathbf{x}(0), \mathbf{k}(0))_{ij} = \mathrm{Tr}[A(\mathbf{x}(0)) \mathbf{u}_0(\mathbf{x}(0)) \mathbf{u}_0^*(\mathbf{x}(0)) A(\mathbf{x}(0)) B^{\tau,ij}(\mathbf{x}(0), \mathbf{k}(0))] \tag{5.3}$$

and where $N^\tau(t) = N^\tau(\mathbf{x}(t), \mathbf{k}(t))$ is the coupling matrix given by (2.18). From (3.19), $\mathbf{g}^\tau$ along the bicharacteristics is governed by

$$\begin{cases} \frac{d}{dt} \mathbf{g}^\tau(t, \mathbf{x}(t), \mathbf{k}(t)) = \mathbf{0} \\ \mathbf{g}^\tau(0, \mathbf{x}(0), \mathbf{k}(0)) = \mathbf{0}. \end{cases} \tag{5.4}$$

For evaluation of the energy density and flux, as shown in (4.1) and (4.2), we also need approximations to $\partial_{k_i} \mathbf{g}^\tau$ at points along the zero set of $\mathbf{g}^\tau$ at the final time. To obtain these, start from (3.19) and take gradients with respect to $\mathbf{x}$ and separately $\mathbf{k}$ to derive, for each component g_i^τ,

$$\begin{cases} \mathcal{L}(\nabla_{\mathbf{x}} g_i^\tau) = -(\nabla_{\mathbf{xk}} \omega_\tau)(\nabla_{\mathbf{x}} g_i^\tau) + (\nabla_{\mathbf{xx}} \omega_\tau)(\nabla_{\mathbf{k}} g_i^\tau) \\ \mathcal{L}(\nabla_{\mathbf{k}} g_i^\tau) = (\nabla_{\mathbf{kx}} \omega_\tau)(\nabla_{\mathbf{k}} g_i^\tau) - (\nabla_{\mathbf{kk}} \omega_\tau)(\nabla_{\mathbf{x}} g_i^\tau) \end{cases} \tag{5.5}$$

where $\mathcal{L}$ is given by (3.1). Then along the characteristics, the above becomes

$$\begin{cases} \frac{d}{dt}(\nabla_{\mathbf{x}} g_i^\tau) = -(\nabla_{\mathbf{xk}} \omega_\tau)(\nabla_{\mathbf{x}} g_i^\tau) + (\nabla_{\mathbf{xx}} \omega_\tau)(\nabla_{\mathbf{k}} g_i^\tau) \\ \frac{d}{dt}(\nabla_{\mathbf{k}} g_i^\tau) = (\nabla_{\mathbf{kx}} \omega_\tau)(\nabla_{\mathbf{k}} g_i^\tau) - (\nabla_{\mathbf{kk}} \omega_\tau)(\nabla_{\mathbf{x}} g_i^\tau), \end{cases} \tag{5.6}$$

with initial conditions given by

$$\begin{cases} \nabla_{\mathbf{x}} g_i^\tau(0, \mathbf{x}(0), \mathbf{k}(0)) = -\partial_{x_i} \nabla_{\mathbf{x}} S_0(\mathbf{x}) \\ \nabla_{\mathbf{k}} g_i^\tau(0, \mathbf{x}(0), \mathbf{k}(0)) = \mathbf{e}_i \end{cases} \tag{5.7}$$

where $\mathbf{e}_i$ is the i^{th} unit vector in $\mathbb{R}^d$. Note that even though we only desire $\nabla_{\mathbf{k}} g_i^\tau$, the fact that (5.6) are coupled requires one to solve for $\nabla_{\mathbf{x}} g_i^\tau$ as well. Now, by solving (3.7), (5.2), and (5.6) for points along the zero set of $\mathbf{g}^\tau$, one can define the *phase space energy density* and *phase space flux* corresponding to eigenvalue ω_τ at $\mathbf{x}(t)$ as

$$\mathcal{E}^\tau(t, \mathbf{x}(t), \mathbf{k}(t)) = \frac{1}{2} \mathrm{Tr} \left(A(\mathbf{x}(\mathbf{t})) \frac{\tilde{U}^\tau(t, \mathbf{x}(t), \mathbf{k}(t))}{\mathrm{vol}\left[\nabla_{\mathbf{k}} \mathbf{g}^\tau(t, \mathbf{x}(t), \mathbf{k}(t))\right]} \right) \tag{5.8}$$

and

$$\mathcal{F}_j^\tau(t, \mathbf{x}(t), \mathbf{k}(t)) = \frac{1}{2} \mathrm{Tr} \left(D^j \frac{\tilde{U}^\tau(t, \mathbf{x}(t), \mathbf{k}(t))}{\mathrm{vol}\left[\nabla_{\mathbf{k}} \mathbf{g}^\tau(t, \mathbf{x}(t), \mathbf{k}(t))\right]} \right) \tag{5.9}$$

respectively with $\tilde{U}^\tau$ defined by (4.3). Note that with the initial condition (5.1), the final point $(\mathbf{x}(t), \mathbf{k}(t))$ is different for each ω_τ so that summing (5.8) and (5.9) over τ is not straight forward as it was in the Eulerian case and may be done analytically via the following construction.

For a given point $\mathbf{x}$, define $(\mathbf{x}_s^\tau(t), \mathbf{k}_s^\tau(t))$ with $s = 1, ..., s_{\mathbf{x}}^\tau$ for some positive integer $s_{\mathbf{x}}^\tau$ as all points with the following properties:

1. The evolution of $(\mathbf{x}_s^\tau(t), \mathbf{k}_s^\tau(t))$ is governed by (3.7) with eigenvalue ω_τ
2. $\mathbf{k}_s^\tau(0) = \nabla S_0(\mathbf{x}_s^\tau(0))$
3. At final time T, $\mathbf{x}_s^\tau(T) = \mathbf{x}$

Note that $s_{\mathbf{x}}^\tau$ denotes the number of branches in the context of multiple valued solutions so that $s_{\mathbf{x}}^\tau = 1$ before caustic formation and $s_{\mathbf{x}}^\tau \geq 0$ after caustic formation (see Figure 4.1 for an illustration in one dimension). Now the energy density and flux at time T may be expressed in terms of phase space energy density and phase space flux ((5.17) and (5.18) respectively) as

$$\mathcal{E}^{(0)}(T, \mathbf{x}) = \sum_\tau \sum_{s=1}^{s_{\mathbf{x}}^\tau} \mathcal{E}^\tau(T, \mathbf{x}, \mathbf{k}_s^\tau(T)) \tag{5.10}$$

and

$$\mathcal{F}_j^{(0)}(T, \mathbf{x}) = \sum_\tau \sum_{s=1}^{s_{\mathbf{x}}^\tau} \mathcal{F}_j^\tau(T, \mathbf{x}, \mathbf{k}_s^\tau(T)) \tag{5.11}$$

respectively. Finding all the points $(\mathbf{x}_s^\tau(t), \mathbf{k}_s^\tau(t))$ which satisfy the above three conditions is not necessarily easy. Because of this, in Section 5.3 we will introduce a more practical method to obtain energy density and flux from these so called phase space energy density and phase space flux before and after $\mathbf{g}^\tau$ forms caustics.

Even though we only need to solve (3.7), (5.2) and (5.6) for points on the set of $\mathbf{g}^\tau$, the addition of the $2d^2$ coupled ordinary differential equations (ODE) in (5.6) is a significant increase in computation. For example, in three dimensions, (5.6) represents 18 coupled ODEs! To avoid solving this considerable number of ODE, we present a geometric method next which avoids these ODEs completely.

5.2 A Geometric Method

Here we present a method that entirely avoids solving any ODE beyond (3.7) and (5.2). In particular, we will show that one may use the solution to (3.7) and (5.2) to solve for the $\text{vol}\left[\nabla_{\mathbf{k}} \mathbf{g}^\tau(t, \mathbf{x}(t), \mathbf{k}(t))\right]$ term needed for evaluating both (5.8) and (5.9).

