Gaussian beam methods for the Schrödinger equation with periodic potentials and strictly hyperbolic systems

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Gaussian beam methods for the Schrödinger equation with periodic potentials and strictly hyperbolic systems

by

Maksym Pryporov

A thesis submitted to the graduate faculty
in partial fulfillment of the requirements for the degree of

DOCTOR OF PHILOSOPHY

Major: Applied Mathematics

Program of Study Committee:
Hailiang Liu, Major Professor
Gary Lieberman
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Paul Sacks
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Iowa State University
Ames, Iowa
2013

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DEDICATION

This work is dedicated to my parents, my sisters, my girlfriend and my niece Alice.
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ABSTRACT

In this dissertation, we study Gaussian beam superposition methods for the computation of high frequency wave fields governed by two important time-dependent partial differential equations, the Schrödinger equation with periodic potentials and strictly hyperbolic systems, both subject to highly oscillatory initial conditions. Gaussian beams form a high frequency asymptotic model which is closely related to geometrical optics. However, unlike geometrical optics, there is no breakdown at caustics. The beam solution is concentrated near a single ray of geometrical optics. The superposition of first order Gaussian beams constitute our asymptotic solution to the underlying initial value problems. Based on the well-posedness result, we obtain optimal error estimates in terms of the high frequency parameter $\varepsilon$. For the Schrödinger equation, our error estimate is obtained in $L^2$ norm, and for hyperbolic systems the energy norm is taken.

For the linear semi-classical Schrödinger equation in periodic media, the geometric optics ansatz together with homogenization leads to the Bloch eigenvalue problem. We provide Gaussian beam evolution equations for each Bloch band, following the idea in the earlier work by M. Dimassi J-C. Guillot and J. Ralston “Gaussian beam construction for adiabatic perturbations” published in the Journal of Mathematical Physics, Analysis and Geometry in 2006, [10]. Our contribution to the analysis of this problem is in obtaining error estimates of the Gaussian beam superposition. Using the superposition principle, we obtain high frequency approximate solutions to the original wave field. When the initial data can be decomposed into a finite number of band eigen-functions and under regularity assumptions for Bloch bands and energy bands, we prove that the first-order Gaussian beam superposition converges to the original wave field at a rate of $\varepsilon^{1/2}$, with $\varepsilon$ the semiclassically scaled constant, as long as the initial data for Gaussian beam components in each band are prepared with same order of error or smaller. For a natural choice of initial approximation, a rate of $\varepsilon^{1/2}$ of initial error is verified.

For the strictly hyperbolic systems we construct Gaussian beam approximations and study the
accuracy of the Gaussian beam superposition. Under some regularity assumptions of data we show error estimates between the exact solution and the Gaussian beam superposition in terms of the high frequency parameter $\varepsilon$. The main result is that the relative local error measured in energy norm in the beam approximations decay as $\varepsilon^{\frac{1}{2}}$ independent of dimension and presence of caustics, for first order beams. This result is shown to be valid when the gradient of the initial phase may vanish on a set of measure zero.
CHAPTER 1. GENERAL INTRODUCTION AND LITERATURE REVIEW

1.1 General Background

The recovery of high frequency waves is a challenging problem from both a theoretical and computational perspective. This type of problem arises in solid states physics, quantum chemistry, acoustic wave propagation, seismology and other fields.

In this thesis, we concentrate on two important wave equations, subject to highly oscillatory initial data. The first one is the semiclassically scaled Schrödinger equation with a periodic potential, which models the dynamics of the Bloch electron in crystals with periodic structure. The second one is the general linear strictly hyperbolic systems.

The common issue is that when the frequency parameter \( \varepsilon \ll 1 \) the wave fields (solutions of the underlying wave equation) become highly oscillatory which makes direct computations prohibitively costly, some asymptotic approach must be used. One classical asymptotic approach to the high frequency problem is to use the WKB (geometric optics) ansatz

\[
\begin{align*}
  u^\varepsilon(t, x) = [A_0(t, x) + A_1(t, x)\varepsilon + \cdots + A_l(t, x)\varepsilon^l]/\varepsilon,
\end{align*}
\]

where the amplitude has been assumed to admit the Debye expansion of finite order. This WKB ansatz is intended to approximate the exact wave field \( u \), when plugged into the underlying wave equation producing a weakly coupled system of equations for the phase and amplitudes. The typical equation for phase is the Hamilton-Jacobi equation

\[
\Phi_t + H(x, \nabla_x \Phi) = 0,
\]

and the transport equations for amplitudes. The equation for \( A_0 \) depends on the phase \( \Phi \) in the following way

\[
A_{0t} + \partial_k H(x, \nabla_x \Phi) \cdot \partial_x A_0 + \frac{1}{2} \partial_x \cdot \partial_k H(x, \nabla_x \Phi) A_0 = 0,
\]
where \( k = \nabla_x \Phi \) and the Hamiltonian varies in its form for different wave equations, for example \( H = \frac{|k|^2}{2} \) for the free Schrödinger equation, and \( H = |k| \) for the wave equation \((\partial_t^2 - \Delta)u = 0\). The advantages of this method is that the obtained equations are independent of \( \varepsilon \) and thus can be computed on uniform grids. The shortcoming lies in the fact that the nonlinearity of the Hamilton-Jacobi equation for phase \( \Phi \) generally leads to finite time singularity formation in phase \( \Phi \), at such a singularity the amplitude \( A_0 \) is forced to be unbounded, therefore unacceptable.

This is the well-known caustic problem, which has been addressed in numerous works, beginning with works by Keller, Maslov and Hörmander, using the classical Fourier integral operator approach, see [14, 17, 26].

Gaussian beams form another high frequency asymptotic model which is closely related to geometrical optics, yet valid at caustics. In this thesis, we are using the method of Gaussian beams. In this approach, the solution is still assumed to be of the WKB form (1.1.1), but it is concentrated on a single ray of geometrical optics. The Gaussian profile is achieved by allowing the phase to be complex away from the central ray so that the solution decays exponentially away from the ray.

To form such a solution we first pick a ray \( \tilde{x} \) and find a Gaussian beam phase as the Taylor expansion in the variables transverse to the ray. For instance, for the first order Gaussian beam, the phase takes the following form

\[
\Phi(t, x; x_0) = S(t; x_0) + p(t; x_0)(x - \tilde{x}(t; x_0)) + \frac{1}{2}(x - \tilde{x}(t; x_0))^\top M(t; x_0)(x - \tilde{x}(t; x_0)),
\]

where \( \tilde{x} \) is the geometrical ray, and \( p \) is the direction of the ray, \( S \) is the phase evaluated on the ray, and \( M \) is a matrix with positive definite imaginary part.

Based on characteristic equations for \( \tilde{x} \) and \( p \), we derive evolution equations for \( S \) and \( M \), so that

\[
\Phi_t + H(x, \nabla_x \Phi) = O((x - \tilde{x})^2).
\]

In the next step, we derive evolution equations for amplitude \( A \).

For the given initial value problem for linear wave equations, the solution is a general high frequency wave field, which is not necessarily concentrated on a single ray. We construct the approximation through the superposition of beams. More precisely, the approximation can be
expressed as a superposition integral

\[ u^\varepsilon = \left( \frac{1}{2\pi \varepsilon} \right)^{d/2} \int_{K_0} A(t, x; x_0) e^{i\Phi(t, x; x_0)}/\varepsilon \, dx_0, \]  

where \( K_0 \) is the support of the initial data.

We choose the initial condition for \( M \) to have positive definite imaginary part, which ensures the existence of the global bounded solution for \( M \), [30].

The main focus is on obtaining the optimal error estimates for Gaussian beam superpositions of the form \( (1.1.2) \) for two wave equations under our investigation. The well-posedness result for both problems state that the total error made by the approximate solutions is controlled by the sum of the initial error and the evolution error. The general result is that the error between the exact wave field and the constructed Gaussian beam approximation using first order beams is of order \( \varepsilon^{1/2} \), when measured in the norm dictated by the wellposedness of the underlying problem.

### 1.2 Literature Review

The origin of the Gaussian beam theory dates back to 1950s, when high frequency problems were studied using the ray theory. In 1956, Babić published his report about the ray method of computation of intensity of wave fronts, [2] which was arguably the first paper concerning Gaussian beams. The existence of Gaussian beam solutions has been known since the 1960's, first in connection with lasers, which is discussed in [3]. In the western literature, Gaussian beams were first used to obtain results on the propagation of singularities in solutions of PDEs in the work of L. Hörmander on the existence and the regularity of solutions of linear pseudo-differential equations in 1971, [14], and Ralston in his work on “Gaussian beams and the propagation of singularities”, published in 1982, [30]. Among other contributions in his paper, Ralston proves that for some choices of the initial data for Gaussian beam components, there exists a global bounded solution of evolution differential equations, governing the Gaussian beam phase, which is an important result for the Gaussian beam construction. The idea of using sums of Gaussian beams to represent more general high frequency solutions was first introduced by Babić and Pankratova in their work on “discontinuities of Green’s function of the wave equation with variable coefficients”, published in 1973, [4].
The first numerical method for computing high frequency wave propagation using Gaussian beams was proposed by Popov in 1982 in his work “A new method of computation of wave fields using Gaussian beams”, [29]. At present there is considerable interest in using superpositions of beams to resolve high frequency waves near caustics. This goes back to the geophysical applications proposed in Červeny et al. 1982, [8] and Hill in 2001, [13]. Recent work in this direction includes Tanushev et al. (2007,2008), Qian et al. (2007), Motamed and Runborg (2009), Jin et al. (2008), see [38, 34, 24, 37, 27, 35] and references therein.

The accuracy of the Gaussian beam superposition to approximate the original wave field is important, but determining the error of the Gaussian beam superposition was thought to be a difficult problem decades ago, see the conclusion section of the review article by Babić and Popov in 1989, [5]. In the past few years, considerable progress on estimates of the error has been made. One of the first results was obtained by Tanushev for the initial error made by \( n \)-th order Gaussian beam approximation for acoustic wave equations in 2008 [37]. Liu and Ralston [21, 22] gave rigorous convergence rates in terms of the small wave length for both the acoustic wave equation in the scaled energy norm and the Schrödinger equation in the \( L^2 \) norm. A damage at caustics was observed when directly estimating the evolution error, leading to a rate of convergence depending on the dimension of the physical space. The main obstacle came from a direct estimate of

\[
\varepsilon^{-d} \int_{\mathbb{R}^d} \left( \int_{K_0} e^{\frac{|x-\tilde{x}|^2}{\varepsilon}} dx_0 \right)^2 dx, \tag{1.2.1}
\]

which when applying Schur’s lemma yields

\[
\varepsilon^{-d} \int_{\mathbb{R}^d} \left( \int_{K_0} G dx_0 \right)^2 dx \leq \sup_x \int_{K_0} |G| dx_0 \cdot \sup_{x_0} \int_{\mathbb{R}^d} |G| dx \leq \varepsilon^{-d} \sup_x \int_{K_0} |G| dx_0, \]

where for \( G \sim e^{-\frac{|x-\tilde{x}|^2}{\varepsilon}} \) the fact \( \varepsilon^{-d/2} \) remains uncanceled.

Error estimates for phase space beam superposition were obtained by Bougacha, Akian and Alexandre in 2009, [7] for the acoustic wave equation. The estimate is carried out in phase space, so there is no damage from caustics. Building upon these advances, Liu, Runborg and Tanushev further obtained optimal error estimates for a class of high-order, strictly hyperbolic partial differential equations [23]. In their work, they developed an elegant non-squeezing argument, with which they were able to obtain optimal estimates. The non-squeezing argument can be summarized as follows. Let \( \tilde{x}(t; x_0) \) be the trajectory of the Gaussian beam issued from \( x_0 \) and \( p(t; x_0) \) be
momentum and assume that \( p(0; x_0) \) is Lipschitz continuous in \( x_0 \in K_0 \). Under those conditions, there exist positive constants \( c_1 \) and \( c_2 \) depending on \( T \), such that
\[
c_1 |x_0 - x'_0| \leq |p(t; x_0) - p(t; x'_0)| + |	ilde{x}(t; x_0) - 	ilde{x}(t; x'_0)| \leq c_2 |x_0 - x'_0|,
\]
(1.2.2)
for all \( x_0, x'_0 \in K_0 \) and \( t \in [0, T] \). This result makes it possible to use cancelations from \( p \) direction when caustics in the \( x \) direction are observed. We are using the non-squeezing argument to prove evolution error estimates in our investigation.

The recovery theory has recently been developed for the Helmholtz equation with a singular source by Liu, Ralston, Runborg and Tanushev in 2013. One of the main challenges in obtaining estimates for the Helmholtz equation was that the ray parameter \( s \) depends on the space variable \( x \), their paper is available at arXiv:1304.1291.

1.3 Bloch Band-Based Gaussian Beam Superposition for the Schrödinger Equation

We study the semiclassically scaled Schrödinger equation
\[
i\varepsilon \partial_t \Psi = -\frac{\varepsilon^2}{2} \Delta \Psi + V\left(\frac{x}{\varepsilon}\right) \Psi + V_e(x) \Psi, \quad x \in \mathbb{R}^d, \quad t > 0,
\]
(1.3.1)
since the two-scale initial condition:
\[
\Psi(0, x) = g\left(\frac{x}{\varepsilon}\right) e^{i S_0(x)/\varepsilon}, \quad x \in \mathbb{R}^d,
\]
(1.3.2)
where \( \Psi(t, x) \) is a complex wave function, \( \varepsilon \) is the re-scaled Planck constant, \( V_e(x) \)– smooth external potential, \( S_0(x) \)– real-valued smooth function, \( g(x, y) = g(x, y + 2\pi) \)– smooth function, compactly supported in \( x \), i.e., \( g(x, y) = 0, \quad x \not\in K_0 \). \( K_0 \)– is a bounded set. \( V(y) \) is periodic with respect to the crystal lattice \( \Gamma = (2\pi \mathbb{Z})^d \). This equation models the electronic potential generated by the lattice of atoms in the crystal [10]. Due to the fast scale \( \frac{x}{\varepsilon} \), we apply a well-known two-scale approach [6] and reformulate the problem in the following way
\[
\begin{cases}
i\varepsilon \partial_t \tilde{\Psi} = -\frac{1}{2} (\varepsilon \nabla_x + \nabla_y)^2 \tilde{\Psi} + V(y) \tilde{\Psi} + V_e(x) \tilde{\Psi}, \\
\tilde{\Psi}(0, x, y) = g(x, y) e^{i S_0(x)/\varepsilon}, \quad x \in \mathbb{R}^d, \quad y \in [0, 2\pi]^d,
\end{cases}
\]
(1.3.3)
where $\Psi(t, x) = \tilde{\Psi}(t, x, y)|_{y = \frac{x}{\varepsilon}}$.

The specifics of this problem is the so-called band structure of the solution, which is closely related to the solution of the eigenvalue problem:

\[
\begin{aligned}
H(k, y)z(k, y) &= E(k)z(k, y), \\
z(k, y) &= z(k, y + 2\pi),
\end{aligned}
\]

(1.3.4)

where $H(k, y)$ is a Hamiltonian operator in the following form:

\[
H(k, y) = \frac{1}{2}(-i\nabla_y + k)^2 + V(y),
\]

(1.3.5)

From the theory of Bloch waves [39], the self-adjoint semi-bounded operator $H(k, y)$ with a compact resolvent has a complete set of orthonormal eigenfunctions $z_n(k, y)$ in $L^2$, called Bloch functions. The correspondent eigenvalues $E_n(k)$ are called band functions. From perturbation theory, [10] $E_n(k)$ is a continuous function of $k$ and real analytic in a neighborhood of any $k$ such that

\[
E_{n-1}(k) < E_n(k) < E_{n+1}(k).
\]

(1.3.6)

We assume that (1.3.6) is satisfied, i.e., all band functions are strictly separated, $\forall n, k$. Under this assumption we can choose $z_n(k, y)$ associated to $E_n(k)$ to be real analytic functions of $k$ [10].