Just as in Section 3.1, define the Hamiltonian flow $H_t(\mathbf{x}_0, \mathbf{k}_0)$ which evolves any point in $(\mathbf{x}_0, \mathbf{k}_0)$ phase space forward to time t according the Hamiltonian system (3.7). Also define the pair of coordinates related by $(t, \mathbf{x}, \mathbf{k}) = (t, H_t(\mathbf{x}_0, \mathbf{k}_0))$ the determinant of the Jacobian of the transform $(t, \mathbf{x}_0, \mathbf{k}_0) \mapsto (t, \mathbf{x}, \mathbf{k})$ is 1. If one parameterizes the zero set of $\mathbf{g}^\tau$ so that $\mathbf{g}^\tau(0, \mathbf{x}_0(\mathbf{s}), \mathbf{k}_0(\mathbf{s})) = \mathbf{0}$, then $\mathbf{g}^\tau(t, H_t(\mathbf{x}_0(\mathbf{s}), \mathbf{k}_0(\mathbf{s}))) = \mathbf{0}$ parameterizes the zero set for all time. At a fixed time t, denote the Jacobian for the transform H_t as DH_t. Then

$$\nabla_{\mathbf{s}} \begin{pmatrix} \mathbf{x} \\ \mathbf{k} \end{pmatrix} = (DH_t) \nabla_{\mathbf{s}} \begin{pmatrix} \mathbf{x}_0 \\ \mathbf{k}_0 \end{pmatrix} \tag{5.12}$$

and

$$\begin{pmatrix} [\nabla_{\mathbf{x_0}} \mathbf{g}^\tau(0, \mathbf{x}_0, \mathbf{k}_0)]^T \\ [\nabla_{\mathbf{k_0}} \mathbf{g}^\tau(0, \mathbf{x}_0, \mathbf{k}_0)]^T \end{pmatrix} = (DH_t)^T \begin{pmatrix} [\nabla_{\mathbf{x}} \mathbf{g}^\tau(t, \mathbf{x}, \mathbf{k})]^T \\ [\nabla_{\mathbf{k}} \mathbf{g}^\tau(t, \mathbf{x}, \mathbf{k})]^T \end{pmatrix}. \tag{5.13}$$

Note that each column vector in $\nabla_{\mathbf{s}} \begin{pmatrix} \mathbf{x} \\ \mathbf{k} \end{pmatrix}$ is perpendicular to each column vector in $\begin{pmatrix} [\nabla_{\mathbf{x}} \mathbf{g}^\tau(t, \mathbf{x}, \mathbf{k})]^T \\ [\nabla_{\mathbf{k}} \mathbf{g}^\tau(t, \mathbf{x}, \mathbf{k})]^T \end{pmatrix}$ and that each column vector in $\nabla_{\mathbf{s}} \begin{pmatrix} \mathbf{x}_0 \\ \mathbf{k}_0 \end{pmatrix}$ is perpendicular to each column vector in $\begin{pmatrix} [\nabla_{\mathbf{x_0}} \mathbf{g}^\tau(0, \mathbf{x}_0, \mathbf{k}_0)]^T \\ [\nabla_{\mathbf{k_0}} \mathbf{g}^\tau(0, \mathbf{x}_0, \mathbf{k}_0)]^T \end{pmatrix}$. We seek to establish useful relationships between the vectors appearing in (5.12) and (5.13) and to this end we prove a few linear algebra results which appear in the Appendix. In light of these results, we note that these sets of vectors seen in (5.12) and (5.13) match the statement of Theorem 8.2 with $\alpha = 2d$ and $\beta = d$ (see the Appendix). Since $\det(DH_t) = 1$, we conclude that

$$\text{vol}\left(\nabla_{\mathbf{s}} \begin{pmatrix} \mathbf{x} \\ \mathbf{k} \end{pmatrix}\right) \text{vol}\begin{pmatrix} [\nabla_{\mathbf{x_0}} \mathbf{g}^\tau(0, \mathbf{x}_0, \mathbf{k}_0)]^T \\ [\nabla_{\mathbf{k_0}} \mathbf{g}^\tau(0, \mathbf{x}_0, \mathbf{k}_0)]^T \end{pmatrix} = \text{vol}\left(\nabla_{\mathbf{s}} \begin{pmatrix} \mathbf{x}_0 \\ \mathbf{k}_0 \end{pmatrix}\right) \text{vol}\begin{pmatrix} [\nabla_{\mathbf{x}} \mathbf{g}^\tau(t, \mathbf{x}, \mathbf{k})]^T \\ [\nabla_{\mathbf{k}} \mathbf{g}^\tau(t, \mathbf{x}, \mathbf{k})]^T \end{pmatrix}. \tag{5.14}$$

Then Corollary 8.3 (see the Appendix) establishes that

$$\mathrm{vol}\left(\nabla_{\mathbf{s}}\mathbf{x}\right)\mathrm{vol}\left(\nabla_{\mathbf{k_0}}\mathbf{g}^{\tau}(0,\mathbf{x}_0,\mathbf{k}_0)\right)=\mathrm{vol}\left(\nabla_{\mathbf{s}}\mathbf{x}_0\right)\mathrm{vol}\left(\nabla_{\mathbf{k}}\mathbf{g}^{\tau}(t,\mathbf{x},\mathbf{k})\right). \tag{5.15}$$

Now every term in (5.15) except the term $\mathrm{vol}\left(\nabla_{\mathbf{k}}\mathbf{g}^{\tau}(t,\mathbf{x},\mathbf{k})\right)$ may be computed exactly or approximately by simply solving (3.7) on a grid of points so that we obtain an approximation to $\mathrm{vol}\left(\nabla_{\mathbf{k}}\mathbf{g}^{\tau}(t,\mathbf{x},\mathbf{k})\right)$ without evolving $\nabla_{\mathbf{k}}\mathbf{g}^{\tau}(t,\mathbf{x},\mathbf{k})$ by the ODE system (5.6)!

We start our computation with the initial grid given by $\mathbf{x}_{\mathbf{z}}(0)=\{h\mathbf{z}:z_1,z_2,...,z_d\in[-N,...,N]\}$ so that the corresponding points for $\mathbf{k}$ are given by $\mathbf{k}_{\mathbf{z}}(0)=\nabla S_0(\mathbf{x}_{\mathbf{z}})$. For each eigenvalue ω_τ define the evolution of the grid points according to (3.7) to a time t as $\mathbf{x}_{\mathbf{z}}^{\tau}(t)$ and $\mathbf{k}_{\mathbf{z}}^{\tau}(t)$. Next solve for $U^{\tau}(t,\mathbf{x}_{\mathbf{z}}^{\tau}(t),\mathbf{k}_{\mathbf{z}}^{\tau}(t))$ using using the ODE (5.2). Then by using the initial conditions for $\mathbf{g}^{\tau}$ given in (3.19), (5.15) may be written as

$$\mathrm{vol}\left(\nabla_{\mathbf{s}}\mathbf{x}\right)\times 1=1\times\mathrm{vol}\left(\nabla_{\mathbf{k}}\mathbf{g}^{\tau}(t,\mathbf{x},\mathbf{k})\right) \tag{5.16}$$

so that for each eigenvalue ω_τ, the phase space energy density and phase space flux on the grid $\mathbf{x}_{\mathbf{z}}^{\tau}(t)$ may be written as

$$\begin{aligned}\mathcal{E}^{\tau}(t,\mathbf{x}_{\mathbf{z}}^{\tau}(t),\mathbf{k}_{\mathbf{z}}^{\tau}(t)) &= \frac{1}{2}\mathrm{Tr}\left(A(\mathbf{x}_{\mathbf{z}}^{\tau}(t))\frac{\tilde{U}^{\tau}(t,\mathbf{x}_{\mathbf{z}}^{\tau}(t),\mathbf{k}_{\mathbf{z}}^{\tau}(t))}{\mathrm{vol}\left[\nabla_{\mathbf{k}}\mathbf{g}^{\tau}(t,\mathbf{x}_{\mathbf{z}}^{\tau}(t),\mathbf{k}_{\mathbf{z}}^{\tau}(t))\right]}\right)\\ &= \frac{1}{2}\mathrm{Tr}\left(A(\mathbf{x}_{\mathbf{z}}^{\tau}(t))\frac{\tilde{U}^{\tau}(t,\mathbf{x}_{\mathbf{z}}^{\tau}(t),\mathbf{k}_{\mathbf{z}}^{\tau}(t))}{\mathrm{vol}\left[\nabla_{\mathbf{s}}\mathbf{x}_{\mathbf{z}}^{\tau}(t)\right]}\right)\end{aligned} \tag{5.17}$$

and

$$\begin{aligned}\mathcal{F}_j^{\tau}(t,\mathbf{x}_{\mathbf{z}}^{\tau}(t),\mathbf{k}_{\mathbf{z}}^{\tau}(t)) &= \frac{1}{2}\mathrm{Tr}\left(D^j\frac{\tilde{U}^{\tau}(t,\mathbf{x}_{\mathbf{z}}^{\tau}(t),\mathbf{k}_{\mathbf{z}}^{\tau}(t))}{\mathrm{vol}\left[\nabla_{\mathbf{k}}\mathbf{g}^{\tau}(t,\mathbf{x}_{\mathbf{z}}^{\tau}(t),\mathbf{k}_{\mathbf{z}}^{\tau}(t))\right]}\right)\\ &= \frac{1}{2}\mathrm{Tr}\left(D^j\frac{\tilde{U}^{\tau}(t,\mathbf{x}_{\mathbf{z}}^{\tau}(t),\mathbf{k}_{\mathbf{z}}^{\tau}(t))}{\mathrm{vol}\left[\nabla_{\mathbf{s}}\mathbf{x}_{\mathbf{z}}^{\tau}(t)\right]}\right)\end{aligned} \tag{5.18}$$

where $\tilde{U}^{\tau}$ is defined by (4.3) and $\nabla_{\mathbf{s}}\mathbf{x}_{\mathbf{z}}^{\tau}(t)$ here may be approximated as the $d\times d$ matrix given by

$$\frac{1}{2h^d}\begin{pmatrix}\mathbf{x}^{\tau}_{(z_1+1,z_2,\ldots,z_d)}(t)-\mathbf{x}^{\tau}_{(z_1-1,z_2,\ldots,z_d)}(t) & \cdots & \mathbf{x}^{\tau}_{(z_1,z_2,\ldots,z_d+1)}(t)-\mathbf{x}^{\tau}_{(z_1,z_2,\ldots,z_d-1)}(t)\end{pmatrix}. \tag{5.19}$$

In summary, for a given eigenvalue ω_τ and by use of Theorem 8.2, $\partial_{k_i}\mathbf{g}^{\tau}(t,\mathbf{x}(t),\mathbf{k}(t))$ may be approximated by simply solving the characteristic equations (3.7) on an initial grid $\mathbf{x}_{\mathbf{z}}$. But this must be done anyway to solve $U^{\tau}(t,\mathbf{x}(t),\mathbf{k}(t))$, thus the approximation to $\partial_{k_i}\mathbf{g}^{\tau}(t,\mathbf{x}(t),\mathbf{k}(t))$ is obtained for free and without additional computation. Again, in Section 5.3 we will show how to obtain energy density and flux from these so called phase space energy density and phase space flux before and after $\mathbf{g}^{\tau}$ forms caustics.

Remark. We observe that some elements of this geometric method relate to those presented in [9] which rely on the property of conservation of "charge", but the equations studied therein are homogeneous scalar Liouville equations whereas here we have introduced a method for coupled systems of inhomogeneous Liouville equations of the form (3.2) in which "charge" is not conserved. Thus this method is more general than that in [9].

5.3 Summing Before or After Caustic Formation

We now show how to obtain energy density (2.21) and flux (2.22) from the phase space energy density and phase space flux defined by (5.17) and (5.18) respectively before or after the formation of caustics.

As in Section 5.2, define an initial mesh $\mathbf{x}_{\mathbf{z}}(0)=\{h\mathbf{z}:z_1,z_2,...,z_d\in[-N,...,N]\}$ so that the corresponding points for $\mathbf{k}$ are given by $\mathbf{k}_{\mathbf{z}}(0)=\nabla S_0(\mathbf{x}_{\mathbf{z}})$. For each eigenvalue ω_τ define the evolution of the grid points according to (3.7) to a time t as $\mathbf{x}_{\mathbf{z}}^{\tau}(t)$ and $\mathbf{k}_{\mathbf{z}}^{\tau}(t)$. Then solving for phase space energy density and flux for the eigenvalue ω_τ is given by (5.17) and (5.18). The grid at the final time T given by $\mathbf{x}_{\mathbf{z}}^{\tau}(T)$ and $\mathbf{k}_{\mathbf{z}}^{\tau}(T)$ is different in general for each τ. Also for each τ, the phase space energy density and flux at final time T give by (5.17) and (5.18) are possibly multiple valued. Thus to evaluate the energy density and flux at any $\mathbf{x}$,

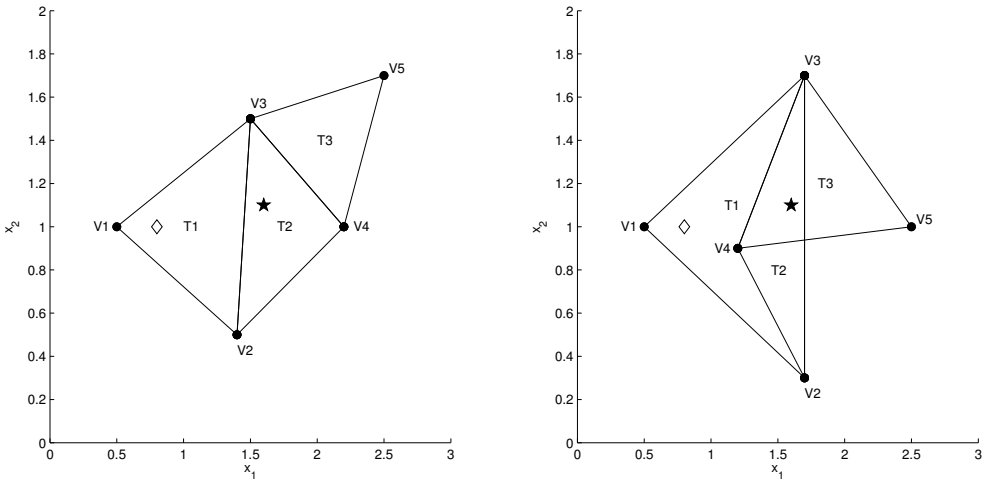

Figure 5.1: The left plot shows a triangulation on an initial grid of 5 points at $t = 0$. The right plot shows the data set at a later time $T > 0$. At the initial time, the three triangles do not overlap whereas at the later time, the solution has become multiple valued and the triangles do overlap (in particular, $T2$ lies completely inside of $T1$). To evaluate the energy density, for example, at the point $\diamondsuit$ at time T, observe that the $\diamondsuit$ lies in triangle $T1$ only. Thus use the energy density at the vertices of $T1$ to interpolate the value at $\diamondsuit$. To evaluate the energy density, at the point $\star$ at time T, however, observe that the $\star$ lies in triangles $T1$, $T2$ and $T3$. Thus one must use the energy density at the vertices of each triangle to interpolate the value at $\star$ three times (once for each triangle) and then sum the results together as indicated by (5.20).

first one must fix τ and sum (5.17) and (5.18) over all of branches and second one must sum all these results over τ. A systematic way to compute this summation is described next.