Using the WKB ansatz

\[
\tilde{\Psi}^\varepsilon(t, x, y) = A(t, x, y)e^{i\Phi(t, x)/\varepsilon},
\]

(1.3.7)

where

\[
A(t, x, y) = A_0(t, x, y) + A_1(t, x, y)\varepsilon + \cdots + A_l(t, x, y)\varepsilon^l,
\]

and the eigenvalue problem (1.3.4) we obtain the system of Hamilton-Jacobi equations

\[
\Phi_{nt} + E_n(\partial_x \Phi_n) + V_\varepsilon(x) = 0,
\]

(1.3.8)

for the leading term. A Bloch band based Gaussian beam approach is described in details in Chapter 2. We build Gaussian beam superposition as in (1.1.2) and present proofs for the initial and evolution errors separately.
For the initial error, we break it into several parts: error made by the phase approximation, error made by the eigenfunction approximation and error made by the amplitude approximation. Taking advantage of finitely many bands, we are able to prove the desired initial error estimate. For the evolution error, the proof is technical, yet the main ingredients we use include: boundedness of the residual terms, the non-squeezing argument and phase estimates, together with the non-stationary phase method.

In order to obtain the main result for the original problem (1.3.1), we also need to convert our estimates from two-scale setting back to one scale. A key estimate we obtain is the following:

$$\left\| f \left( x, \frac{x}{\varepsilon} \right) \right\|_{L^2_x} \leq \frac{1}{\pi \varepsilon^2} \left\| f(x,y) \right\|_{L^2_{x,y}}.$$

for sufficiently small $\varepsilon$.

### 1.4 Strictly Hyperbolic Systems

Our second project is concerned with the study of asymptotic solutions for symmetric systems of strictly hyperbolic equations

$$A(x) \frac{\partial u}{\partial t} + \sum_{j=1}^{n} D^j \frac{\partial u}{\partial x_j} = 0,$$

subject to the highly oscillatory initial condition,

$$u(0,x) = B_0(x)e^{iS_0(x)/\varepsilon},$$

where $x \in \mathbb{R}^n$, $S_0(x)$ is a scalar smooth function, $B_0 : \mathbb{R}^n \to \mathbb{C}^m$ is a smooth vector function, compactly supported in $K_0 \subset \mathbb{R}^n$, $A(x)$ is an $m \times m$ symmetric strictly positive definite matrix, and $D^j$ are $m \times m$ symmetric constant coefficient matrices, $j = 1, \ldots, n$.

The well-wellposedness estimate for the symmetric hyperbolic system is based on the following energy norm:

$$\|u\|^2_E := \int_{\mathbb{R}^n} \langle Au, u \rangle dx,$$

where $\langle Au, u \rangle$ is a dot product of vector functions $Au$ and $u$.

For the strictly hyperbolic system (1.4.1-1.4.2) we use the fact that the dispersive matrix $L(x,k)$:

$$L(x,k) = A^{-1}(x) \sum_{j=1}^{n} D^j k_j,$$
is symmetric with respect to the weighted inner product
\[ \langle u, v \rangle_A := \langle Au, v \rangle. \]

Thus, \( L(x, k) \) has real eigenvalues \( \{ \lambda_i(x, k) \}_{i=1}^m \), satisfying
\[ L(x, k)b_i(x, k) = \lambda_i(x, k)b_i(x, k), \quad i = 1, \ldots, m, \]
where \( \{ b_i(x, k) \}_{i=1}^m \) are eigenvectors, forming an orthonormal basis in \( l_2 \) equipped with a weight function \( A(x) \), i.e., \( \langle b_i, b_j \rangle_A = \delta_{ij} \), and \( \lambda_i(x, k) \) are scalar smooth functions. The geometric optics ansatz for this problem has the following form
\[ u^\varepsilon = (v_0(t, x) + \varepsilon v_1(t, x) + \cdots + \varepsilon^l v_l(t, x)) e^{i \Phi(t, x) / \varepsilon}, \]
where \( v_j(x, k) \) are vector-functions \( j = 0, \cdots, l \). Insertion of \( u^\varepsilon \) into (1.4.1) yields
\[ A^{-1}(x) P[u^\varepsilon] = (1 + c_0 + c_1 + \cdots + \varepsilon^{l-1} c_l) e^{i \Phi / \varepsilon} = 0. \]

By geometric optics, the leading term is required to vanish,
\[ c_0 = i(\Phi_t + L(x, \partial_x \Phi)) v_0 = 0. \]

This when combined with an eigen-vector decomposition of \( v_0 \) leads to the Hamilton-Jacobi equation
\[ \Phi_t + \lambda(x, \partial_x \Phi) = 0 \]
for each \( \lambda \in \{ \lambda_j \}_{j=1}^m \). We assume that all eigenvalues are simple (i.e., system (1.4.1) is strictly hyperbolic) and the following holds:
\[ \lambda_{i-1}(x, k) < \lambda_i(x, k) < \lambda_{i+1}(x, k), \quad i = 2, \ldots, m - 1, \]
in a neighborhood of any \((x, k)\).

Borrowing some similar techniques developed for the Schrödinger equation with finite energy bands, we construct the Gaussian beam superposition and estimate the error, to be detailed in Chapter 3. For the proof of initial error, we carefully apply the eigen-decomposition upon the involved vector functions. For the evolution error, we estimate all terms componentwise assuming the initial phase gradient to be away from zero. Also we extend our results to the case when the initial phase gradient vanishes on a set of measure zero. By eliminating a small set from Gaussian beam superposition, we still can obtain the same estimates.
1.5 Thesis Organization

The organization of this thesis is as follows. In Chapter 2 we present our paper “Error Estimates of the Bloch Band-Based Gaussian Beam Superposition for the Schrödinger Equation”, which was submitted to SIAM MMS Journal. This is a joint paper with my advisor Prof. Liu. In this paper we formulate Gaussian beam superposition and prove error estimates for the case when the initial data can be decomposed into finitely many bands. Chapter 3 is devoted to a preprint on “Gaussian Beam Methods for Strictly Hyperbolic Systems”, where we formulate Gaussian beam superpositions and prove error estimates as well. This work is done under the supervision of Prof. Liu. In Chapter 4, we discuss applications of the Gaussian beam method, developed in Chapter 3 to the case of acoustic waves. We provide general conclusions and discussions on some open problems that are likely to be addressed in the future in Chapter 5.
CHAPTER 2. ERROR ESTIMATES OF THE BLOCH BAND-BASED
GAUSSIAN BEAM SUPERPOSITION FOR THE SCHRÖDINGER
EQUATION

A paper submitted to SIAM MMS Journal

Hailiang Liu, Maksym Pryporov

Abstract

This work is concerned with asymptotic approximations of the semi-classical Schrödinger equation in periodic media using Gaussian beams. For the underlying equation, subject to a highly oscillatory initial data, a hybrid of the Gaussian beam approximation and homogenization leads to the Bloch eigenvalue problem and associated evolution equations for Gaussian beam components in each Bloch band. We formulate a superposition of Bloch-band based Gaussian beams to generate high frequency approximate solutions to the original wave field. For initial data of a sum of finite number of band eigen-functions, we prove that the first-order Gaussian beam superposition converges to the original wave field at a rate of $\epsilon^{1/2}$, with $\epsilon$ the semiclassically scaled constant, as long as the initial data for Gaussian beam components in each band are prepared with same order of error or smaller. For a natural choice of initial approximation, a rate of $\epsilon^{1/2}$ of initial error is verified.

2.1 Introduction

We consider the semiclassically scaled Schrödinger equation with a periodic potential:

$$i\varepsilon \partial_t \Psi = -\frac{\varepsilon^2}{2} \Delta \Psi + V \left(\frac{x}{\varepsilon}\right) \Psi + V_e(x) \Psi, \quad x \in \mathbb{R}^d, \quad t > 0,$$

subject to the two-scale initial condition:

$$\Psi(0, x) = g \left(x + \frac{x}{\varepsilon}\right) e^{i S_0(x)/\varepsilon}, \quad x \in \mathbb{R}^d,$$
where $\Psi(t, x)$ is a complex wave function, $\varepsilon$ is the re-scaled Planck constant, $V_0(x)$—smooth external potential, $S_0(x)$—real-valued smooth function, $g(x, y) = g(x, y + 2\pi)$—smooth function, compactly supported in $x$, i.e., $g(x, y) = 0$, $x \not\in K_0$, $K_0$—is a bounded set. $V(y)$ is periodic with respect to the crystal lattice $\Gamma = (2\pi \mathbb{Z})^d$, it models the electronic potential generated by the lattice of atoms in the crystal [10].

This type of Schrödinger equations models the quantum dynamics of a Bloch electron in a crystal subjected to an external field [36]. This problem has been studied rigorously from both mathematical and physical points of view in recent years, see, e.g., [1, 9, 10, 12, 25, 35].

The main feature of this type of problems is the “band structure” of solutions. For suitable initial data, the solution depends on the semi-classical Hamiltonian operator

$$H(k, y) = \frac{1}{2}(-i \nabla_y + k)^2 + V(y),$$

and the solution of the eigenvalue problem:

$$\begin{cases} 
H(k, y)z(k, y) = E(k)z(k, y), \\
z(k, y) = z(k, y + 2\pi),
\end{cases}$$

where $k \in [-1/2, 1/2]$—called Brillouin zone, see [40].

According to the theory of Bloch waves [39], the self-adjoint semi-bounded operator $H(k, y)$ with a compact resolvent has a complete set of orthonormal eigenfunctions $z_n(k, y)$ in $L^2$ called Bloch functions. The correspondent eigenvalues $E_n(k)$ are called band functions. Standard perturbation theory [10] shows that $E_n(k)$ is a continuous function of $k$ and real analytic in a neighborhood of any $k$ such that

$$E_{n-1}(k) < E_n(k) < E_{n+1}(k).$$

We assume that (2.1.5) is satisfied, i.e., all band functions are strictly separated, $\forall n$, $k$. Under this assumption we can choose $z_n(k, y)$ associated to $E_n(k)$ to be real analytic functions of $k$ [10]. We also assume that

$$\sum_{|\alpha|\leq d+2, \beta\leq 3} \|\partial_k^\alpha \partial_y^\beta z_n(k, y)\|_{L^2_y} \leq Z < \infty.$$
A direct computation of the problem is prohibitively costly because of the small parameter $\varepsilon$. A classical approach to solve this problem asymptotically is by the Bloch band decomposition based WKB method [6, 12], which leads to Hamilton-Jacobi and transport equations valid up to caustics. The Bloch-band based level set method was introduced in [25] to compute crossing rays and position density beyond caustics. However, at caustics, neither method gives correct prediction for the amplitude. A closely related alternative to the WKB method is the construction of approximations based on Gaussian beams. Gaussian beams are asymptotic solutions concentrated on classical trajectories for the Hamiltonian $H(x,p)$, and they remain valid beyond “caustics”. The existence of Gaussian beam solutions has been known since sometime in the 1960’s, first in connection with lasers, see Babič and Buldyrev [2, 3]. Later, they were used to obtain results on the propagation of singularities in solutions of PDEs [14, 30]. The idea of using sums of Gaussian beams to represent more general high frequency solutions was first introduced by Babič and Pankratova in [4] and was later proposed as a method for wave propagation by Popov in [29]. At present there is considerable interest in using superpositions of beams to resolve high frequency waves near caustics. This goes back to the geophysical applications in [8, 13]. Recent work in this direction includes [38, 34, 24, 37, 27, 35].

The accuracy of the Gaussian beam superposition to approximate the original wave field is important, but determining the error of the Gaussian beam superposition is highly non-trivial, see the conclusion section of the review article by Babič and Popov [5]. In the past few years, some significant progress on estimates of the error has been made. One of the first results was obtained by Tanushev for the initial error in 2008 [37]. Liu and Ralston [21, 22] gave rigorous convergence rates in terms of the small wave length for both the acoustic wave equation in the scaled energy norm and the Schrödinger equation in the $L^2$ norm. At about the same time, error estimates for phase space beam superposition were obtained by Bougacha, Akian and Alexandre in [7] for the acoustic wave equation. Building upon these advances, Liu, Runborg and Tanushev further obtained sharp error estimates for a class of high-order, strictly hyperbolic partial differential equations [23].

In this paper, we develop a convergence theory for the Gaussian beam superposition as a valid approximate solution of problem (2.1.1)-(2.1.2). We have two objectives:

(i) to present the construction of beam superpositions;
(ii) to estimate the error between the exact wave field and the asymptotic ones.

The construction for (i) is based on Gaussian beams in each Bloch band, and carried out by using
the two scale expansion approach, as in [10] for adiabatic perturbations. Our approximate solution
is thus formulated as a superposition of Bloch band-based Gaussian beams. Numerical results
based on this type of superpositions were presented in [35].

Our focus in this work is mainly on (ii). The main result can be stated as follows.

**Theorem 2.1.1.** Suppose that $S_0 \in C_b^3(\mathbb{R}^d)$, $E_n, V_e \in C_b^{d+4}(\mathbb{R}^d), n = 1, \ldots, N$, $V(y)$ and $g(x,y)$
are periodic in $y$ with respect to the crystal lattice $\Gamma = (2\pi \mathbb{Z})^d$, $V(y) \in C^2((2\pi \mathbb{Z})^d)$ and $g(x,y)$ has
compact support in $x$. Also assume that $g$ has the following expression

$$g(x,y) = \sum_{n=1}^N a_n(x) z_n(\nabla_x S_0(x), y),$$

where $z_n(k,y)$ are eigenfunctions of (2.1.4) with eigenvalues $E_n(k)$ satisfying (2.1.5) and (2.1.6).

Let $\Psi(t,x)$ be the solution to (2.1.1)-(2.1.2), and

$$\Psi^\varepsilon(t,x) = \tilde{\Psi}^\varepsilon(t,x, x_\varepsilon)$$

be the Gaussian beam superposition defined by (2.3.35) for $0 < t \leq T$, then

$$\|\Psi - \Psi^\varepsilon\|_{L_x^2} \leq C\varepsilon^{1/2},$$

where $C$ may depend on $Z$, $T$, $N$ and data given, but independent of $\varepsilon$.

We prove this result in several steps. We first reformulate the problem using the two scale
expansion method [6, 10], in which both $x$ and $y = \frac{x}{\varepsilon}$ are regarded as two independent variables.
The well-posedness estimate for this reformulated problem tells that the total error is bounded by
the sum of initial and evolution error. For initial error, we use some techniques similar to those
developed by Tanushev [37], keeping in mind that here we have to deal with the band structure.
The band structure induces additional technical difficulties, which we solve in several steps. As
for evolution error part, we rely on the non-squeezing argument proved in [23], which is the key
technique for the proof. After we obtain estimate in $L_{x,y}^2$, we convert to $L_x^2$.

This paper has the following structure: in section 2 we use the two scale method to reformulate
our problem and state the corresponding results; in the end of this section we prove Theorem 1.1
for the original problem. In section 3 we review Gaussian beam constructions and formulate our Gaussian beam superposition. Justifications of main results are presented in section 4 and section 5. In section 6 we discuss possible extensions of our results and some remaining challenges.