Define a triangulation of the initial grid $\mathbf{x}_{\mathbf{z}}^{\tau}(0)$ as $\mathcal{T}_{\tau}(0)$ where each member of $\mathcal{T}_{\tau}(0)$ is a simplex of dimension d denoted by its $d+1$ vertices which are members of $\mathbf{x}_{\mathbf{z}}^{\tau}(0)$. Then denote by $\mathcal{T}_{\tau}(t)$ the collection of simplices who have the corresponding vertices in $\mathbf{x}_{\mathbf{z}}^{\tau}(t)$. Note that for $t > 0$, $\mathcal{T}_{\tau}(t)$ may not be a proper triangulation since its simplices may overlap one another (see Figure 4.1 for a one dimensional illustration and Figure 5.1 for a two dimensional illustration). Further note that such an overlap occurs exactly when $\mathbf{g}^{\tau}$ becomes multiple valued. If a point $\mathbf{x}$ falls inside of a simplex $\mathcal{S} \in \mathcal{T}_{\tau}(t)$ then since the solution to (5.17) and (5.18) has been computed at the vertices of $\mathcal{S}$, denote the linear interpolation of phase space energy density and phase space flux onto the point $\mathbf{x}$ relative to the vertices of $\mathcal{S}$ as $\mathcal{LI}[\mathcal{E}^{\tau}(t, \mathbf{x}_{\mathbf{z}}^{\tau}(t), \mathbf{k}_{\mathbf{z}}^{\tau}(t)), \mathcal{S}, \mathbf{x}]$ and $\mathcal{LI}[\mathcal{F}_j^{\tau}(t, \mathbf{x}_{\mathbf{z}}^{\tau}(t), \mathbf{k}_{\mathbf{z}}^{\tau}(t)), \mathcal{S}, \mathbf{x}]$ respectively. Then finally one obtains the energy density and flux at the point $\mathbf{x}$ by

$$\mathcal{E}^{(0)}(T, \mathbf{x}) = \sum_{\tau} \left[\sum_{\{S \in \mathcal{T}_{\tau}(t) : \mathbf{x} \in S\}} \mathcal{LI}[\mathcal{E}^{\tau}(T, \mathbf{x}_{\mathbf{z}}^{\tau}(T), \mathbf{k}_{\mathbf{z}}^{\tau}(T)), \mathcal{S}, \mathbf{x}] \right] \tag{5.20}$$

and

$$\mathcal{F}_j^{(0)}(T, \mathbf{x}) = \sum_{\tau} \left[\sum_{\{S \in \mathcal{T}_{\tau}(t) : \mathbf{x} \in S\}} \mathcal{LI}[\mathcal{F}_j^{\tau}(T, \mathbf{x}_{\mathbf{z}}^{\tau}(T), \mathbf{k}_{\mathbf{z}}^{\tau}(T)), \mathcal{S}, \mathbf{x}] \right] \tag{5.21}$$

respectively.

Remark. This triangulation method has been implemented in our numerical examples and some additional details about this approach can be found in [9].

6 Numerical Results

The following few examples show the effectiveness of the Eulerian and Lagrangian formulations in one and two dimensions and are based on two model problems shown below.

6.1 One-Dimensional Model Problem

The following model system is one of the most simple one-dimensional systems which has repeated eigenvalues of the dispersion matrix as well as a nontrivial coupling matrix.

In reference to (1.1) define $D^1 = I$ and $A(x)$ where

$$A^{-1} = RMR^T \tag{6.1}$$

with

$$M = \begin{pmatrix} a & b & b \\ b & a & b \\ b & b & a \end{pmatrix} \tag{6.2}$$

and

$$R = \begin{pmatrix} \cos(\theta) & -\sin(\theta) & 0 \\ \sin(\theta) & \cos(\theta) & 0 \\ 0 & 0 & 1 \end{pmatrix} \tag{6.3}$$

where we assume that $0 < b < a$ and that a, b, θ are arbitrary function of x. The eigenvalues and eigenvectors of the dispersion matrix L orthonormal with respect to $\langle \cdot, \cdot \rangle_A$ are

$$\begin{cases} \omega_1 = k(a-b) & \mathbf{b}^{1,1} = \sqrt{a-b} R \mathbf{v}_{1,1} \\ & \mathbf{b}^{1,2} = \sqrt{a-b} R \mathbf{v}_{1,2} \\ \omega_2 = k(a+2b) & \mathbf{b}^{2} = \sqrt{a+2b} R \mathbf{v}_{2} \end{cases} \tag{6.4}$$

where

$$\begin{cases} \mathbf{v}_{1,1} = \frac{1}{\sqrt{2}}(1, 0, -1) \\ \mathbf{v}_{1,2} = \frac{1}{\sqrt{6}}(1, -2, 1) \\ \mathbf{v}_{2} = \frac{1}{\sqrt{3}}(1, 1, 1). \end{cases} \tag{6.5}$$

The coupling matrix for ω_1 is

$$N^1 = \begin{pmatrix} 0 & \frac{(a-b)\theta'}{\sqrt{3}} \\ -\frac{(a-b)\theta'}{\sqrt{3}} & 0 \end{pmatrix}. \tag{6.6}$$

Example 1

In this example we demonstrate the convergence of the full solution of (1.1) to the solution obtained via our new method in the high frequency limit ($\varepsilon \to 0$). We take the following parameters

- $\theta(x) = 10 \sin(2\pi x)$
- $a = 2$, $b = 1$
- domain: $x \in [-.5, .5]$
- boundary conditions: periodic in x and not needed in k
- Initial conditions $\mathbf{u}_0(x) = (e^{-40 \tan(\pi x)^2}, 0, 0)$, $S_0(x) = x$, $\varepsilon = 1/(40\pi)$ and $\varepsilon = 1/(100\pi)$
- Final time: $t_f = .05$

Remark. Boundary conditions are not needed in k because of the reduction of dimension we derived in Section 4.

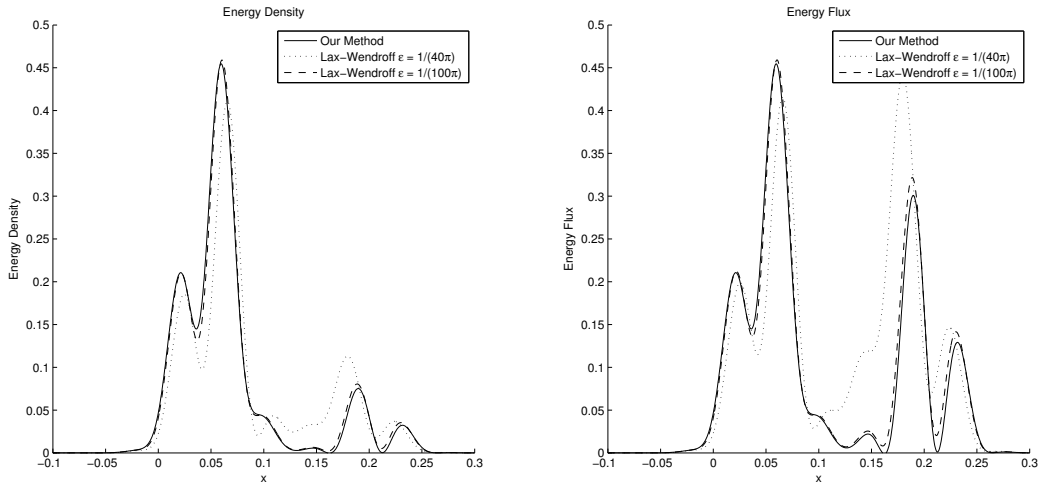

Figure 6.1: (Example 1) Energy density and energy flux of the one-dimensional model problem comparing the full solution to our new method's solution in the high frequency limit.

The full solution on the original system was computed using the Lax-Wendroff scheme and the solution from our new method was computed in the Eulerian frame using the simplifications outlined in Sections 3 and 4. The results are shown in Figure 6.1 where the Lax-Wendroff solution is seen to be converging to our new method's solution as ε decreases.

Example 2

Next we show an example where a, b are no longer constants and take the following parameters:

- $\theta(x) = \sin(2\pi x)$
- $a = 2(.5 + .4\sin(4\pi x))$, $b = (.5 + .4\sin(4\pi x))$
- domain: $x \in [-.5, .5]$
- boundary conditions: periodic in x and not needed in k
- Initial conditions $\mathbf{u}_0(x) = (e^{-40\tan(\pi x)^2}, 0, 0)$, $S_0(x) = x$, $\epsilon = 1/(40\pi)$
- Final time: $t_f = .05$

The full solution on the original system was computed using the Lax-Wendroff scheme while our new method's solution was computed in the Eulerian frame using the simplifications outlined in Section 3. The results (which show as good agreement) are shown in Figure 6.2.