### 2.2 Set-up and Main Results

In order to construct an asymptotic solution of (2.1.1) we use the two-scale method as in [6, 10]. We regard \( x \) and \( y = \frac{x}{\varepsilon} \) as independent variables and introduce a new function

\[
\tilde{\Psi}(t, x, y) \equiv \Psi(t, x),
\]

equation (2.1.1) can be rewritten in the form:

\[
\begin{cases}
    i\varepsilon \partial_t \tilde{\Psi} = -\frac{1}{2}(\varepsilon \nabla_x + \nabla_y)^2 \tilde{\Psi} + V(y)\tilde{\Psi} + V_\varepsilon(x)\tilde{\Psi}, \\
    \tilde{\Psi}(0, x, y) = g(x, y)e^{iS_0(x)/\varepsilon}, \quad x \in \mathbb{R}^d, \quad y \in [0, 2\pi]^d.
\end{cases}
\]

(2.2.1)

We assume that the initial amplitude \( g(x, y) \) can be decomposed into \( N \) bands,

\[
g(x, y) = \sum_{n=1}^{N} a_n(x)z_n(\nabla_x S_0, y),
\]

(2.2.2)

where \( a_n \) is determined by

\[
a_n(x) = \int_{[0, 2\pi]^d} g(x, y)z_n(\nabla_x S_0, y)dy,
\]

(2.2.3)

and \( \{ z_n(\partial_x S_0, y) \}_{n=1}^{\infty} \) are eigenfunctions of the self-adjoint second order differential operator \( H(k, y) \) defined by (2.1.3). \( \{ z_n(\partial_x S_0, y) \}_{n=1}^{\infty} \) form an orthonormal basis in \( L^2(0, 2\pi) \).

For each energy band, the Gaussian beam ansatz was constructed in [10], which we will review in section 3:

\[
\tilde{\Psi}^n_{GB}(t, x, y; x_0) = A^n(t, x, y; x_0)e^{i\Phi_n(t, x; x_0)/\varepsilon},
\]

(2.2.4)

where \( \Phi_n \) and \( A^n \) are Gaussian beam phases and amplitudes, respectively, \( n = 1, \ldots N \). The Gaussian beam phase is defined as:

\[
\Phi_n(t, x; x_0) = S_n(t; x_0) + p_n(t; x_0)(x - \tilde{x}_n(t; x_0)) + \frac{1}{2}(x - \tilde{x}_n(t; x_0))\top M_n(t; x_0)(x - \tilde{x}_n(t; x_0)),
\]

(2.2.5)
where $\tilde{x}_n, p_n, S_n$ and $M_n$, as well as the amplitude $a_n$ satisfy corresponding evolution equations (see section 3 for details). Using the fact that the Schrödinger equation is linear, we sum the Gaussian beam ansatz for each band to obtain the approximate solution along the ray:

$$\tilde{\Psi}_{GB}(t, x, y; x_0) = \sum_{n=1}^{N} \tilde{\Psi}_{GB}^n(t, x, y; x_0).$$

(2.2.6)

Using $\tilde{\Psi}_{GB}(t, x, y; x_0)$ as a building block of the approximate solution, we have the following superposition of Gaussian beams:

$$\tilde{\Psi}^\varepsilon(t, x, y) = \frac{1}{(2\pi\varepsilon)^{d/2}} \int_{K_0} \sum_{n=1}^{N} A^n(0, x, y; x_0) e^{i\Phi^0(x; x_0)/\varepsilon} dx_0,$$

(2.2.7)

where $\frac{1}{(2\pi\varepsilon)^{d/2}}$ is a normalizing constant which is needed for matching the initial data of problem (2.2.1). The initial data is approximated by:

$$\tilde{\Psi}^\varepsilon(0, x, y) = \frac{1}{(2\pi\varepsilon)^{d/2}} \int_{K_0} \sum_{n=1}^{N} A^n(0, x, y; x_0) e^{i\Phi^0(x; x_0)/\varepsilon} dx_0,$$

(2.2.8)

where $A^n(0, x, y; x_0)$ is the initial data for the amplitude, and $\Phi^0$ is the initial Gaussian beam phase for all bands, chosen as follows:

$$\Phi^0(x; x_0) = S_0(x_0) + \nabla_x S_0(x_0) \cdot (x - x_0) + \frac{1}{2}(x - x_0)^\top \cdot (\nabla_x^2 S_0(x_0) + iI)(x - x_0).$$

(2.2.9)

We address the two-scale problem, with $y = \frac{x}{\varepsilon}$ considered to be independent variables, and then convert to the original problem. The norm $L^2_{x,y}$ is defined as follows:

$$\|u\|_{L^2_{x,y}}^2 = \int_{[0, 2\pi]^d} \int_{\mathbb{R}^d} |u(x, y)|^2 dx dy.$$

(2.2.10)

We obtain two major results formulated in the following theorems:

**Theorem 2.2.1.** [Initial error estimate] Let $K_0 \subset \mathbb{R}^d$ be a bounded measurable set, $g(x, y) \in H^1(K_0 \times [0, 2\pi]^d)$, $S_0(x) \in C^3_b(\mathbb{R}^d)$. Then the initial error made by the Gaussian beam superposition (2.2.8) is as follows:

$$\|\tilde{\Psi}(0, x, y) - \tilde{\Psi}^\varepsilon(0, x, y)\|_{L^2_{x,y}} \leq C\varepsilon^{1/2},$$

where constant $C$ depends only on the initial amplitude $g(x, y)$ and the initial phase $S_0(x)$. 
The proof is split in two parts, see Lemma 2.4.1 and Lemma 2.4.2.

In order to measure the evolution error, we define $P$ the two-scale Schrödinger operator,

$$ P(\Psi) = i\varepsilon \partial_t \Psi + \frac{1}{2} (\varepsilon \nabla_x + \nabla_y)^2 \Psi - V(y) \Psi - V_\epsilon(x) \Psi. \quad (2.2.11) $$

**Theorem 2.2.2.** [Evolution error estimate] Let $K_0$ be a bounded set, conditions (2.1.5) and (2.1.6) are satisfied, the external potential $V_\epsilon(x) \in C_b^{d+4}(\mathbb{R}^d)$. Then the evolution error is

$$ \sup_{0 \leq t \leq T} \| P(\tilde{\Psi}^\varepsilon(t, \cdot)) \|_{L^2_{x,y}} \leq C \varepsilon^{3/2}, $$

where constant $C$ depends on the measure of set $K_0$, finite time $T$, the number of bands $N$, and external potential $V_\epsilon$.

The proof of this theorem is done in several steps, one step requires a phase estimate which uses essentially the “Non-squeezing” result obtained by Liu et al. [23].

Finally we recall the well-posedness estimate for the two-scale Schrödinger equation (2.1.1).

**Lemma 2.2.1.** The $L^2$–norm of the difference between the exact solution $\tilde{\Psi}$ and an approximate solution $\tilde{\Psi}^\varepsilon$ of the problem (2.1.1) is bounded above by the following estimate:

$$ \| \tilde{\Psi}(t,x,y) - \tilde{\Psi}^\varepsilon(t,x,y) \|_{L^2_{x,y}} \leq \| \tilde{\Psi}(0,x,y) - \tilde{\Psi}^\varepsilon(0,x,y) \|_{L^2_{x,y}} + \frac{1}{\varepsilon} \int_0^T \| P(\tilde{\Psi}^\varepsilon) \|_{L^2_{x,y}} \, dt, \quad 0 < t \leq T, $$

(2.2.12)

where $T$ is a finite time, $\tilde{\Psi}(0,\cdot), \tilde{\Psi}^\varepsilon(0,\cdot)$ are initial values of the exact and approximate solution respectively.

This result when combined with both initial error and evolution error gives the following.

**Corrolary 2.2.1.** The total error made by the first order Gaussian beam superposition method is of order $\varepsilon^{1/2}$ in the following sense

$$ \| \tilde{\Psi} - \tilde{\Psi}^\varepsilon \|_{L^2_{x,y}} \leq C \varepsilon^{1/2}. $$

**Remark 2.2.1.** For an infinite number of bands we need to have a uniform bound for $|\partial_k^\alpha E_n(k)|$ for $|\alpha| \leq 3$ as well as for the eigenfunctions $z_n(k,y)$ and its derivatives uniformly in band index $n$. This has not been verified yet.
In order to convert the two-scale result stated in Corollary 2.2.1 to the original problem, we prepare the following lemma.

**Lemma 2.2.2.** Assume that $f(x,y) \in L^2(\mathbb{R}^d, [-\pi, \pi]^d)$ and $f$ is $2\pi$ periodic in $y$. Then for sufficiently small $\varepsilon$,

$$
\left\| f \left( x, \frac{x}{\varepsilon} \right) \right\|_{L^2_x} \leq \frac{1}{\pi^\frac{d}{2}} \|f(x,y)\|_{L^2_{x,y}}. 
$$

(2.2.13)

**Proof.** Denote $Y^k_\varepsilon = [2\pi k \varepsilon, 2\pi (k+1) \varepsilon]$ and let $I_\varepsilon = \{ k \in \mathbb{Z}^d, \quad Y^k_\varepsilon \cap [-R,R]^d \neq \emptyset \}$ for any fixed $R > 0$. Then,

$$
\int_{|x| \leq R} f^2 \left( x, \frac{x}{\varepsilon} \right) dx \leq \sum_{k \in I_\varepsilon} \int_{Y^k_\varepsilon} f^2 \left( x, \frac{x}{\varepsilon} \right) dx.
$$

Here $|x|$ denotes $l^\infty$- norm of the vector $x$, hence $|x| \leq R$ corresponds to a $d$-dimensional cube. Introducing a change of variable $y = \frac{x}{\varepsilon}$ and taking advantage of the periodicity in $y$, one can rewrite the right hand side of the above expression in the shifted cell form:

$$
\int_{|x| \leq R} f^2 \left( x, \frac{x}{\varepsilon} \right) dx \leq \sum_{k \in I_\varepsilon} \varepsilon^d \int_{|y| \leq \pi} f^2(\varepsilon(y + 2\pi k), y) dy.
$$

For fixed $y$ the right hand side corresponds to the Riemann sum of the function

$$
g^2(x) = \int_{|y| \leq \pi} f^2(x + \varepsilon y, y) dy
$$

sampled at $x_k = 2\pi k \varepsilon$. Note that the step size in all direction $\Delta x_k = (2\pi \varepsilon)^d$, hence

$$
\sum_{k \in I_\varepsilon} \varepsilon^d \int_{|y| \leq \pi} f^2(\varepsilon(y + 2\pi k), y) dy = \frac{1}{(2\pi)^d} \sum_{k \in I_\varepsilon} g^2(x_k) \Delta x_k 
$$

$$
\rightarrow \frac{1}{(2\pi)^d} \int_{|x| \leq R} \int_{|y| \leq \pi} f^2(x,y) dy dx
$$

as $\varepsilon \to 0$.

with the first order of convergence. Therefore,

$$
\int_{|x| \leq R} f^2 \left( x, \frac{x}{\varepsilon} \right) dx \leq \frac{1}{(2\pi)^d} \int_{|x| \leq R} \int_{|y| \leq \pi} f^2(x,y) dy dx + C \varepsilon.
$$

Taking $C = (2\pi)^{-d} \|f\|^2_{L^2_{x,y}}$ and $\varepsilon < 1$, then the right hand side is bounded above by

$$
\frac{1}{2d-1-\pi^d} \int_{\mathbb{R}} \int_{|y| \leq \pi} f^2(x,y) dy dx.
$$

Passing limit $R \to \infty$ leads to the desired estimate (2.2.13). \qed
Set the error in two scale setting as

\[ e(t, x, y) = \tilde{\Psi}(t, x, y) - \tilde{\Psi}^\varepsilon(t, x, y), \]

then the error in original variable gives

\[ \Psi(t, x) - \Psi^\varepsilon(t, x) = e(t, x, x/\varepsilon). \]

Applying Lemma 2.2.2 and using Corollary 2.2.1 we prove Theorem 1.1 for the original problem.

### 2.3 Construction

In this section we first review the classical asymptotic approach and the band structure, then the Gaussian beam construction following [10]. For simplicity, the construction and proofs are presented in one-dimensional setting.

**Asymptotic Approach**

We look for an approximate solution to (2.1.1) of the form:

\[ \tilde{\Psi}^\varepsilon(t, x, y) = A(t, x, y)e^{i\Phi(t,x)/\varepsilon}, \]

where

\[ A(t, x, y) = A_0(t, x, y) + A_1(t, x, y)\varepsilon + \cdots + A_l(t, x, y)\varepsilon^l, \]

with \( A_i \) satisfying:

\[ A_i(t, x, y) = A_i(t, x, y + 2\pi), \quad i = 0, \ldots l. \]

Then the two-scale Schrödinger operator \( P \) defined in (2.2.11) when applied upon \( \tilde{\Psi}^\varepsilon \) gives

\[ P(\tilde{\Psi}^\varepsilon) = (c_0 + c_1\varepsilon + c_2\varepsilon^2 + \cdots + c_l\varepsilon^{l+2})e^{i\Phi/\varepsilon}, \]

where by a direct calculation,

\[ c_0 = [-\partial_t\Phi - \frac{1}{2}(-i\partial_y + \partial_x\Phi)^2 - V(y) - V_\varepsilon(x)]A_0 =: G(t, x, y)A_0, \]  

\[ c_1 = i\partial_tA_0 + \frac{1}{2}(2\partial_x \cdot \partial_y + 2i\partial_x\Phi \cdot \partial_x + i\partial_x^2\Phi)A_0 + G(t, x, y)A_1 =: iLA_0 + GA_1, \]

\[ c_j = \partial_x^2A_{j-2} + iLA_{j-1} + GA_j, \quad j = 2, 3, \ldots, l + 2. \]
Here

\[ L := \partial_t + (-i\partial_y + \partial_x \Phi)\partial_x + \frac{1}{2}\partial_x^2 \Phi. \]

Observe that, when \( \Phi \) is real valued, (2.3.1) is a standard ansatz of the geometric optics [10]. In the construction of geometric optic solutions it is required that \( c_j = 0, j = 0,1,\ldots,l + 2 \), which gives PDEs for \( \Phi, A_0, \cdots, A_l \). However, \( \Phi \) may develop finite time singularities at ‘caustics’ and equations for \( A_j \) then become undefined [10].

**Band Structure/Bloch Decomposition**

The relation \( c_0 = 0 \) can be rewritten as

\[ (\Phi_t + H(\partial_x \Phi, y) + V_e(x))A_0 = 0, \]

where \( H(k,y) \) with \( k = \partial_x \Phi \) is a self-adjoint differential operator,

\[ H(k,y) = \frac{1}{2}(-i\partial_y + k)^2 + V(y). \]

We let \( z_n \) be the normalized eigenfunction corresponding to \( E_n(k) \):

\[ H(k,y)z_n = E_n(k)z_n, \quad \langle z_n, z_n \rangle = 1. \]

From now on we will suppress the index \( n \), since the construction for each band remains the same.

We set the leading amplitude as

\[ A_0(t,x,y) = a(t,x)z(k(t,x),y), \]

where \( k = \partial_x \Phi \), hence (2.3.5) is satisfied as long as \( \Phi \) solves the Hamilton-Jacobi equation:

\[ F(t,x) := \partial_t \Phi + E(\partial_x \Phi) + V_e(x) = 0. \]

**A Bloch Decomposition-Based Gaussian Beam Method**

Let \((x,p) = (\tilde{x}(t), p(t))\) be a bicharacteristics of (2.3.8), then

\[ \dot{\tilde{x}} = E'(p), \quad \dot{p} = -V_e'(\tilde{x}). \]

From now on, we fix a bi-characteristics \( \{(\tilde{x}(t), p(t)), t > 0\} \) with initial data \((x_0, \partial_x S_0(x_0))\) for any \( x_0 \in K_0 = \text{supp}_x(g(x,y)) \). We denote by \( \gamma \) its projection into the \((x,t)\) space.
The idea underlying the Gaussian beam method is to build asymptotic solutions concentrated on a single ray \( \gamma \) so that \( \Phi(t, \tilde{x}(t)) \) is real and \( \text{Im}\{\Phi(t, y)\} > 0 \) for \( y \neq \tilde{x}(t) \). We are going to choose \( \Phi \) so that \( \text{Im}(\Phi) \geq cd(x, \gamma)^2 \), where \( d(x, \gamma) \) is a distance from \( x \) to the central ray \( \gamma \) [31]. Therefore, instead of solving (2.3.8) exactly, we only need to have \( F(x, t) \) vanish to higher order on \( \gamma \). For the first order Gaussian beam approximation we choose the phase \( \Phi(t, x) \) a quadratic function:

\[
\Phi(t, x) = S(t) + p(t)(x - \tilde{x}(t)) + \frac{1}{2}M(t)(x - \tilde{x}(t))^2. \tag{2.3.10}
\]

With this choice we have

\[
F(t, x) = \dot{S} + \dot{p}(x - \tilde{x}) - p\dot{x} + \frac{1}{2}\dot{M}(x - \tilde{x})^2 - M(x - \tilde{x})\dot{x} + E(p + M(x - \tilde{x})) + V_e(x). \tag{2.3.11}
\]

We see that \( F(t, \tilde{x}(t)) = 0 \) gives the evolution equation for \( S \),

\[
\dot{S} = pE'(p) - E(p) - V_e'(\tilde{x}).
\]

It can be verified \( \partial_x F(t, \tilde{x}(t)) = 0 \) is equivalent to \( \dot{p} = -V_e'(\tilde{x}) \), which is the second equation in (2.3.9). From \( \partial_x^2 F(t, \tilde{x}(t)) = 0 \) we obtain the equation for \( M \):

\[
\dot{M} = -E''(p)M^2 - V_e''(\tilde{x}). \tag{2.3.12}
\]

It is clear that we should set initial condition for the phase as

\[
S(0) = S_0(x_0), \tag{2.3.13}
\]

where \( S_0 \) is a given initial phase in (2.1.2). Note that equation (2.3.12) is a nonlinear Ricatti type equation. The important result about \( M \) is given in [10], proving that global solution for \( M \) exists and \( \text{Im}(M) \) remains positive (positive definite in multi-dimensional setting) for all time \( t \) as long as \( \text{Im}(M(0)) \) is positive. Therefore we choose

\[
M(0) = \partial_x^2 S_0(x_0) + i, \tag{2.3.14}
\]

which satisfies \( \text{Im}(M(0)) > 0 \) as required in the Gaussian beam approximation.

It follows from our construction that \( c_0 \) vanishes up to third order on \( \tilde{x} \). In fact,

\[
c_0 = G(az(k(t, x), y)) \tag{2.3.15}
\]

\[
= a(t, x)F(t, x)z(k(t, x), y)
\]

\[
= {\frac{a(t, x)}{3!}} \partial_x^2 F(t, x^*)z(k(t, x), y)(x - \tilde{x})^3,
\]
where \(x^*\) is an intermediate value between \(x\) and \(\tilde{x}\). A simple calculation gives

\[
\partial_t^3 F(t, x^*) = (V_e^{(3)}(x^*) + E^{(3)}(p + M(x^* - \tilde{x})))M^3(t),
\]

(2.3.16)

which is uniformly bounded near the ray \(\tilde{x}\) since \(V_e \in C^5_b(\mathbb{R})\) and (2.1.5) holds. Hence \(c_0\) will be bounded by \(O(|x - \tilde{x}|^3)\) as long as the amplitude is bounded.

**Equation for the amplitude**

For the first order Gaussian beam construction, we shall determine the amplitudes so that \(c_1\) vanishes to the first order on \(\gamma\). Note that

\[
c_1 = iLA_0 + GA_1,
\]

where

\[
G = -(\Phi_t + H(k, y) + V_e(x)) = -F(t, x) + E(k) - H(k, y).
\]

On the ray \(x = \tilde{x}(t)\), we require that \(c_1 = 0\), that is

\[
iLA_0 + (E(k) - H(k, y))A_1 = 0.
\]

In order for \(A_1\) to exist, it is necessary that

\[
\langle LA_0, z \rangle |_{x = \tilde{x}(t)} = 0.
\]

(2.3.17)

For \(x \neq \tilde{x}(t)\), we have

\[
c_1 = iL(A_0) - FA_1 + (E(k) - H(k, y))A_1^\top,
\]

where \(A_1^\top\) contains the orthogonal compliment of \(z\), satisfying \(\langle A_1^\top, z \rangle = 0\). We let

\[
A_1^\top = i(E(k) - H)^{-1}[(LA_0, z)z - L(A_0)].
\]

(2.3.18)

Therefore using (2.3.17) and Taylor expansion at \(\tilde{x}\),

\[
c_1 = i\langle LA_0, z \rangle - FA_1 = i\partial_x \langle LA_0, z \rangle(t, x^*)(x - \tilde{x}) - FA_1.
\]

(2.3.19)

With further refined calculation, (2.3.17) and (2.3.19) yield the following result.
Lemma 2.3.1. For the first order Gaussian beam construction, \( a(t, x) = a(t; x_0) \) and satisfies the following evolution equation along the ray \( x = \tilde{x}(t) \):

\[
a_t = a \left( V'_e(\tilde{x}) \langle \partial_k z(p, \cdot), z(p, \cdot) \rangle - \frac{1}{2} E''(p) M \right). \tag{2.3.20}
\]

Moreover, for \( x \neq \tilde{x}(t) \) we have

\[
c_0 = \frac{a(t; x_0)}{3!} \partial_k^3 F(t, x^*) z(k, y)(x - \tilde{x})^3, \tag{2.3.21}
\]

\[
c_1 = -ia \langle \partial_k z(p, \cdot), z(p, \cdot) \rangle (E''(p) M^2 + V'_e(\tilde{x}))(x - \tilde{x}) - F(t, x) A_1, \tag{2.3.22}
\]

\[
c_2 = a(t; x_0) M^2 \partial_k^2 z(k, y) + i L A_1, \tag{2.3.23}
\]

where \( A_1 \in \text{span}\{A_1^\top, z\} \).

Proof. Recall that

\[
A_0 = az(k(t, x), y), \quad k(t, x) = p(t) + M(t)(x - \tilde{x}(t))
\]

and

\[
L = \partial_t + H_k(k, y) \partial_x + \frac{1}{2} \partial_x^2 \Phi = \partial_t + H_k(k, y) \partial_x + \frac{1}{2} M.
\]

We take \( a(t, x) = a(t; x_0) \), and calculate

\[
\langle L(az), z \rangle = \partial_t a + \frac{1}{2} a M + a \langle \partial_t z, z \rangle + a \langle H_k \partial_x z, z \rangle
\]

\[
= \partial_t a + a \left( \frac{1}{2} M + k_t \langle \partial_k z, z \rangle + k_x \langle H_k \partial_k z, z \rangle \right).
\]

We observe that the eigenvalue identity \( H z = E z \) holds for any \( k \), implying

\[
H_k k_z + 2H_k \partial_k z + H \partial_k^2 z = E''(k) z + 2E' \partial_k z + E \partial_k^2 z.
\]

This against \( z \) using \( H_{kk} = 1 \) and \( \langle (H - E) \partial_k^2 z, z \rangle = 0 \) leads to

\[
E''(k) = 1 + 2 \langle H_k \partial_k z, z \rangle - 2E' \langle \partial_k z, z \rangle.
\]

Hence using \( k_x = M \) we have

\[
\frac{1}{2} M + k_x \langle H_k \partial_k z, z \rangle = \frac{1}{2} E''(k) M + E' M \langle \partial_k z, z \rangle.
\]

Putting together we obtain

\[
\langle L(az), z \rangle = \partial_t a + a \left( \frac{1}{2} E''(k) M + (k_t + E' M) \langle \partial_k z, z \rangle \right),
\]
where
\[ k_t = -V_e'(\tilde{x}) - E'(p)M + \dot{M}(x - \tilde{x}(t)). \]

Thus (2.3.17) gives the desired amplitude equation. Recalling (2.3.15) and (2.3.16) we have (2.3.21). (2.3.19) yields
\[ c_1 = ia\dot{M}(\partial_k z, z)(x - \tilde{x}) - FA_1, \]
which in virtue of (2.3.12) gives (2.3.22). From (2.3.4) it follows that
\[ c_2 = \partial_x^2(az) + iLA_1 = a(k_x)^2\partial_x^2 z + iLA_1 \]
which gives (2.3.23).

Therefore, the system of ODEs for GB components is set up:

\[
\begin{cases}
\dot{x} = E'(p), & x|_{t=0} = x_0, \\
\dot{p} = -V'_e(\tilde{x}), & p|_{t=0} = \partial_x S_0(x_0), \\
\dot{S} = pE'(p) - E(p) - V_e(\tilde{x}), & S|_{t=0} = S_0(x_0), \\
\dot{M} = -E''(p)M^2 - V''_e(\tilde{x}), & M|_{t=0} = \partial_x^2 S_0(x_0) + i, \\
\dot{a} = a(V'_e(\tilde{x})\langle \partial_k z(p,\cdot), z(p,\cdot) \rangle - \frac{1}{2}E''(p)M), & a|_{t=0} = a(x_0),
\end{cases}
\]

where the initial value for the amplitude \(a(t; x_0)\) is taken as
\[ a|_{t=0} = a(x_0) = \int_0^{2\pi} g(x, y)z(\partial_x S_0, y)dy. \]

Remark 2.3.1. For the derivation of the equations for the Gaussian beam components for the higher order approximations, we refer the reader to [10].

In order to complete the estimate for \(c_i\), we still need to estimate \(A_1\). The following result will be used later in the estimate of the evolution error.

Lemma 2.3.2. If eigenvector \(z(k, y)\) satisfies the following condition:
\[
\sum_{\beta_1 \leq 2, \beta_1 + \beta_2 \leq 4} \|\partial_k^{\beta_1} \partial_y^{\beta_2} z(k, y)\|_{L_2^y} \leq Z < \infty.
\]
Then for \(\alpha = 0, 1\),
\[
\sup_{t, x_0} \int_0^{2\pi} |L^\alpha A_1|^2 dy \leq C Z(1 + Z + Z^2),
\]
where \(C\) depends on the spectral gap \(\Delta E = \min_{i \neq j} |E_i - E_j| > 0\) and the Gaussian beam components.
Proof. Since $A_1$ is a linear combination of $A_1^\top$ and $z$, we will prove (2.3.27) for $A_1^\top$ only. Set

$$B := i(LA_0 - (LA_0, z))z,$$

we have

$$A_1^\top = (H - E)^{-1}B.$$  \hfill (2.3.28)

We proceed in two steps:

**Step 1.** Estimate of $LA_1^\top$ in terms of $B$.

A careful calculation gives that

$$(H - E)LA_1^\top = LB - k_t (H_k - E_k)A_1^\top - k_x H_k (H_k - E_k) A_1^\top + iV'(y) \partial_x A_1^\top.$$ \hfill (2.3.29)

In fact, applying $L$ to (2.3.28) gives

$$(H_k - E_k)k_t A_1^\top + (H - E) \partial_t A_1^\top + H_k \partial_x [(H - E) A_1^\top] + \frac{1}{2} k_x (H - E) A_1^\top = LB.$$ \hfill (2.3.29)

Note that

$$\partial_x [(H - E) A_1] = (H_k - E_k) k_x A_1 + (H - E) \partial_x A_1.$$ \hfill (2.3.29)

Using the definition of operators $H$ and $H_k$ we also have

$$H_k(H - E) = (H - E)H_k - iV'(y).$$

These together verifies (2.3.29). From (2.3.29) it follows that

$$\|LA_1^\top\| \leq \frac{C}{\Delta E}(\|LB\| + \sum_{j=0}^{2} \|\partial^j_y A_1^\top\| + \|\partial_x A_1^\top\|),$$ \hfill (2.3.30)

here $C$ depends on $k_t, k_x, E_k$ and $V'(y)$, and we have used the following resolvent estimate,

$$\|(H - E)^{-1}\| \leq \frac{1}{\Delta E}.$$ \hfill (2.3.30)

Next we estimate the right hand of (2.3.30) in terms of $B$. From here on we use $C$ to denote a generic constant depending on $\Delta E, k, E, z$ and their derivatives. We note that

$$LB = B_t + H_k B_x + \frac{1}{2} k_x B = B_t - iB_{xy} + k B_x + \frac{1}{2} k_x B,$$
which yields
\[ \|LB\| \leq C(\|B\| + \|B_t\| + \|B_x\| + \|B_{xy}\|). \]

From (2.3.28) it follows that
\[ B_y = (H - E)A_{1y} - iV'(y)A_1, \]
\[ B_{yy} = (H - E)A_{1yy} - 2iV'(y)A_{1y} - iV''(y)A_1, \]
\[ B_x = (H - E)A_{1x} + k_x(H_k - E_k)A_1. \]

Again from (2.3.28) we obtain \( \|A_{1y}\| \leq C\|B\| \), which when combined with the above gives
\[ \|A_{1y}\| \leq C(\|B\| + \|B_y\|), \]
\[ \|A_{1yy}\| \leq C(\|B_{yy}\| + \|A_{1y}\| + \|A_1\|) \leq C \sum_{j=0}^{2} \|\partial_j^2 B\|, \]
\[ \|A_{1x}\| \leq C(\|B_x\| + \|A_{1y}\| + \|A_1\|) \leq C(\|B\| + \|B_y\| + \|B_x\|). \]

Therefore,
\[ \|LA_{1\top}\| \leq C(\|B\| + \|B_t\| + \|B_x\| + \|B_{xy}\| + \|B_y\| + \|B_{yy}\|). \]  

(2.3.31)

**Step 2. Estimate of \( B \).**

Note that
\[ B = L(az) - \langle L(az), z \rangle z \]
\[ = ak_t(z_k - \langle z_k, z \rangle) + ak_x(H_k z_k - \langle H_k z_k, z \rangle)z \]
\[ = ak_t \tilde{f}_1 + ak_x \tilde{f}_2, \]
where \( \tilde{f}_i \) are of the form
\[ \tilde{f}(k, y) = f(k, y) - \langle f(k, \cdot), z(k, \cdot) \rangle z(k, y), \]
with \( f_1 = z_k \) and \( f_2 = H_k z_k = -iz_{ky} + kz_k \). The right hand side of (2.3.31) is majored by
\[ I_1 + I_2 := C \sum_{i=1}^{2} (\|\tilde{f}_i\| + \|\partial_t \tilde{f}_i\| + \|\partial_x \tilde{f}_i\| + \|\partial_{xy} \tilde{f}_i\| + \|\partial_y \tilde{f}_i\| + \|\partial_{yy} \tilde{f}_i\|). \]
We apply Lemma 2.3.3 below to bound both $I_1$ and $I_2$.

\[
I_1 \leq C(\|z_k\| + \|z_{kk}\| + \|z_k\|^2 + (1 + \|z_k\|)(\|z_{ky}\| + \|z_{kyy}\|)) + \|z_{kk}\|
\]
\[
\|z_{kk}\| \|z_y\| + \|z_{ky}\| \|z_k\| + \|z_k\|^2 \|z_y\|
\]
\[
\leq CZ(1 + Z + Z^2).
\]

Since $f_2 = -iz_{ky} + kf_1$, it suffices to bound $I_2$ by considering only $f_2 = z_{ky}$. By Lemma 2.3.3 we have

\[
I_2 \leq C(\|z_{ky}\| + \|z_{kk}\| + \|z_{ky}\||z_k||z_k|
\]
\[
+ \|z_{kyy}\| + \|z_{kky}\| \|z_y\| + \|z_{kyy}\| \|z_k\| + \|z_{ky}\|^2 + \|z_{ky}\| \|z_k\| \|z_y\|
\]
\[
\leq CZ(1 + Z + Z^2).
\]

These together with (2.3.31) yield

\[
\|LA_1\| \leq CZ(1 + Z + Z^2).
\]

This proves the boundedness of $\|LA_1\|$. \hfill \Box

**Lemma 2.3.3.** Let $f(k, y)$ be smooth and integrable in $y$ and

\[
\tilde{f}(k, y) = f(k, y) - \langle f(k, \cdot), z(k, \cdot) \rangle z(k, y).
\]

Then for $k = k(t, x)$ the following estimates hold:

1. $\|\tilde{f}_t, \tilde{f}_x\| \leq C(\|f_k\| + \|f\| \|z_k\|),$

2. $\|\partial^j_y \tilde{f}\| \leq \|\partial^j_y f\| + \|f\| \|\partial^j_y z\|$, \quad $j = 1, 2,$

3. $\|\tilde{f}_{xy}\| \leq C(\|f_{ky}\| + \|f_k\| \|z_y\| + \|f_y\| \|z_k\| + \|f\| \|z_{ky}\| + \|f\| \|z_k\| \|z_y\|),$

where constant $C$ depends on $k_t$ and $k_x$. 