Remark. We also computed Example 1 and 2 with the Lagrangian formulation of our method using the interpolation described in Section 5.3 and we obtained similar results.

6.2 Two-Dimensional Model Problem

The following model system is a two-dimensional analogue of Maxwell's equations which are shown in [12].

In reference to (1.1) define

$$A = \begin{pmatrix} 1/a & 0 & 0 & 0 \\ 0 & 1/a & 0 & 0 \\ 0 & 0 & 1/b & 0 \\ 0 & 0 & 0 & 1/b \end{pmatrix}, \quad D^1 = \begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{pmatrix}, \quad D^2 = \begin{pmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & -1 & 0 \\ 0 & -1 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{pmatrix} \tag{6.7}$$

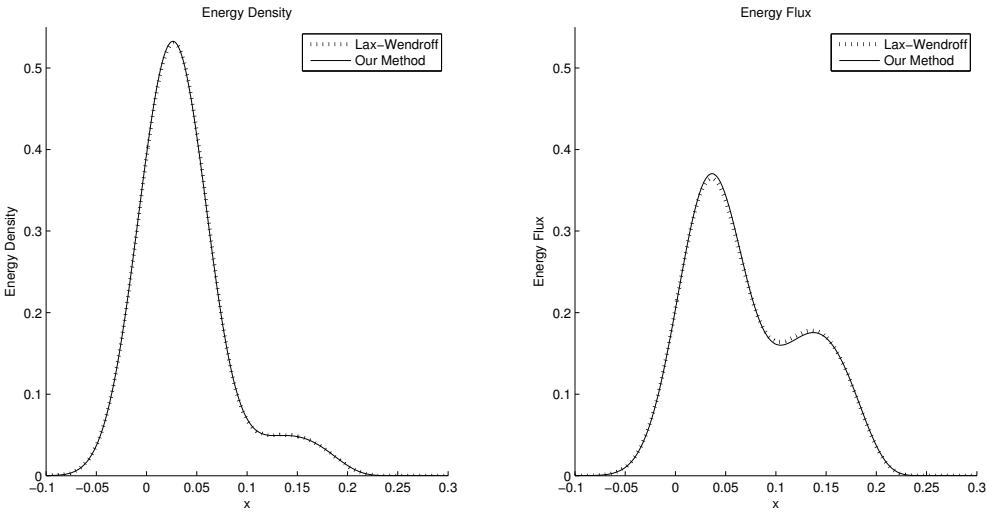

Figure 6.2: (Example 2) Energy density of the one-dimensional model problem with non-constant a and b functions.

where $a, b > 0$ are arbitrary functions of $\mathbf{x}$. The dispersion matrix is

$$L(\mathbf{x}, \mathbf{k}) = \begin{pmatrix} 0 & 0 & ak_1 & ak_2 \\ 0 & 0 & -ak_2 & ak_1 \\ bk_1 & -bk_2 & 0 & 0 \\ bk_2 & bk_1 & 0 & 0 \end{pmatrix} \tag{6.8}$$

The eigenvalues and eigenvectors of the dispersion matrix orthonormal with respect to $\langle \cdot, \cdot \rangle_A$ are

$$\begin{cases} \omega_1 = -\sqrt{ab}\sqrt{k_1^2 + k_2^2} & \mathbf{b}^{1,1} = \left(-\sqrt{\frac{a}{2}} \frac{k_2}{\sqrt{k_1^2+k_2^2}}, -\sqrt{\frac{a}{2}} \frac{k_1}{\sqrt{k_1^2+k_2^2}}, 0, \sqrt{\frac{b}{2}} \right) \\ & \mathbf{b}^{1,2} = \left(-\sqrt{\frac{a}{2}} \frac{k_1}{\sqrt{k_1^2+k_2^2}}, \sqrt{\frac{a}{2}} \frac{k_2}{\sqrt{k_1^2+k_2^2}}, \sqrt{\frac{b}{2}}, 0 \right) \\ \omega_2 = \sqrt{ab}\sqrt{k_1^2 + k_2^2} & \mathbf{b}^{2,1} = \left(\sqrt{\frac{a}{2}} \frac{k_2}{\sqrt{k_1^2+k_2^2}}, \sqrt{\frac{a}{2}} \frac{k_1}{\sqrt{k_1^2+k_2^2}}, 0, \sqrt{\frac{b}{2}} \right) \\ & \mathbf{b}^{2,2} = \left(\sqrt{\frac{a}{2}} \frac{k_1}{\sqrt{k_1^2+k_2^2}}, -\sqrt{\frac{a}{2}} \frac{k_2}{\sqrt{k_1^2+k_2^2}}, \sqrt{\frac{b}{2}}, 0 \right) \end{cases} \tag{6.9}$$

The coupling matrix for ω_1 is

$$N^1 = \begin{pmatrix} 0 & \frac{1}{2}\sqrt{\frac{b}{a}} \frac{1}{\sqrt{k_1^2+k_2^2}} (a_{x_1} k_2 - a_{x_2} k_1) \\ -\frac{1}{2}\sqrt{\frac{b}{a}} \frac{1}{\sqrt{k_1^2+k_2^2}} (a_{x_1} k_2 - a_{x_2} k_1) & 0 \end{pmatrix} \tag{6.10}$$

and $N^2 = -N^1$.

Remark. When $\mathbf{k} = \mathbf{0}$ in the one and two-dimensional model problems, the multiplicity of the eigenvalues changes; This violates the assumption we made when we developed our new method. This issue is resolved by the fact that in solving via our new method, $\mathbf{g}(t, \mathbf{x}, \mathbf{k})$ given by (3.19) is initialized with zero set away from the origin so conservation of energy of Hamiltonian flows guarantees that this zero set stays away from the origin for all time. Thus even though the origin may be part of the computational domains of (3.18) and (3.19), it will not be used for evaluating the physical observables via (2.7) and (2.8). [5] also discusses this issue in further detail.

Example 3

In this example, we show a solution to the two-dimensional model problem computed with the Lagrangian formulation of our new method outlined in Section 5. Since our new method is tailored to compute multiple valued observables, we choose an example where the solution to (3.4) becomes multiple valued; something that never happens in one dimension. We take the following parameters:

- $a(x_1, x_2) = .5 + .4\cos(4\pi x_1)\sin(4\pi(x_2))$, $b(x_1, x_2) = 1$
- domain: $(x_1, x_2) \in [-.5, .5] \times [-.5, .5]$
- boundary conditions: periodic in x_1 and x_2.
- Initial conditions $\mathbf{u}_0(x_1, x_2) = (e^{-5(\tan(\pi x_1)^2 + \tan(\pi(x_2+.05))^2)}, 0, 0, 0)$, $S_0(x_1, x_2) = x_1 + x_2$
- Final time: $t_f = .08, .16, .24, .32$

The result is shown in Figure 6.3 where we have chosen to plot the energy density. The two components of the flux for the final time $t = .32$ are shown in Figure 6.4. A three-dimensional projection of the zero set of $\mathbf{g}^1$ corresponding to ω_1 at the final time is shown in Figure 6.5, as well as a contour plot of the same surface. The contour plot shows the multiple valued regions in the $\mathbf{x}$ space which correspond to the caustics appearing in Figure 6.3. A reference solution with $\varepsilon = 1/(80\pi)$ was computed and found to have a good agreement with our method until time neared the caustic formation time $t = .24$ which is what we expect. Computing a reference solution with a standard finite difference method for $\varepsilon = 1/(80\pi)$ after caustic formation was not computationally feasible due to heavy diffusion of these methods for this example. Thus we computed, for sake of comparison, the exact solution for $t = .32$ and $\varepsilon = 1/(80\pi)$ using a Gaussian beam type method which we will introduce in a forthcoming paper. The result may be seen in Figure 6.6 where one sees interference fringes appearing in the multiple valued region of the solution. As ε shrinks, the interference fringes in this region is expected to limit weakly to the solution shown in Figure 6.3.