Proof. By the chain rule,
\[ \dot{\tilde{f}}_t = k_t f_k - k_t \langle f_k, z \rangle z - \bar{k}_t (f, z_k) z - k_t \langle f, z \rangle z_k. \]
Using the Cauchy inequality together with the fact that $z$ is normalized, we obtain
\[ \|\dot{\tilde{f}}_t\| \leq C(\|f_k\| + 2\|f\|\|z_k\|). \]
Same estimate follows for $f_x$.

For differentiation in $y$ we have
\[ \partial^j_y \tilde{f} = \partial^j_y f - \langle f, z \rangle \partial^j_y z, \]
leading to
\[ \|\partial^j_y \tilde{f}\| \leq \|\partial^j_y f\| + \|f\|\|\partial^j_y z\|. \]
Finally,
\[ \tilde{f}_{xy} = k_x f_{k_y} - k_x \langle f_k, z \rangle z_y - \bar{k}_x (f, z_k) z_y - k_x \langle f, z \rangle z_{k_y}. \]
Hence
\[ \|\tilde{f}_{xy}\| \leq C(\|f_{k_y}\| + \|f_k\|\|z_y\| + \|f\|\|z_k\|\|z_y\| + \|f\|\|z_{k_y}\|) \]
which concludes the proof of the lemma. \[\]

Gaussian Beam Superposition and Residuals

We solve ODE system (2.3.24) for each band, and obtain a band based Gaussian beam approximation along a given ray:
\[ \tilde{\Psi}^{\varepsilon n}_{GB}(t, x, y; x_0) = (a_n(t; x_0) z_n(k_n, y) + \varepsilon A_1^n(t, x, y; x_0)) e^{i\Phi_n(t, x; x_0)/\varepsilon}. \]
Since the Schrödinger equation is linear, the approximate solution can be generated by a superposition of neighboring Gaussian beams and over all available bands
\[ \tilde{\Psi}(t, x, y) = \frac{1}{\sqrt{2\pi \varepsilon}} \int_{K_0} \sum_{n=1}^{N} \tilde{\Psi}^{\varepsilon n}_{GB}(t, x, y; x_0) dx_0, \]
where $\frac{1}{\sqrt{2\pi \varepsilon}}$ is a normalized constant chosen to match initial data against the Gaussian profile. Let us use the notation
\[ \tilde{\Psi}^{\varepsilon n}(t, x, y) := \frac{1}{\sqrt{2\pi \varepsilon}} \int_{K_0} \tilde{\Psi}^{\varepsilon n}_{GB}(t, x, y; x_0) dx_0, \]
then Lemma 2.3.1 yields the following residual representation:

\[ P(\tilde{\Psi}^{\varepsilon n}) = \frac{1}{\sqrt{2\pi \varepsilon}} \int_{K_0} (c_{0n} + \varepsilon c_{1n} + \varepsilon^2 c_{2n}) e^{i\Phi_n(t,x,x_0)/\varepsilon} \, dx_0. \]  

(2.3.36)

In next two sections we provide proofs of the accuracy results. We start with the initial error estimation.

### 2.4 Initial Error - Proof of Theorem 2.2.1.

For simplicity of presentation, we only give the one dimensional estimate with \( d = 1 \). The initial phase can be expressed as

\[ S_0(x) = S_0(x_0) + S_0'(x_0)(x - x_0) + \frac{S_0''(x_0)(x - x_0)^2}{2} + R_2^{x_0}[S_0] = T_2^{x_0}[S_0](x) + R_2^{x_0}[S_0](x), \]

where

\[ R_2^{x_0}[S_0] = \frac{|S_0^{(3)}(\eta(x,x_0))|(x - x_0)^3}{3!} \]

is the remainder of the Taylor expansion. The idea of the proof of Theorem 2.2.1 is to introduce

\[ \Psi^* = \frac{1}{\sqrt{2\pi \varepsilon}} \int g(x_0,y) e^{iT_2^{x_0}[S_0](x)/\varepsilon} e^{-\frac{(x-x_0)^2}{2\varepsilon}} \, dx_0, \]

(2.4.1)

so that

\[ \|\tilde{\Psi}_0 - \tilde{\Psi}_0^\varepsilon\| \leq \|\tilde{\Psi}_0 - \Psi^*\| + \|\Psi^* - \tilde{\Psi}_0^\varepsilon\|, \]

(2.4.2)

where the initial condition \( \tilde{\Psi}_0 = \tilde{\Psi}(0,x,y) \) defined in (2.2.1), \( \tilde{\Psi}_0^\varepsilon = \tilde{\Psi}^\varepsilon(0,x,y) \) defined in (2.2.8) is the the Gaussian beam superposition evaluated at \( t = 0 \),

\[ \tilde{\Psi}_0^\varepsilon = \frac{1}{\sqrt{2\pi \varepsilon}} \int_{K_0} \sum_{n=1}^N a_n(x_0)z_n(\partial_x \Phi^0(x;x_0),y) + \varepsilon A_1^n(0,x,y;x_0))e^{i\Phi^0(x;x_0)/\varepsilon} \, dx_0, \]

(2.4.3)

where from (2.2.9) we have

\[ \Phi^0(x,x_0) = T_2^{x_0}[S_0](x) + \frac{i(x-x_0)^2}{2}. \]

Here and in what follows, the unmarked norm \( \| \cdot \| \) denotes \( \| \cdot \|_{L_2^{x,y}} \) - norm unless otherwise specified.

The rest of this section is to estimate two terms on the right of (2.4.2), which will be given in Lemma 4.1 and Lemma 4.2 below, respectively.
Lemma 2.4.1. Let $\Psi^*$ be defined in (2.4.1), $g(x, y) \in H^1(K_0 \times [0, 2\pi])$, then

$$\|\Psi^* - \tilde{\Psi}_0\| \leq \left( \|\partial_x g\| + \sqrt{\frac{5}{12}} \max_{x \in \mathbb{R}} |S_0^{(3)}(x)| \|g\| \right) \varepsilon^{1/2}. $$

Proof. Using that

$$\Psi^* - \tilde{\Psi}_0 = \frac{1}{\sqrt{2\pi} \varepsilon} \int_{\mathbb{R}} \left( g(x, y) - g(x, y) \right) e^{iT^a_{2\varepsilon} [S_0](x)/\varepsilon} e^{-\left(\frac{x-x_0}{2\varepsilon}\right)^2} dx_0 = I + J, \tag{2.4.4}$$

where

$$I = \frac{1}{\sqrt{2\pi} \varepsilon} \int_{\mathbb{R}} \left( g(x, y) - g(x, y) \right) e^{iT^a_{2\varepsilon} [S_0](x)/\varepsilon} e^{-\left(\frac{x-x_0}{2\varepsilon}\right)^2} dx_0,$$

$$J = \frac{1}{\sqrt{2\pi} \varepsilon} \int_{\mathbb{R}} \left( g(x, y) - g(x, y) \right) e^{iS_0(x)/\varepsilon} e^{-\left(\frac{x-x_0}{2\varepsilon}\right)^2} dx_0.$$

Our next step is to find estimates for $\|I\|$ and $\|J\|.$

$$\|I\|^2 = \frac{1}{\pi} \int_{0}^{2\pi} \int_{\mathbb{R}} \left( \int_{\mathbb{R}} g(x, y) \right) e^{iT^a_{2\varepsilon} [S_0](x)/\varepsilon} e^{-\left(\frac{x-x_0}{2\varepsilon}\right)^2} dx_0 \right]^2 dx_0.$$

For fixed $x,$ we introduce a new variable $\xi = \frac{x-x_0}{\sqrt{2\varepsilon}}, \quad d\xi = -\sqrt{2\varepsilon} d\xi$ to obtain

$$\|I\|^2 = \frac{1}{\sqrt{2\pi} \varepsilon} \int_{0}^{2\pi} \int_{\mathbb{R}} \left( \int_{\mathbb{R}} g(x, y) \right) e^{iS_0(x)/\varepsilon} e^{-\left(\frac{x-x_0}{2\varepsilon}\right)^2} dx_0 \right]^2 dx_0.$$

By the Hölder inequality,

$$\|I\|^2 \leq \frac{1}{\pi} \int_{0}^{2\pi} \int_{\mathbb{R}} \int_{\mathbb{R}} |g(x, y)|^2 e^{-\xi^2} d\xi d\xi dy.$$

Using the mean value theorem for $g,$ we have

$$g(x - \sqrt{2\varepsilon} \xi, y) - g(x, y) = -\partial_x g(x - \eta^*(x - x_0), y) \sqrt{2\varepsilon} \xi = -\partial_x g(x - \eta^*(x - x_0), y) \sqrt{2\varepsilon} \xi.$$

Hence,

$$\|I\|^2 \leq \frac{2\varepsilon}{\sqrt{\pi}} \int_{0}^{2\pi} \int_{\mathbb{R}} \int_{\mathbb{R}} \left| \partial_x g(x - \eta^*(x - x_0), y) \right|^2 d\xi d\xi dy = \frac{2\varepsilon}{\sqrt{\pi}} \|\partial_x g\|^2 \int_{\mathbb{R}} \xi^2 e^{-\xi^2} d\xi = \varepsilon \|\partial_x g\|^2.$$
Now we turn to the estimation of $\|J\|$:

$$
\|J\|^2 = \frac{1}{2\pi \varepsilon} \left| \int_{\mathbb{R}} g(x, y) \left( e^{iT_2^0[S_0(x)/\varepsilon]} - e^{iS_0(x)/\varepsilon} \right) e^{-\frac{-(x-x_0)^2}{4\varepsilon}} dx_0 \right|^2 \\
\leq \frac{1}{2\pi \varepsilon} \int_{0}^{2\pi} \int_{\mathbb{R}} |g(x, y)| |e^{iS_0(x)/\varepsilon}| |e^{-iR_2^0[S_0(x)/\varepsilon]} - 1| e^{-\frac{(x-x_0)^2}{4\varepsilon}} dx_0 dy.
$$

Since $S_0$ is real, $|e^{iS_0(x)/\varepsilon}| = 1$. The above is further bounded by

$$
\|J\|^2 \leq \frac{1}{2\pi \varepsilon} \int_{0}^{2\pi} \int_{\mathbb{R}} |g(x, y)| \left[ \left( \cos \left( \frac{R_2^0[S_0(x)]}{\varepsilon} \right) - 1 \right)^2 + \sin^2 \left( \frac{R_2^0[S_0(x)]}{\varepsilon} \right) \right] e^{-\frac{(x-x_0)^2}{4\varepsilon}} dx_0 dy.
$$

Using a half-angle formula for $\sin x$ and that $|\sin x| \leq |x|$, we obtain:

$$
\|J\|^2 \leq \frac{1}{2\pi \varepsilon} \int_{0}^{2\pi} \int_{\mathbb{R}} |g(x, y)|^2 e^{-\frac{(x-x_0)^2}{4\varepsilon}} dx_0 dy \int_{\mathbb{R}} \frac{|S_0^{(3)}(\eta)|^2}{36} |x-x_0|^6 e^{-\frac{(x-x_0)^2}{4\varepsilon}} dx_0 dy.
$$

Using the remainder formula and the Hölder inequality,

$$
\|J\|^2 \leq \frac{1}{2\pi \varepsilon} \int_{0}^{2\pi} \int_{\mathbb{R}} |g(x, y)|^2 e^{-\frac{(x-x_0)^2}{4\varepsilon}} dx_0 \int_{\mathbb{R}} \frac{|S_0^{(3)}(\eta)|^2}{36} |x-x_0|^6 e^{-\frac{(x-x_0)^2}{4\varepsilon}} dx_0 dy.
$$

Now, applying the same change of variable as for the term $I$, $\xi = \frac{x-x_0}{\sqrt{2\varepsilon}}$, $(x$ variable is fixed) we get:

$$
\|J\|^2 \leq \frac{1}{2\pi \varepsilon} \left\| g \right\|^2 \frac{\left( \max_{\mathbb{R}} |S_0^{(3)}(x)| \right)^2}{36} \sqrt{2\pi} \int_{\mathbb{R}} 8\sqrt{2\varepsilon}^{-2+3+1/2} |\xi|^6 e^{-\varepsilon^2} d\xi \
\leq \frac{\sqrt{2\pi} \max_{x \in \mathbb{R}} |S_0^{(3)}(x)|^2}{72\pi} \times 8\sqrt{2} \times \frac{15}{8} \sqrt{\pi}\|g\|^2 \varepsilon.
$$

Hence, summing both parts, we conclude that:

$$
\|\Psi^* - \tilde{\Psi}_0\| \leq \|I\| + \|J\| \\
\leq \left( \|\partial_x g\| + \sqrt{\frac{5}{12}} \max_{x \in \mathbb{R}} |S_0^{(3)}(x)| \|g\| \right)^{1/2} \varepsilon^{1/2}.
$$

□

Our next step is to find an estimate for the difference between GB ansatz and $\Psi^*$. 
Lemma 2.4.2. The following estimate holds:

\[ \| \tilde{\Psi}_0 - \Psi^* \| \leq C \varepsilon^{1/2}, \]

where

\[ C = 2\pi \max_{k, 1 \leq n \leq N} \| \partial_k z_n(k, y) \|_{L^2_{xy}}^2 \int_{K_0} \left| \sum_{n=1}^{N} a_n(x_0) \right|^2 (S_0''(x_0) + 1) dx_0, \]

can be computed from the initial data.

Proof. According to our construction,

\[ \| \tilde{\Psi}_0 - \Psi^* \|^2 = \left\| \tilde{\Psi}_0 - \frac{1}{\sqrt{2\pi\varepsilon}} \int_{\mathbb{R}} g(x_0, y) e^{i\mathbb{R}^2 \eta_0(x_0)/\varepsilon} e^{-\frac{(x-x_0)^2}{2\varepsilon}} dx_0 \right\|^2 \]

\[ = \frac{1}{2\pi\varepsilon} \int_0^{2\pi} \int_{\mathbb{R}} \left[ \int_{K_0} \left| \sum_{n=1}^{N} (a_n(x_0)(z_n(\partial_x \Phi^0(x, x_0), y) - z_n(\partial_x S_0(x_0), y))) + \varepsilon A_n^0(0, x, y; x_0) \right|^2 dx_0 \right] dy. \]

Then, putting the absolute value sign inside the integral over \( K_0 \), we observe that

\[ \| \tilde{\Psi}_0 - \Psi^* \|^2 \leq \frac{1}{2\pi\varepsilon} \int_0^{2\pi} \int_{\mathbb{R}} \left[ \int_{K_0} \left| \sum_{n=1}^{N} (a_n(x_0)(z_n(\partial_x \Phi^0(x, x_0), y) - z_n(\partial_x S_0(x_0), y))) + \varepsilon A_n^0(0, x, y; x_0) \right|^2 dx_0 \right] dy. \]

By the Hölder inequality,

\[ \| \tilde{\Psi}_0 - \Psi^* \|^2 \leq \frac{1}{2\pi\varepsilon} \int_0^{2\pi} \int_{\mathbb{R}} \left[ \int_{K_0} \left| \sum_{n=1}^{N} \varepsilon A_n^0(0, x, y; x_0) \right|^2 e^{-\frac{(x-x_0)^2}{2\varepsilon}} dx_0 \right] \int_{K_0} \left| \sum_{n=1}^{N} (a_n(x_0)(z_n(\partial_x \Phi^0(x, x_0), y) - z_n(\partial_x S_0(x_0), y))) \right|^2 dx_0 dxdy. \]

Using that

\[ z_n(\partial_x \Phi^0(x, x_0), y) - z_n(\partial_x S_0(x_0), y) = z_n(S_0''(x_0) + (S_0''(x_0) + i)(x - x_0), y) - z_n(S_0''(x_0), y) = \partial_k z_n(\eta_n(x, x_0), y)(S_0''(x_0) + i)(x - x_0), \]
we obtain:

\[
\| \tilde{\Psi}_0 - \Psi^* \|^2 \leq \frac{1}{\sqrt{2\pi}} \int_0^{2\pi} \int_{K_0} \int_{\mathbb{R}} \left| \sum_{n=1}^{N} (a_n(x_0) \partial_k z_n(\eta_n(x, x_0), y)(S_0''(x_0) + i)(x - x_0) \right|^2 e^{-(x-x_0)^2/2\varepsilon} dx dy \\
+ \varepsilon A_1^n(0, x_0; y; x_0) \right|^2 e^{-(x-x_0)^2/2\varepsilon} dx_0 dy \\
\leq \frac{2}{\sqrt{2\pi}} \max_{k, 1 \leq n \leq N} \| \partial_k z_n(k, y) \|_{L^\infty}^2 \int_0^{2\pi} \int_{K_0} \sum_{n=1}^{N} \left| \right|^2 \left| (S_0''(x_0) + 1) dx_0 dy \\
\leq 2\varepsilon \max_{k, 1 \leq n \leq N} \| \partial_k z_n(k, y) \|_{L^\infty}^2 \int_0^{2\pi} \int_{K_0} \sum_{n=1}^{N} a_n(x_0) \left| (S_0''(x_0) + 1) dx_0 dy \\
= I_1 + I_2.
\]

Switching the order of integration and applying the change of variable for fixed \( x_0 \),

\[
\xi = \frac{x - x_0}{\sqrt{2\varepsilon}}, \quad dx = \sqrt{2\varepsilon} d\xi
\]

together with the fact that \( S_0''(x_0) \) is real,

\[
I_1 \leq \frac{1}{\sqrt{2\pi}} \int_0^{2\pi} \int_{K_0} \int_{\mathbb{R}} \left| \sum_{n=1}^{N} a_n(x_0) \partial_k z_n(\eta_n(x_0), y)(S_0''(x_0) + i)(x - x_0) \right|^2 \varepsilon^2 \xi^2 e^{-\xi^2} dx_0 dy \\
\leq \frac{2\varepsilon}{\sqrt{\pi}} \max_{k, 1 \leq n \leq N} \| \partial_k z_n(k, y) \|_{L^\infty} \int_0^{2\pi} \int_{K_0} \sum_{n=1}^{N} a_n(x_0) \left| (S_0''(x_0) + 1) dx_0 dy \\
\leq 2\varepsilon \max_{k, 1 \leq n \leq N} \| \partial_k z_n(k, y) \|_{L^\infty} \int_0^{2\pi} \int_{K_0} \sum_{n=1}^{N} a_n(x_0) \left| (S_0''(x_0) + 1) dx_0 dy \\
\]

Since \( N < \infty \) is finite, the right hand side is bounded by \( C\varepsilon \) where constant \( C \) depends on the initial data.

As for \( I_2 \),

\[
I_2 = \frac{\varepsilon^2}{\sqrt{2\pi}} \int_0^{2\pi} \int_{K_0} \int_{\mathbb{R}} \left| \sum_{n=1}^{N} A_1^n(0, x, y; x_0) \right|^2 e^{-(x-x_0)^2/2\varepsilon} dx_0 dy,
\]

we use the definition of \( A_1 \) in (2.3.18), where we use that \((H(k, y) - E(k))^{-1}\) is bounded operator (moreover, it is compact), hence \( A_1 \) is bounded. Also, the same change of variable as in the case of \( I_1 \) estimate will produce the additional rate of convergence.

Hence,

\[
I_2 \leq C\varepsilon^2
\]

and may be neglected since its order of convergence is higher than for \( I_1 \).
Using the triangle inequality, we thus get the estimate for the initial error:

$$\|\tilde{\Psi}_0 - \tilde{\Psi}_0^{\epsilon}\| \leq \|\tilde{\Psi}_0 - \Psi^*\| + \|\Psi^* - \tilde{\Psi}_0^{\epsilon}\| \leq C\varepsilon^{1/2}.$$ 

### 2.5 Evolution Error - Proof of Theorem 2.2.2

We prove Theorem 2.2.2 in several steps, in one dimensional setting; an extension to multi-dimensions will be given in next section. Taking advantage of the band structure of the asymptotic construction and the linearity of the Schrödinger operator, we rewrite

$$P(\tilde{\Psi}^\varepsilon) = P\left(\sum_{n=1}^{N} \tilde{\Psi}^{\varepsilon n}\right) = \sum_{n=1}^{N} P(\tilde{\Psi}^{\varepsilon n}),$$

where $\tilde{\Psi}^{\varepsilon n}$ is defined in (2.3.35). By the Minkowski inequality,

$$\|P(\tilde{\Psi}^\varepsilon)\| \leq \sum_{n=1}^{N} \|P(\tilde{\Psi}^{\varepsilon n})\|.$$ 

Using residual representation of $P(\tilde{\Psi}^{\varepsilon,n})$ from (2.3.36) in section 3, we have

$$P(\tilde{\Psi}^{\varepsilon n}) = \sum_{j=0}^{2} I_{jn},$$

where

$$I_{jn} = \frac{\varepsilon^{j-\frac{1}{2}}}{(2\pi)^{\frac{3}{2}}} \int_{K_0} G_{jn}(t, x; x_0, y)\left(x - \tilde{x}_n(t; x_0)\right)^{(3-2j)}e^{i\Phi_n(t,x_{x0})/\varepsilon} dx_0,$$  (2.5.1)

$$G_{0n}(t, x; x_0, y) = \frac{1}{3!}a_n(t; x_0)\partial^3_z F_n(t, x^*) z_n(k_n, y),$$  (2.5.2)

$$G_{1n}(t, x; x_0) = (i\partial_k z_n, z_n)\tilde{M} - \frac{1}{3!}\partial^3_x F_n(t, x^*) A_{1n}(x - \tilde{x}_n)^2.$$  (2.5.3)

$$G_{2n}(t, x; x_0, y) = a_n(t; x_0)M^2_n\partial^2_k z_n(k_n, y) + iLA_{1n}.$$  (2.5.4)

Let ' denote quantities defined on the ray emanating from $x'_0$ such as $\tilde{x}_n', c_{jn}'$ and $\Phi'_n$.

From Lemma 2.3.1 and Lemma 2.3.2 it follows the following bound:

$$\int_{0}^{2\pi} |G_{jn} G_{jn}'| dy \leq C_1.$$  (2.5.5)

Here we note that $G_{1n}$ contains a term involving $(x - \tilde{x}_n)^2$ which becomes unbounded when $x$ is far away from the ray $\tilde{x}_n$. In such case, the Gaussian beam factor $e^{-\delta|\tilde{x}_n|^2/\varepsilon}$ needs to be taken into account.
We compute the $L^2$ norm of $I_{jn}$ by
\[
\|I_{jn}\|^2 = \int_0^{2\pi} \int_{\mathbb{R}} I_{jn}(t, x; x_0, y) \cdot I_{jn}(t, x; x_0', y) \, dx \, dy \\
= \int_0^{2\pi} \int_{K_0} \int_{K_0} J_{jn}(x, y, x_0, x_0') \, dx_0 \, dx_0' \, dx \, dy,
\]
where
\[
J_{jn}(x, y, x_0, x_0') = \frac{\varepsilon^{2j-1}}{2\pi} G_{jn} \overline{G'_{jn}} (x - \tilde{x}_n)(3 - 2j) + (x - \tilde{x}_n')(3 - 2j) + e^{i\psi_n/\varepsilon} \tag{2.5.6}
\]
with
\[
\psi_n(t, x, x_0, x_0') = \Phi_n(t, x; x_0) - \Phi'_n(t, x; x_0'). \tag{2.5.7}
\]
Let $\rho_j(x, x_0, x_0') \in C^\infty$ be a partition of unity such that
\[
\rho_2 = \begin{cases} 
1, & |x - \tilde{x}_n| \leq \eta \cap |x - \tilde{x}'_n| \leq \eta, \\
0, & |x - \tilde{x}_n| \geq 2\eta \cup |x - \tilde{x}'_n| \geq 2\eta,
\end{cases} \tag{2.5.8}
\]
and $\rho_1 + \rho_2 = 1$. Moreover, let
\[
J_{jn}^1 = \rho_1 J_{jn}(x, y, x_0, x_0'), \quad J_{jn}^2 = \rho_2 J_{jn}(x, y, x_0, x_0'),
\]
so that $J_{jn}(x, y, x_0, x_0') = J_{jn}^1 + J_{jn}^2$.

The rest of this section is to establish the following
\[
\left| \int_0^{2\pi} \int_{K_0} \int_{K_0} J_{jn}^i \, dx_0 \, dx_0' \, dx \, dy \right| \leq C\varepsilon^3 \tag{2.5.9}
\]
for $i = 1, 2$. With this estimate we have $\|I_{jn}\| \leq C\varepsilon^{3/2}$, leading to the desired estimate. Since for $j = 2$ we already have the needed convergence rate, the following proof will be concerned with $j = 0$ or $j = 1$ cases.

### 2.5.0.1 Estimate of $J_{jn}^1$

Using that $\Im \psi_n = \Im \Phi_n + \Im \Phi'_n \geq \delta(|x - \tilde{x}_n|^2 + |x - \tilde{x}'_n|^2)$ and the definition of $\rho_1$, in $J_{jn}^1$ either $|x - \tilde{x}_n(t; x_0)|$ or $|x - \tilde{x}_n(t; x_0')|$ is greater than $2\eta$, hence
\[
\int_0^{2\pi} |J_{jn}^1| \, dy \leq C e^{-\frac{\delta}{\pi} |x - \tilde{x}_n|^2} e^{-\frac{2\eta^2}{\varepsilon}},
\]
we thus obtain an exponential decay
\[
\left| \int_0^{2\pi} \int_{K_0} \int_{K_0} J_{jn}^1 \, dx_0 \, dx_0' \, dx \, dy \right| \leq C \left( \frac{2\pi \varepsilon}{\delta} \right)^{1/2} |K_0|^2 e^{-\frac{2\eta^2}{\varepsilon}} \leq C\varepsilon^s \quad \forall s.
\]
2.5.0.2 Estimation of $J_{jn}^2$

Using the estimate

$$s^p e^{-as^2} \leq \left( \frac{p}{e} \right)^{p/2} a^{-p/2} e^{-a s^2/2},$$

with $s = |x - \tilde{x}_n|$ or $s = |x - \tilde{x}'_n|$, $p = 3, 1$, or 0, $a = \frac{\delta}{2\varepsilon}$, we have

$$\int_0^{2\pi} |J_{jn}|dy \leq CC_2e^{-\frac{\delta}{2\varepsilon}|(x-\tilde{x}_n)^2 + |x-\tilde{x}'_n|^2|},$$

where

$$C_2 \leq \frac{1}{2\pi} \left( \frac{6}{e\delta} \right)^{3/2}.$$

Next we note that

$$|x - \tilde{x}_n(t; x_0)|^2 + |x - \tilde{x}_n(t; x_0')|^2 = 2\left| x - \frac{\tilde{x}_n(t; x_0) + \tilde{x}_n(t; x_0')}{2} \right|^2 + \frac{1}{2}|\tilde{x}_n(t; x_0) - \tilde{x}_n(t; x_0')|^2,$$

(2.5.10)

with which we have

$$\int_0^{2\pi} \int_{R} |J_{jn}^2|dxdy \leq C\varepsilon^2 \int_{R} e^{-\frac{\delta}{4\varepsilon} x^2} dx e^{-\frac{\delta}{4\varepsilon} |\tilde{x}_n(t; x_0) - \tilde{x}_n(t; x_0')|^2}. $$

Hence,

$$\left| \int_0^{2\pi} \int_{R} \int_{K_0} J_{jn}^2 dx_0 dx_0' dxdy \right| \leq C\varepsilon^2 \int_{K_0} \int_{K_0} e^{-\frac{\delta}{4\varepsilon} |\tilde{x}_n(t; x_0) - \tilde{x}_n(t; x_0')|^2} dx_0 dx_0'. $$

(2.5.11)

In order to obtain (2.5.9), we need to recover an extra $\varepsilon^\frac{1}{2}$ from the integral on the right hand side, which is difficult when $|\tilde{x}_n(t; x_0) - \tilde{x}_n(t; x_0')|$ is small.

Following [23], we split the set $K_0 \times K_0$ into

$$D_1(t, \theta) = \left\{ (x_0, x_0') : |\tilde{x}_n(t; x_0) - \tilde{x}_n(t; x_0')| \geq \theta |x_0 - x_0'| \right\},$$

which corresponds to the non-caustic region of the solution, and the set associated with the caustic region

$$D_2(t, \theta) = \left\{ (x_0, x_0') : |\tilde{x}_n(t; x_0) - \tilde{x}_n(t; x_0')| < \theta |x_0 - x_0'| \right\}.$$

For the former we have

$$\int_{D_1} e^{-\frac{\delta}{4\varepsilon} |\tilde{x}_n(t; x_0) - \tilde{x}_n(t; x_0')|^2} dx_0 dx_0' \leq \int_{D_1} e^{-\frac{\delta}{4\varepsilon} |x_0 - x_0'|^2} dx_0 dx_0'.$$
Letting \( \Lambda = \sup_{x_0, x_0' \in K_0} |x_0 - x_0'| < \infty \) be the diameter of \( K_0 \), we continue to estimate the above \( D_1 \)-integral
\[
\int_{D_1} e^{-\frac{4\pi^2}{\varepsilon} |x_0-x_0'|^2} dx_0 dx_0' \leq C \int_0^\Lambda e^{-\frac{4\pi^2}{\varepsilon} \tau^2} d\tau \leq C \varepsilon^{1/2},
\]
which concludes the estimate of \( J_{jn}^2 \) when restricted on \( D_1 \) in (2.5.11).

To estimate \( J_{jn}^2 \) restricted on \( D_2 \), we need the following result on phase estimate.

**Lemma 2.5.1. (Phase estimate)** For \( (x_0, x_0') \in D_2 \), it holds
\[
|\partial_x \psi_n(t, x, x_0, x_0')| \geq C(\theta, \eta) |x_0 - x_0'|,
\]
where \( C(\theta, \eta) \) is independent of \( x \) and positive if \( \theta \) and \( \eta \) are sufficiently small.

The proof of this result is due to [23], where the non-squeezing lemma is crucial. Since all requirements for the non-squeezing argument are satisfied by the construction of Gaussian beam solutions in present work, we therefore omit details of the proof.