7 Conclusion

We have extended the singularity decomposition idea in [5] to the case of high frequency solutions of symmetric hyperbolic systems with repeated eigenvalues of the dispersion matrix in both Eulerian and Lagrangian frameworks. Such problems arise in many physically important problems such as Maxwell's equations and the elastic wave equations. Furthermore we introduce a highly efficient Lagrangian method with a geometric reduction of computational complexity to the numerical evaluation of the energy and energy flux. Numerical examples in both one and two space dimensions are given to show the validity of the new computational methods.

8 Appendix: A Few Linear Algebra Identities

Lemma 8.1. *Suppose M is an $\alpha \times \alpha$ matrix with $\det(M) \neq 0$. Write M and M^{-1} in block form as*

$$M = \begin{pmatrix} A & B \\ C & D \end{pmatrix} \quad \text{and} \quad M^{-1} = \begin{pmatrix} \tilde{A} & \tilde{B} \\ \tilde{C} & \tilde{D} \end{pmatrix} \tag{8.1}$$

where A and $\tilde{A}$ are $\beta \times \beta$ matrices for some $\beta < \alpha$. Then

$$\det(A) = \det(M)\det(\tilde{D}). \tag{8.2}$$

Proof. Examine the two cases:
Case: Assume that $\det(A) = 0$. Then there exists $\mathbf{v}_a \neq \mathbf{0}$ where $A\mathbf{v}_a = \mathbf{0}$ so take

$$\begin{pmatrix} A & B \\ C & D \end{pmatrix} \begin{pmatrix} \mathbf{v}_a \\ \mathbf{0} \end{pmatrix} = \begin{pmatrix} \mathbf{0} \\ C\mathbf{v}_a \end{pmatrix} \tag{8.3}$$

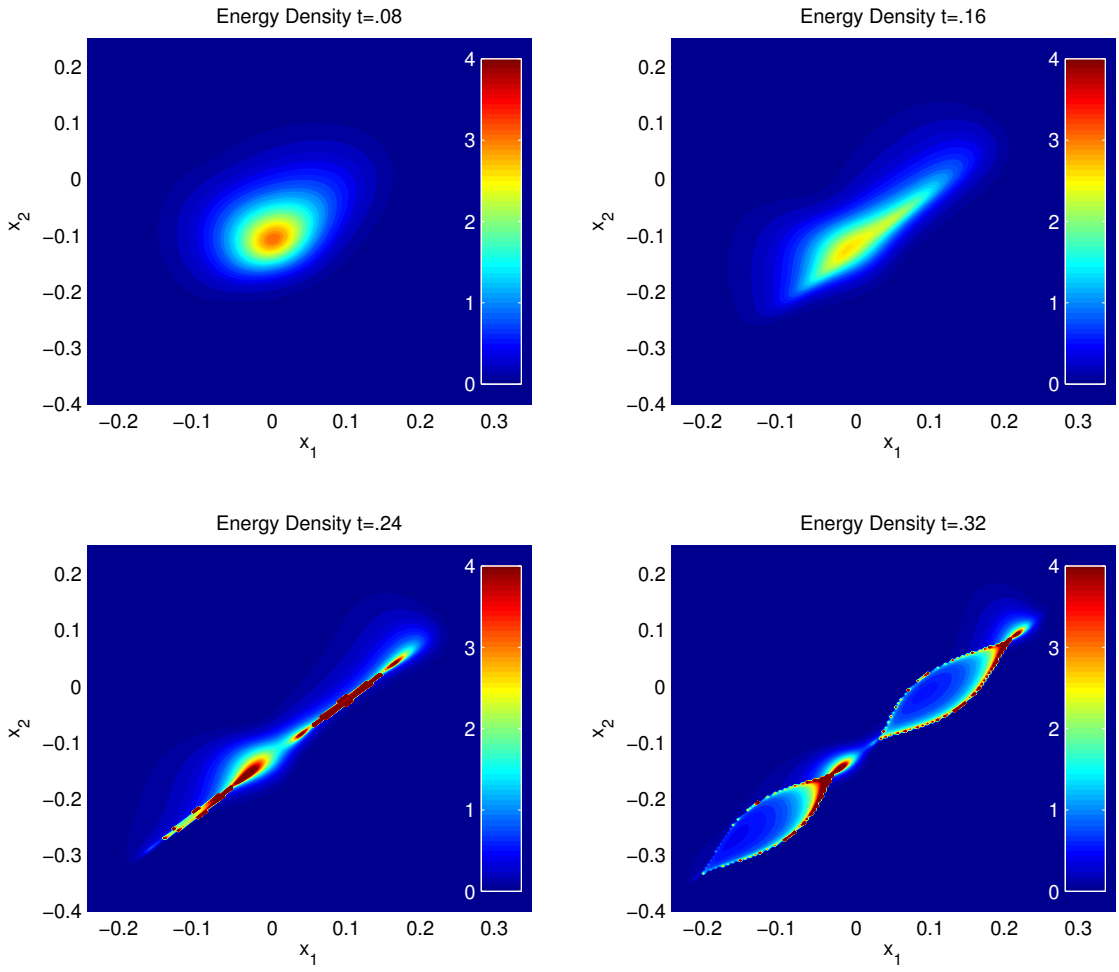

Figure 6.3: (Example 3) Energy density plotted at different times. Caustics form around $t = .24$.

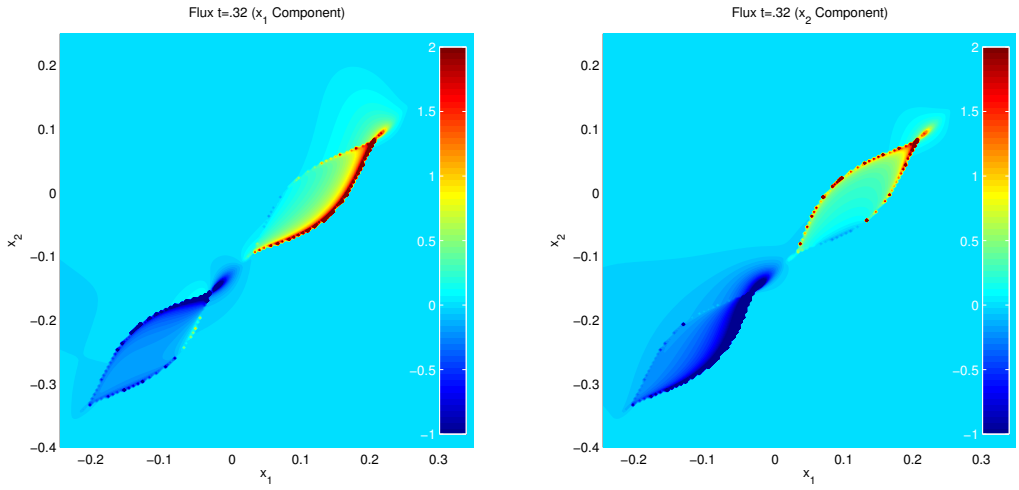

Figure 6.4: (Example 3) The two components of energy flux at time $t = .32$.

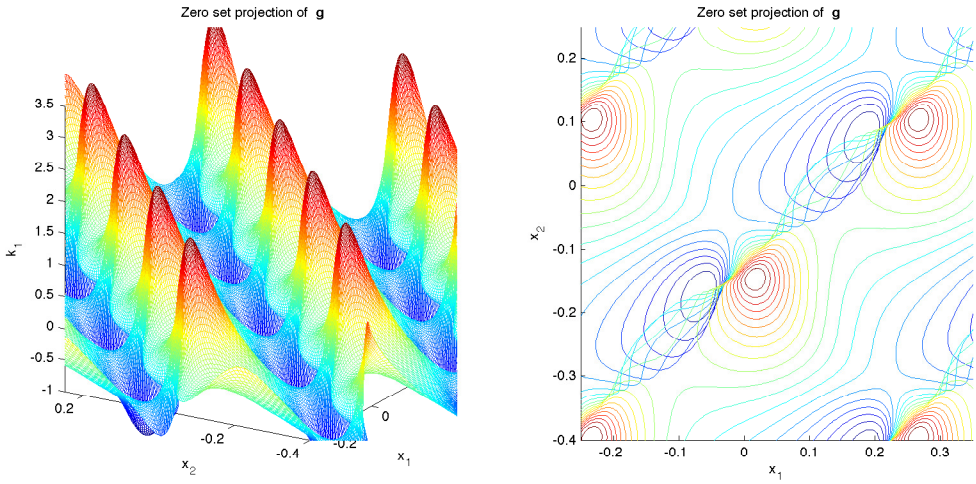

Figure 6.5: (Example 3) Zero set projection of the $\mathbf{g}^1$ function corresponding to ω_1. On the left, the multiple valued surface is projected into three dimensions by plotting x_1, x_2 versus k_1. On the right, the same surface is represented as a contour plot with axis limits set equal to those in Figure 6.3 and Figure 6.4 for comparison.

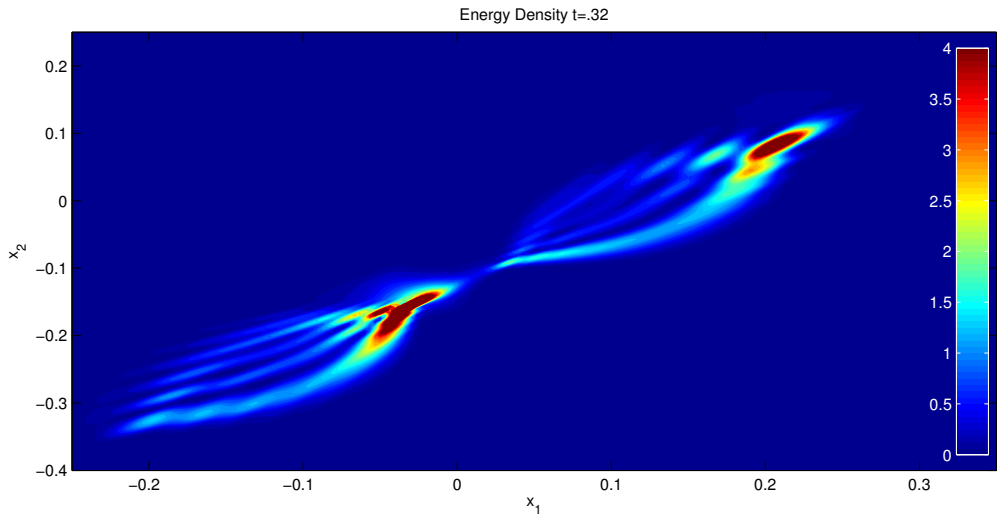

Figure 6.6: (Example 3) Energy density at $t = .32$ with $\varepsilon = 1/(80\pi)$ computed with Gaussian beams.

where $C\mathbf{v}_a \neq \mathbf{0}$ since $\det(M) \neq 0$. Then by definition

$$\begin{pmatrix} \tilde{A} & \tilde{B} \\ \tilde{C} & \tilde{D} \end{pmatrix} \begin{pmatrix} \mathbf{0} \\ C\mathbf{v}_a \end{pmatrix} = \begin{pmatrix} \tilde{B}C\mathbf{v}_a \\ \tilde{D}C\mathbf{v}_a \end{pmatrix} = \begin{pmatrix} \mathbf{v}_a \\ \mathbf{0} \end{pmatrix} \tag{8.4}$$

which implies that $\det(\tilde{D}) = 0$ since $C\mathbf{v}_a \neq \mathbf{0}$. Thus (8.2) holds in this case.
Case: Assume that $\det(A) \neq 0$. Then note first that

$$\det \begin{pmatrix} A & B \\ C & D \end{pmatrix} = \det \left(\begin{pmatrix} A & 0 \\ C & I \end{pmatrix} \begin{pmatrix} I & A^{-1}B \\ 0 & D - CA^{-1}B \end{pmatrix} \right) = \det(A) \det(D - CA^{-1}B) = \det(M) \tag{8.5}$$

where we point out for the sake of the following steps that (8.5) implies $\det(D - CA^{-1}B) \neq 0$. Then, from the block matrix inversion formula:

$$\begin{pmatrix} A & B \\ C & D \end{pmatrix} \begin{pmatrix} -A^{-1}B(D - CA^{-1}B)^{-1} \\ (D - CA^{-1}B)^{-1} \end{pmatrix} = \begin{pmatrix} 0 \\ I \end{pmatrix}. \tag{8.6}$$

In particular $\tilde{D} = (D - CA^{-1}B)^{-1}$ so that

$$\det(M) \det(\tilde{D}) = \det(M) \det((D - CA^{-1}B)^{-1}) = \frac{\det(M)}{\det(D - CA^{-1}B)} = \det(A). \tag{8.7}$$

Thus (8.2) again holds. □

Theorem 8.2. *Given $\beta, \alpha \in \mathbb{N}$ with $\beta < \alpha$, let $\{\mathbf{v}_1, ..., \mathbf{v}_\beta, \mathbf{v}_{\beta+1}, ..., \mathbf{v}_\alpha\}$ and $\{\mathbf{w}_1, ..., \mathbf{w}_\beta, \mathbf{w}_{\beta+1}, ..., \mathbf{w}_\alpha\}$ be sets of linearly independent vectors in $\mathbb{R}^\alpha$ where*

$$\mathbf{w}_i \cdot \mathbf{w}_j = 0 \quad \textit{for all} \quad i \in \{1, ..., \beta\}, j \in \{\beta + 1, ..., \alpha\} \ . \tag{8.8}$$

Let M be an $\alpha \times \alpha$ matrix with $\det(M) \neq 0$ and where

$$\mathbf{v}_i = M\mathbf{w}_i \quad \textit{for all} \quad i \in \{1, ..., \beta\} \tag{8.9}$$

and

$$\mathbf{w}_j = M^T\mathbf{v}_j \quad \textit{for all} \quad j \in \{\beta + 1, ..., \alpha\}. \tag{8.10}$$

Then

$$\text{vol}(\mathbf{v}_1, ..., \mathbf{v}_\beta)\text{vol}(\mathbf{w}_{\beta+1}, ..., \mathbf{w}_\alpha) = |\det(M)| \, \text{vol}(\mathbf{v}_{\beta+1}, ..., \mathbf{v}_\alpha)\text{vol}(\mathbf{w}_1, ..., \mathbf{w}_\beta) \tag{8.11}$$

Proof. Because of (8.8), without loss of generality we may choose an orthonormal basis wherein

$$(\mathbf{w}_1, ..., \mathbf{w}_\beta) = \begin{pmatrix} W_1 \\ 0 \end{pmatrix}_{\alpha \times \beta} \quad \text{and} \quad (\mathbf{w}_{\beta+1}, ..., \mathbf{w}_\alpha) = \begin{pmatrix} 0 \\ W_4 \end{pmatrix}_{\alpha \times (\alpha-\beta)}. \tag{8.12}$$

where W_1 is a $\beta \times \beta$ matrix and W_4 is an $(\alpha - \beta) \times (\alpha - \beta)$ matrix. The matrices M and M^{-1} may be written in bock form as

$$M = \begin{pmatrix} A & B \\ C & D \end{pmatrix} \quad \text{and} \quad M^{-1} = \begin{pmatrix} \tilde{A} & \tilde{B} \\ \tilde{C} & \tilde{D} \end{pmatrix} \tag{8.13}$$

where A and $\tilde{A}$ are $\beta \times \beta$ matrices. Then from the definitions,

$$(\mathbf{v}_1, ..., \mathbf{v}_\beta) = \begin{pmatrix} AW_1 \\ CW_1 \end{pmatrix} \quad \text{and} \quad (\mathbf{v}_{\beta+1}, ..., \mathbf{v}_\alpha) = \begin{pmatrix} \tilde{C}^T W_4 \\ \tilde{D}^T W_4 \end{pmatrix}. \tag{8.14}$$