To continue, we note that the phase estimate ensures that for \( (x_0, x_0') \in D_2, x_0 \neq x_0' \), \( \partial_x \psi_n(t, x, x_0, x_0') \neq 0 \). Therefore, in order to estimate \( J_{jn}^2 \) on \( D_2 \), we shall use the following non-stationary phase lemma.

**Lemma 2.5.2. (Non-stationary phase lemma)** Suppose that \( u(x, \xi) \in C_0^\infty(\Omega \times Z \) where \( \Omega \) and \( Z \) are compact sets and \( \psi(x; \xi) \in C^\infty(\Omega) \) for some open neighborhood \( \Omega \times Z \). If \( \partial_x \psi \) never vanishes in \( \Omega \), then for any \( K = 0, 1, \ldots \),
\[
\left| \int_{\Omega} u(x; \xi) e^{i\psi(x; \xi)/\varepsilon} dx \right| \leq C_K \varepsilon^K \sum_{\alpha=1}^{K} \int_{\Omega} \frac{|\partial_x^\alpha u(x; \xi)|}{|\partial_x \psi(x; \xi)|^{2K-\alpha}} e^{-\Im \psi(x; \xi)/\varepsilon} dx,
\]
where \( C_K \) is a constant independent of \( \xi \).

Using the non-stationary lemma, we obtain for \( (x_0, x_0') \in D_2 \),
\[
\left| \int_0^{2\pi} \int_{\mathbb{R}} J_{jn}^2 dx dy \right| = \frac{C_K \varepsilon^{K+2j-1}}{2\pi} \times \int_0^{2\pi} \sum_{\alpha=1}^{K} \frac{|{\partial_x^\alpha [\rho G_{jn} G_{jn}^\prime (x-x_0) (3-2j)]}|}{|\partial_x \psi_n(t, x; x_0, x_0')|^{2K-\alpha}} e^{-\Im \psi_n(x; \xi)/\varepsilon} dx dy.
\]
By Leibniz’s rule,

\[ \partial_x^{\alpha_1} [\rho_1 G_{jn} G_{jn}'] (x - \tilde{x}_n)^{3-2j} (x - \tilde{x}'_n)^{3-2j} \]

\[ = \sum_{\alpha_1 + \alpha_2 = \alpha} (\partial_x^{\alpha_1} [\rho_1 G_{jn} G_{jn}']) + \partial_x^{\alpha_2} ((x - \tilde{x}_n)^{3-2j} (x - \tilde{x}'_n)^{3-2j}). \]

Here we take a detailed look at the term \( \int_0^{2\pi} \partial_x^{\alpha_1} [\rho_1 G_{jn} G_{jn}'] dy \), for each case when \( j = 0, 1 \). For \( j = 0 \), we have

\[ \int_0^{2\pi} \partial_x^{\alpha_1} [\rho_1 G_{0n} G_{0j}'] dy = \int_0^{2\pi} a_n a_n' \partial_x^{\alpha_1} [\rho_1 \partial_x^3 F_n z_n \partial_x^3 F_n'] dy \]

\[ = \sum_{\alpha_{11} + \alpha_{12} = \alpha_1} a_n a_n' \partial_x^{\alpha_{11}} [\rho_1 \partial_x^3 F_n] \cdot \int_0^{2\pi} \partial_x^{\alpha_{12}} [z_n z_n'] dy \]

\[ \leq |a_n|^2 |M_n|^{\alpha_{12}} \cdot \sum_{\alpha_{11} + \alpha_{12} = \alpha_1} |\partial_x^{\alpha_{11}} [\rho_1 \partial_x^3 F_n] \partial_x^{\alpha_{12}} [z_n z_n']| \]

\[ \leq C Z^2 := C_2. \]

For \( j = 1 \), we notice that \( G_{1n} \) does not depend on \( y \),

\[ |\partial_x^{\alpha_1} [\rho_1 G_{1n} G_{1n}']| \sim |a_n a_n' \partial_x^{\alpha_1} (\rho_1 \partial_k z_n, z_n) M_n' \partial_k z_n' z_n'| \]

\[ = \sum_{\alpha_{11} + \alpha_{12} = \alpha_1} a_n a_n' \partial_x^{\alpha_{11}} [\rho_1 \partial_x^3 F_n] \cdot \partial_x^{\alpha_{12}} [\partial_k z_n, z_n] \]

\[ \leq |a_n|^2 |M_n|^{\alpha_{12}} \cdot \sum_{\alpha_{11} + \alpha_{12} = \alpha_1} |\partial_x^{\alpha_{11}} [\rho_1 \partial_x^3 F_n] \partial_x^{\alpha_{12}} [\rho_1 \partial_k z_n, z_n]| \]

\[ \leq C Z^2 := C_2. \]

Here we used the fact that indices \( \alpha_{12} \) and \( \alpha_{13} \) are not greater than 2 and \( j \) is either 0 or 1, which is consistent with the boundedness requirement in (2.1.6).

Going further,

\[ \partial_x^{\alpha_2} [(x - \tilde{x}_n)^{3-2j} (x - \tilde{x}'_n)^{3-2j}] \leq C \sum_{\alpha_{21} + \alpha_{22} = \alpha_2} (x - \tilde{x}_n)^{3-2j - \alpha_{21}} \]

\[ \cdot (x - \tilde{x}'_n)^{3-2j - \alpha_{22}}, \]
we have
\[
\int_0^{2\pi} \int_{R} |\partial_x^{\alpha_1} [\rho_1 G_{jn} \bar{G}_{jn}'] | \partial_x^{\alpha_2} [(x - \bar{x}_n)^{3-2j} (x - \bar{x}_n')^{3-2j}] |e^{-3\psi_n/\varepsilon} dx dy 
\leq C \sum_{\alpha_1 + \alpha_2 = \alpha} \int_{R} |x - \bar{x}_n|^{3-2j-\alpha_2} |x - \bar{x}_n'|^{3-2j-\alpha_2} e^{-3\psi_n/\varepsilon} dx 
\leq C \varepsilon^{-\frac{\alpha \alpha_2}{\varepsilon}} \int_{r} e^{-\frac{\delta}{\varepsilon} (|x - \bar{x}_n|^2 + |x - \bar{x}_n'|^2)} dx 
\leq C \left( \frac{\pi}{\delta} \right)^{1/2} \varepsilon^{-\frac{1 - \alpha_2}{2} + 3 - 2j} e^{-\frac{\delta}{2\varepsilon} |\bar{x}_n - \bar{x}_n'|^2},
\]

where (2.5.10) has been used. Hence,
\[
\left| \int_{D_2} \int_{D_2'} J_{jn}^2 dx_0 dx_0' \right| \leq \int_{D_2} e^{-\frac{\delta}{\varepsilon} |\bar{x}_n - \bar{x}_n'|^2} \sum_{\alpha = 1}^{K} \inf |\partial_x \psi_n / \sqrt{\varepsilon}|^{2K-\alpha} dx_0 dx_0' 
\leq C \varepsilon^{\frac{2}{\varepsilon}} \int_{D_2} e^{-\frac{\delta}{\varepsilon} |\bar{x}_n - \bar{x}_n'|^2} \sum_{\alpha = 1}^{K} \frac{1}{\inf |\partial_x \psi_n / \sqrt{\varepsilon}|^{2K-\alpha}} dx_0 dx_0'.
\]

The last estimate together with (2.5.11) yields:
\[
\left| \int_{D_2} \int_{D_2'} J_{jn}^2 dx_0 dx_0' \right| \leq C \varepsilon^{\frac{2}{\varepsilon}} \int_{D_2} e^{-\frac{\delta}{\varepsilon} |\bar{x}_n - \bar{x}_n'|^2} \min \left[ 1, \sum_{\alpha = 1}^{K} \frac{1}{\inf |\partial_x \psi_n / \sqrt{\varepsilon}|^{2K-\alpha}} \right] dx_0 dx_0' 
\leq C \varepsilon^{\frac{2}{\varepsilon}} \int_{K_0} \int_{K_0} e^{-\frac{\delta}{\varepsilon} |\bar{x}_n - \bar{x}_n'|^2} \sum_{\alpha = 1}^{K} \frac{1}{\inf |\partial_x \psi_n / \sqrt{\varepsilon}|^{2K-\alpha}} dx_0 dx_0' 
\leq C \varepsilon^{\frac{2}{\varepsilon}} \int_{K_0} \int_{K_0} \sum_{\alpha = 1}^{K} \frac{1}{1 + (C(\theta, \eta)|x_0 - x_0'|/\sqrt{\varepsilon})^{2K-\alpha}} dx_0 dx_0'.
\]

Taking $K = 2$ and changing variable $\xi = \frac{x_0 - x_0'}{\sqrt{\varepsilon}}$, we compute
\[
\left| \int_{D_2} \int_{D_2'} J_{jn}^2 dx_0 dx_0' \right| \leq C \varepsilon^{\frac{2}{\varepsilon}} \int_{K_0 \times K_0} \frac{1}{1 + (|x_0 - x_0'|/\sqrt{\varepsilon})^{2K}} dx_0 dx_0' 
\leq C \varepsilon^{3} \int_{0}^{\infty} \frac{1}{1 + \xi^2} d\xi = \frac{\pi}{2} C \varepsilon^{3},
\]

which gives (2.5.9) when restricted to the caustic region.

Putting all together we complete the proof of (2.5.9), hence Theorem 2.2.2.
2.6 Extensions

The extension of the one-dimensional results to multidimensional case is straightforward. We still have the two-scale formulation,

$$i\varepsilon \frac{\partial \tilde{\Psi}}{\partial t} = -\frac{1}{2}(\varepsilon \nabla_x + \nabla_y)^2 \tilde{\Psi} + V(x) \tilde{\Psi} + V_e(x) \tilde{\Psi}, \quad x \in \mathbb{R}^d,$$

$$\Psi(0, x, y) = g(x, y)e^{iS_0(x)/\varepsilon}, \quad x \in K_0 \subset \mathbb{R}^d, \quad y \in [0, 2\pi]^d. \quad (2.6.1)$$

The Gaussian beam construction of the phase will have the following form:

$$\Phi(t, x; x_0) = S(t; x_0) + p(t; x_0) \cdot (x - \tilde{x}(t; x_0)) + \frac{1}{2}(x - \tilde{x}(t; x_0))^{\top} \cdot M(x - \tilde{x}(t; x_0)). \quad (2.6.3)$$

Following the procedure of the Gaussian beam construction in section 3, we only check possible different formulations in the multidimensional setting. For instance, equation (2.3.4) will take a form:

$$c_j = \Delta x A_{j-2} + iLA_{j-1} + GA_j, \quad j = 2, 3, \ldots, l + 2,$$

where $L$ reads

$$L = \partial_t + (-i\nabla_y + \nabla_x \Phi) \cdot \nabla_x + \frac{1}{2} \Delta_x \Phi. \quad (2.6.4)$$

An equation for the amplitude can be derived from (2.3.19), however because of the matrix $M$, it has more sophisticated form than in 1-dimensional case:

$$\dot{a} = a(\langle (\nabla_k z \cdot (\nabla_x V_e(\tilde{x}) + M\nabla_k E(p)), z \rangle - \langle (-i\nabla_y + p) \cdot M\nabla_k z, z \rangle - \frac{1}{2} Tr(M)). \quad (2.6.5)$$

One can easily verify that the amplitude equation for $d = 1$ follows from (2.6.5).

The superposition formula (2.3.35) for the approximate solution is:

$$\tilde{\Psi}^\varepsilon(t, x, y) = \frac{1}{(2\pi\varepsilon)^{d/2}} \int_{K_0} \tilde{\Psi}^\varepsilon_{GB}(t, x, y, x_0) dx_0. \quad (2.6.6)$$
The technique for estimating the initial error can be carried out in multi-dimensional setting, without any further difficulty.

As for the evolution error, some clarification of the notation needs to be done. For example, the main representations (2.5.1)-(2.5.6), can be reformulated as follows:

\[ I_{jn} = \frac{\varepsilon \beta^d}{(2\pi)^{d/2}} \int_{K_0} \sum_{|\beta|=(3-2j)_+} G_{jn\beta}(t, x, y; x_0)(x - \tilde{x}_n(t; x_0))^\beta e^{i\Phi_n(t;x;x_0)/\varepsilon} dx_0, \tag{2.6.7} \]

where

\[ G_{0n\beta}(t, x; x_0, y) = \frac{1}{\beta!} a_n(t; x_0) \partial_x^\beta F_n(t, x^*) z_n(k, y), \quad |\beta| = 3, \tag{2.6.8} \]

\[ G_{1n\beta}(t, x; x_0) = (ia\langle \partial_k z_n, z_n \rangle \dot{M}_n(t; x_0) - \sum_{|\beta|=3} \frac{1}{\beta!} \partial_x^\beta F_n(t, x^*) A_{1n}(x - \tilde{x})^{(\beta-1)_+}), \tag{2.6.9} \]

\[ G_{2n}(t, x; x_0, y) = a_n(t; x_0)(Tr(M_n))^2 \Delta_k z_n(k_n, y) + iLA_{1n}. \tag{2.6.10} \]

Finally,

\[ J_{jn}(x, y, x_0, x'_0) = \frac{\varepsilon^{2j-d}}{(2\pi)^{d/2}} \sum_{|\beta|=(3-2j)_+} (G_{jn\beta}(t, x, y; x_0))(x - \tilde{x}_n(t; x_0))^\beta \]

\[ \times \sum_{|\beta|=(3-2j)_+} \frac{(G_{jn\beta}(t, x, y; x'_0))(x - \tilde{x}_n(t; x'_0))^\beta e^{i\psi_n/\varepsilon}}{\varepsilon}. \]

The rest of the ingredients of the proof remain unchanged, except when using the non-stationary phase method \( K \) need to be taken as \( d + 1 \).

Another possible extension of this result is to apply our technique to higher order Gaussian beam superpositions, using the Gaussian beam construction in [10].

Our results valid for finite number of bands can be used in practice by approximating a given high frequency initial data by finite number of bands within certain accuracy. An open question in our Gaussian beam theory is to deal with infinite number of bands, which is left in a future work.
CHAPTER 3. GAUSSIAN BEAM METHODS FOR STRICTLY HYPERBOLIC SYSTEMS

Preprint
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Abstract

In this work we construct Gaussian beam approximations to solutions of the strictly symmetric hyperbolic system with highly oscillatory initial data. The evolution equations for each Gaussian beam component are derived. Under some regularity assumptions of the data we obtain an optimal error estimate between the exact solution and the Gaussian beam superposition in terms of the high frequency parameter $\varepsilon$. The main result is that the relative local error measured in the energy norm in the beam approximation decays as $\varepsilon^{-\frac{1}{2}}$ independent of dimension and presence of caustics, for first order beams. This result is shown to be valid when the gradient of the initial phase may vanish on a set of measure zero.

3.1 Introduction

In this article we are interested in the accuracy of Gaussian beam approximations to solutions of the symmetric hyperbolic system:

$$A(x)\frac{\partial u}{\partial t} + \sum_{j=1}^{n} D^j \frac{\partial u}{\partial x_j} = 0,$$

subject to the highly oscillatory initial condition,

$$u(0, x) = B_0(x)e^{iS_0(x)/\varepsilon},$$
where \( x \in \mathbb{R}^n \), \( S_0(x) \) is a scalar smooth function, \( B_0 : \mathbb{R}^n \to \mathbb{C}^m \) is a smooth vector function, compactly supported in \( K_0 \subset \mathbb{R}^n \), \( A(x) \) is an \( m \times m \) symmetric positive definite matrix, and \( D^j \) are \( m \times m \) symmetric constant coefficient matrices, \( j = 1, \ldots, n \).