Next note that

$$M^T M = \begin{pmatrix} A^T A + C^T C & A^T B + C^T D \\ B^T A + D^T C & B^T B + D^T D \end{pmatrix} \tag{8.15}$$

and

$$M^{-1} \left(M^{-1}\right)^T = \begin{pmatrix} \tilde{A}\tilde{A}^T + \tilde{B}\tilde{B}^T & \tilde{A}\tilde{C}^T + \tilde{B}\tilde{D}^T \\ \tilde{C}\tilde{A}^T + \tilde{D}\tilde{B}^T & \tilde{C}\tilde{C}^T + \tilde{D}\tilde{D}^T \end{pmatrix} \tag{8.16}$$

so that since $\det(M^T M) = \det(M)^2$ Lemma 8.1 gives that

$$\det(A^T A + C^T C) = \det(M)^2 \det(\tilde{C}\tilde{C}^T + \tilde{D}\tilde{D}^T). \tag{8.17}$$

Then

$$\begin{aligned} \operatorname{vol}(\mathbf{v}_1, ..., \mathbf{v}_\beta)\operatorname{vol}(\mathbf{w}_{\beta+1}, ..., \mathbf{w}_\alpha) &= \operatorname{vol}\begin{pmatrix} AW_1 \\ CW_1 \end{pmatrix} \operatorname{vol}\begin{pmatrix} 0 \\ W_4 \end{pmatrix} \\ &= \sqrt{\det(W_1^T A^T A W_1 + W_1^T C^T C W_1)}\, |\det(W_4)| \\ &= \sqrt{\det(A^T A + C^T C)}\, |\det(W_1)|\, |\det(W_4)| \\ &= |\det(M)| \sqrt{\det(\tilde{C}\tilde{C}^T + \tilde{D}\tilde{D}^T)}\, |\det(W_1)|\, |\det(W_4)| \\ &= |\det(M)| \sqrt{\det(W_4^T \tilde{C}\tilde{C}^T W_4 + W_4^T \tilde{D}\tilde{D}^T W_4)}\, |\det(W_1)| \\ &= |\det(M)| \operatorname{vol}\begin{pmatrix} \tilde{C}^T W_4 \\ \tilde{D}^T W_4 \end{pmatrix} \operatorname{vol}\begin{pmatrix} W_1 \\ 0 \end{pmatrix} \\ &= |\det(M)| \operatorname{vol}(\mathbf{v}_{\beta+1}, ..., \mathbf{v}_\alpha)\operatorname{vol}(\mathbf{w}_1, ..., \mathbf{w}_\beta) \end{aligned} \tag{8.18}$$

which proves the result. □

Corollary 8.3. *Let $\mathbf{w}_i$ and $\mathbf{v}_i$ be the vectors given in Theorem 8.2. Written in block form they become*

$$(\mathbf{w}_1, ..., \mathbf{w}_\beta) = \begin{pmatrix} W_1 \\ W_2 \end{pmatrix}_{\alpha \times \beta}, \quad (\mathbf{w}_{\beta+1}, ..., \mathbf{w}_\alpha) = \begin{pmatrix} W_3 \\ W_4 \end{pmatrix}_{\alpha \times (\alpha-\beta)} \tag{8.19}$$

and

$$(\mathbf{v}_1, ..., \mathbf{v}_\beta) = \begin{pmatrix} V_1 \\ V_2 \end{pmatrix}_{\alpha \times \beta}, \quad (\mathbf{v}_{\beta+1}, ..., \mathbf{v}_\alpha) = \begin{pmatrix} V_3 \\ V_4 \end{pmatrix}_{\alpha \times (\alpha-\beta)}, \tag{8.20}$$

where W_1 and V_1 are both $\beta \times \beta$ matrices while W_4 and V_4 are both $(\alpha - \beta) \times (\alpha - \beta)$. Then

$$\operatorname{vol}(V_1)\operatorname{vol}(W_4) = |\det(M)| \operatorname{vol}(V_4)\operatorname{vol}(W_1). \tag{8.21}$$

Proof. By orthogonality

$$W_1^T W_3 + W_2^T W_4 = 0. \tag{8.22}$$

If $\text{vol}(W_1) = \text{vol}(W_4) = 0$, (8.21) holds trivially. Thus assume $\text{vol}(W_1) \neq 0$ so that

$$\begin{aligned}
\text{vol}(W_4)\text{vol}\begin{pmatrix} W_1 \\ W_2 \end{pmatrix} &= |\det(W_4)| \sqrt{\det(W_1^T W_1 + W_2^T W_2)} \\
&= |\det(W_4)|\,|\det(W_1)| \sqrt{\det(I + (W_1^{-1})^T W_2^T W_2 W_1^{-1})} \\
&= |\det(W_4)|\,|\det(W_1)| \sqrt{\det(I + W_2 W_1^{-1} (W_1^{-1})^T W_2^T)} \\
&= |\det(W_1)| \sqrt{\det(W_4^T W_4 + W_4^T W_2 W_1^{-1} (W_1^{-1})^T W_2^T W_4)} \\
&= |\det(W_1)| \sqrt{\det(W_4^T W_4 + W_3^T W_1 W_1^{-1} (W_1^{-1})^T W_1^T W_3)} \\
&= |\det(W_1)| \sqrt{\det(W_4^T W_4 + W_3^T W_3)} \\
&= \text{vol}(W_1)\text{vol}\begin{pmatrix} W_3 \\ W_4 \end{pmatrix}
\end{aligned} \tag{8.23}$$

where the third line of (8.23) follows from Sylvester's determinant theorem and the fifth line follows from (8.22). Note that linear independence implies that $\text{vol}\begin{pmatrix} W_1 \\ W_2 \end{pmatrix} \neq 0$ and $\text{vol}\begin{pmatrix} W_3 \\ W_4 \end{pmatrix} \neq 0$ so that (8.23) gives $\text{vol}(W_4) \neq 0$. Since similar steps give the same result as (8.23) in the case where $\text{vol}(W_4) \neq 0$, one gets that $\text{vol}(W_1) \neq 0$ iff $\text{vol}(W_4) \neq 0$. By first noting that

$$\mathbf{v}_i \cdot \mathbf{v}_j = 0 \quad \text{for all} \quad i \in \{1, ..., \beta\}, j \in \{\beta + 1, ..., \alpha\} \tag{8.24}$$

is also guaranteed by the statement of Theorem 8.2, an equivalent result to (8.23) then holds for the $\mathbf{v}_i$ vectors so that in summary

$$\text{vol}(W_4)\text{vol}\begin{pmatrix} W_1 \\ W_2 \end{pmatrix} = \text{vol}(W_1)\text{vol}\begin{pmatrix} W_3 \\ W_4 \end{pmatrix} \quad \text{and} \quad \text{vol}(V_4)\text{vol}\begin{pmatrix} V_1 \\ V_2 \end{pmatrix} = \text{vol}(V_1)\text{vol}\begin{pmatrix} V_3 \\ V_4 \end{pmatrix}. \tag{8.25}$$

Finally, from Theorem 8.2

$$\text{vol}\begin{pmatrix} V_1 \\ V_2 \end{pmatrix} \text{vol}\begin{pmatrix} W_3 \\ W_4 \end{pmatrix} = |\det(M)|\,\text{vol}\begin{pmatrix} V_3 \\ V_4 \end{pmatrix} \text{vol}\begin{pmatrix} W_1 \\ W_2 \end{pmatrix}. \tag{8.26}$$

Multiplying both sides of (8.26) by $\text{vol}(V_1)\text{vol}(W_4)$ and using (8.25) gives

$$\text{vol}(V_1)\text{vol}(W_4)\text{vol}\begin{pmatrix} V_1 \\ V_2 \end{pmatrix} \text{vol}\begin{pmatrix} W_3 \\ W_4 \end{pmatrix} = |\det(M)|\,\text{vol}(V_4)\text{vol}(W_1)\text{vol}\begin{pmatrix} V_1 \\ V_2 \end{pmatrix} \text{vol}\begin{pmatrix} W_3 \\ W_4 \end{pmatrix} \tag{8.27}$$

which after cancelation gives (8.21). □

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