Symmetric hyperbolic systems represent a wide area of research in PDE theory itself, in particular, the high frequency problem arises in several areas of continuum physics including acoustic waves and the research in this field can give some insight in the study of some significant physical systems such as the Maxwell system of equations. The symmetry of the hyperbolic system ensures the existence of an orthogonal basis in \( \mathbb{R}^n \) formed by its eigenvectors, and this spectral decomposition will be used in our construction of the approximate solution. It is well known that high frequency wave propagation problems create severe numerical challenges that make direct computations unfeasible for multidimensional settings. Asymptotic approaches for high frequency problems can be found in some classical literature (see [6]). The level set framework to compute multi-valued phases in the high frequency regime was presented in [19]. In this paper we are going to use the Gaussian beam approach. This approach gained a lot of attention in recent years from both computational and theoretical points of view. For an overview of the history and the latest development of this method we refer the reader to [23].

In this paper we formulate a Gaussian beam superposition for symmetric hyperbolic systems and prove error estimates. Also we prove several minor results: the leading Gaussian beam phase is shown to be stationary (which is related to the Huygens principle) along the Hamiltonian flow, and the momentum does not vanish as long as it is nonzero initially. Another significant improvement of the Gaussian beam theory, we are presenting here, is that we can formulate and prove our main result for a more general initial phase in the sense that we allow the gradient of the initial phase to vanish on a set of measure zero; this question was considered open in previous works [21], [23].

The organization of this paper is as follows: In section 2, we start with the problem formulation and state the main results, then we proceed with Gaussian beam construction which is new for this problem but quite straightforward and simple for those familiar with the Gaussian beam method. In section 3 we prove our main results for initial phase with non-vanishing gradient everywhere in \( K_0 \). Finally, in section 4, we extend our results to a more general phase as stated in section 2. To keep our computations less lengthy, we consider quite simple hyperbolic systems, although we
believe that our results can be generalized to some extent.

3.2 Problem Formulation and Main Result

Consider the initial value problem (3.1.1)-(3.1.2). We define the dispersion matrix \( L(x, k) \):

\[
L(x, k) = A^{-1}(x) \sum_{j=1}^{n} D^j k_j, \tag{3.2.1}
\]

and introduce the following inner product in \( \mathbb{R}^n \):

\[
\langle u, v \rangle_A := \langle Au, v \rangle.
\]

It is known that (see, e.g., [6], [19]) \( L \) is symmetric with respect to the inner product \( \langle \cdot, \cdot \rangle_A \):

\[
\langle Lu, v \rangle_A = \langle u, Lv \rangle_A.
\]

Hence, \( L \) has real eigenvalues \( \{\lambda_i(x, k)\}_{i=1}^{m} \), satisfying

\[
L(x, k) b_i(x, k) = \lambda_i(x, k) b_i(x, k), \quad i = 1, \ldots m,
\tag{3.2.2}
\]

where \( \{b_i(x, k)\}_{i=1}^{m} \) are eigenvectors, forming an orthonormal basis in \( l_2 \) equipped with a weight function \( A(x) \), i.e., \( \langle b_i, b_j \rangle_A = \delta_{ij} \), and \( \lambda_i(x, k) \) are scalar smooth functions. We assume that all eigenvalues are simple (i.e., system (3.1.1) is strictly hyperbolic) and the following holds:

\[
\lambda_{i-1}(x, k) < \lambda_i(x, k) < \lambda_{i+1}(x, k), \quad i = 2, \ldots, m-1,
\tag{3.2.3}
\]

in a neighborhood of any \( (x, k) \) in phase space.

For the initial data (3.1.2) we assume that the amplitude \( B_0(x) \) has compact support in a bounded domain \( K_0 \subset \mathbb{R}^n \), and the phase \( S_0(x) \) is smooth.

Let \( B_0(x) \) have the following eigenvector decomposition

\[
B_0(x) = \sum_{i=1}^{m} a_i(x) b_i(x, \partial_x S_0(x)),
\tag{3.2.4}
\]

then

\[
a_i(x) = \langle B_0(x), b_i(x, \partial_x S_0(x)) \rangle_A, \quad i = 1, \ldots, m.
\tag{3.2.5}
\]

For each wave field associated with \( b_i \), we construct a Gaussian beam approximation

\[
u^i_{GB} = A^i(t, x; x_0)e^{i\Phi_i(t,x;x_0)/\varepsilon},
\tag{3.2.6}
\]
where $A^i(t, x; x_0)$ and $\Phi_i(t, x; x_0)$ are Gaussian beam phases and amplitudes, respectively, based on a central ray starting from $x_0 \in K_0$ with $p_0 = \partial_x S_0(x_0)$. By the linearity of the hyperbolic system, we then sum the Gaussian beam ansatz (3.2.6) over $i = 1, \ldots, m$ and $x_0 \in K_0$ to define the approximate solution

$$u^\varepsilon(t, x) = \frac{1}{(2\pi \varepsilon)^{\frac{n}{2}}} \int_{K_0} \sum_{i=1}^{m} A^i_{GB}(x_0) e^{i\Phi^0(x_0)/\varepsilon} dx_0, \quad (3.2.7)$$

where $(2\pi \varepsilon)^{-\frac{n}{2}}$ is a normalizing constant which is needed for matching the initial data in (3.1.2).

Indeed the initial data can be approximated by the same form of the Gaussian beam superposition (3.2.7),

$$u^\varepsilon(0, x) = \frac{1}{(2\pi \varepsilon)^{\frac{n}{2}}} \int_{K_0} \sum_{i=1}^{m} A^i(0, x; x_0)e^{i\Phi^0(x_0)/\varepsilon} dx_0, \quad (3.2.8)$$

where $\Phi^0$ is the initial Gaussian beam phase, which is assumed to be the same for each wave field. By the classical Gaussian beam theory [30], the initial phase can be taken of the form

$$\Phi^0(x; x_0) = S_0(x_0) + \partial_x S_0(x_0) \cdot (x - x_0) + \frac{1}{2} (x - x_0)^\top \cdot (\partial^2_x S_0(x_0) + iI) (x - x_0). \quad (3.2.9)$$

with coefficients that serve as initial data for ODEs of the Gaussian beam components. The amplitude $A^i(0, x; x_0)$ are defined later in (3.4.1) using $a_i(x_0)$ in (3.2.5).

We are going to use the following notations in this work. The energy norm:

$$\|u\|_E^2 := \int_{\mathbb{R}^n} \langle Au, u \rangle dx. \quad (3.2.10)$$

$L^\infty$ norm of function $f$ and its derivatives:

$$|f(x)|_{C^\beta} := \max_x |\partial^\beta_x f(x)|.$$

$L^\infty$ matrix norm:

$$\|A\|_{L^\infty} := \sup_{|v|=1} |Av|, \quad v \in \mathbb{R}^m.$$
the exact solution to (3.1.1)-(3.1.2) for $0 < t \leq T$, and $u^\varepsilon$ be the first order Gaussian beam superposition (3.2.7). Then

$$\|u - u^\varepsilon\|_E \leq C \varepsilon^{1/2}, \quad (3.2.11)$$

where the constant $C$ is independent of $\varepsilon$, but may depend on the finite time $T$ and the data given.

The proof of this result is based on the following well-posedness estimate.

**Proposition 3.2.1. (Well-posedness)**

Let $u, u^\varepsilon$ be an exact and approximate solution of (3.1.1) with initial data $u_0$ and $u_0^\varepsilon$, respectively. Then the following error estimate holds:

$$\|u - u^\varepsilon\|_E \leq \|u_0 - u_0^\varepsilon\|_E + C \int_0^T \|P[u^\varepsilon]\|_{L^2} dt, \quad (3.2.12)$$

where $C$ is independent of $\varepsilon$, but may depend on the matrix $A$ and $P = A(x) \partial_t + \sum_{j=1}^n D^j \frac{\partial}{\partial x_j}$.

This is a classical result, which can be found, for example, in [15]. The well-posedness estimate tells that the energy norm of the total error is bounded by the sum of initial and evolution error.

An improvement of the above results is that we may allow more general initial phase with possible vanishing phase gradient on a small set. More precisely, we have

**Corrolary 3.2.1.** Under the assumption of Theorem 3.2.1, if the measure of the set $\sigma := \{x, \ |\partial_x S_0(x)| = 0\}$ is zero, then the error estimate (3.2.11) remains valid if the superposition is over beams issued from points in $K_0/\Sigma$.

We proceed to construct Gaussian beam asymptotic solutions and obtain the desired error estimate in several steps. First, we present the construction for the Gaussian beam phase components which is a straightforward extension of the the Gaussian beam approach developed for hyperbolic and Schrödinger equations, see for example, [23]. While constructing the Gaussian beam amplitude, we address some solvability difficulties and show the way to solve it using the approach developed in [10] and verifying the boundedness of the additional terms. For the error estimate, we rely on the well-posedness argument and prove initial and evolution errors separately. For the initial error, we use some techniques similar to those developed by Tanushev in [37], keeping in mind that here we have to deal with vector valued functions. As for the evolution error estimate, we rely on some phase estimates proved in [23], which is a key technique for the proof.
3.3 Gaussian Beam Construction

Let $P$ be the differential operator in (3.1.1). We look for an approximate solution to (3.1.1), which has the form

$$u^\varepsilon = (v_0 + \varepsilon v_1 + \cdots + \varepsilon^l v_l(t,x))e^{i\Phi(t,x)}/\varepsilon.$$  \hfill (3.3.1)

Inserting $u^\varepsilon$ into (3.1.1), we obtain:

$$A^{-1}(x)P[u^\varepsilon] = \left(\frac{1}{\varepsilon}c_0 + c_1 + \cdots + \varepsilon^{l-1} c_l\right)e^{i\Phi(t,x)}/\varepsilon = 0,$$  \hfill (3.3.2)

where

$$c_0 = i(\Phi_t + L(x,\partial_x \Phi))v_0,$$  \hfill (3.3.3)

$$c_1 = (\partial_t + L(x,\partial_x ))v_0 + i(\Phi_t + L(x,\partial_x \Phi))v_1,$$  \hfill (3.3.4)

$$c_i = (\partial_t + L(x,\partial_x ))v_{i-1} + i(\Phi_t + L(x,\partial_x \Phi))v_i, \quad i = 2, \ldots, l.$$  \hfill (3.3.5)

By geometric optics, the leading term is required to vanish,

$$c_0 = i(\Phi_t + L(x,\partial_x \Phi))v_0 = 0,$$  \hfill (3.3.6)

where $L(x,k)$ is the dispersion matrix defined in (3.2.1). We set the leading amplitude as

$$v_0(t,x) = \sum_{i=1}^{m} a_i(t,x)b_i(x,k(t,x)), \quad k(t,x) := \partial_x \Phi(t,x),$$  \hfill (3.3.7)

to infer from (3.2.2) that

$$c_0 = \sum_{i=1}^{m} ia_i(t,x)(\partial_t \Phi + \lambda_i)b_i(x,k(t,x)),$$

which vanishes as long as $\Phi$ solves the Hamilton-Jacobi equation:

$$G(t,x) := \Phi_t + \lambda(x,\partial_x \Phi) = 0,$$  \hfill (3.3.8)

for each $\lambda = \lambda_i$. From now on we shall suppress the index $i$, since the construction is the same for each eigenvalue $\lambda_i$, $i = 1, \ldots m$. 
3.3.1 Construction of the Gaussian Beam Phase

Let \((\tilde{x}(t; x_0), p(t; x_0))\) be the phase space trajectory governed by the Hamiltonian in (3.3.8), then

\[
\dot{\tilde{x}} = \partial_k \lambda(\tilde{x}, p), \quad \dot{p} = -\partial_x \lambda(\tilde{x}, p),
\]

(3.3.9)
satisfying \(\tilde{x}(0, x_0) = x_0 \in K_0\) and \(p(0; x_0) = \partial_x S_0(x_0)\). Next we introduce an approximation of the phase:

\[
\Phi(t, x; x_0) = S(t; x_0) + p(t; x_0) \cdot (x - \tilde{x}(t; x_0)) + \frac{1}{2} (x - \tilde{x}(t; x_0))^\top \cdot M(t; x_0) \cdot (x - \tilde{x}(t; x_0)),
\]

(3.3.10)

where \(S\) and \(M\) are to be chosen so that \(G(t, x)\) vanishes on \(x = \tilde{x}(t; x_0)\) to higher order. From (3.3.8) and (3.3.10) we derive:

\[
G(t, x; x_0) = \dot{S} + \dot{p} \cdot (x - \tilde{x}) - p \cdot \dot{x} + \frac{1}{2} (x - \tilde{x})^\top \cdot \dot{M} (x - \tilde{x}) - \tilde{x}^\top \cdot M (x - \tilde{x}) + \lambda.
\]

(3.3.11)

Setting \(G(t, x; x_0) = 0\) at \(x = \tilde{x}\), we obtain

\[
\dot{S} = p \cdot \partial_k \lambda(\tilde{x}, p) - \lambda(\tilde{x}, p).
\]

(3.3.12)

We can actually show that \(\dot{S} = 0\) as stated below.

**Lemma 3.3.1.** Let \(\lambda(x, k)\) be an eigenvalue of \(L(x, k)\) associated with the eigenvector \(b(x, k)\), then

\[
\lambda(x, k) = k \cdot \partial_k \lambda(x, k)
\]

(3.3.13)

holds for any \(x, k\), and

\[
|\lambda(x, k)| \leq C|k|, \quad x \in \mathbb{R}^n,
\]

(3.3.14)

if \(|A(x)| \geq \delta > 0\).

**Proof.** Differentiation of (3.2.2) with respect to \(k_j\) leads to the following:

\[
A^{-1}(x) D^j b(x, k) + L(x, k) \frac{\partial}{\partial k_j} b(x, k) = \partial_k \lambda(x, k) b(x, k) + \lambda(x, k) \frac{\partial}{\partial k_j} b(x, k).
\]

(3.3.15)

Multiplying (3.3.15) by \(k_j\) and summing up in \(j, j = 1, \ldots m\), we obtain

\[
L(x, k) b(x, k) + \sum_{j=1}^{m} k_j L(x, k) \frac{\partial}{\partial k_j} b(x, k) = k \cdot \partial_k \lambda(x, k) b(x, k) + \sum_{j=1}^{m} k_j \lambda(x, k) \frac{\partial}{\partial k_j} b(x, k).
\]

(3.3.16)
Hence,

$$\lambda(x,k)b(x,k) = \sum_{j=1}^{m} k_j (\lambda(x,k) - L(x,k)) \frac{\partial}{\partial k_j} b(x,k) + k \cdot \partial_k \lambda(x,k)b(x,k). \quad (3.3.17)$$

Taking inner product with $b(x,k)$ and using that matrix $L(x,k)$ is symmetric, we prove (3.3.13).

The estimate (3.3.14) follows from the relation $\lambda(x,k) = b^\top \cdot L(x,k)b(x,k)$ and the assumption $|A| \geq \delta > 0$.

The identity (3.3.13) when applied to (3.3.12) yields $\dot{S} = 0$.

We observe that $\partial_x G(t, \tilde{x}, x_0) = 0$ is equivalent to the $p$ equation in (3.3.9).

Next, we set $\partial_x^2 G(t, \tilde{x}, x_0) = 0$, to obtain

$$\dot{M} + \partial_x^2 (\lambda(x,k)) \bigg|_{(x,k)=(\tilde{x},p)} = 0,$$

which is equivalent to

$$\dot{M} + K_1 + K_2 M + MK_2^\top + MK_3 M = 0, \quad (3.3.18)$$

where $K_1, K_2$ and $K_3$ are matrices with the correspondent entries:

$$K_{1ij} = \frac{\partial^2 \lambda}{\partial x_i \partial x_j}, \quad K_{2ij} = \frac{\partial^2 \lambda}{\partial x_i \partial k_j}, \quad K_{3ij} = \frac{\partial^2 \lambda}{\partial k_i \partial k_j}$$

which are evaluated on the ray trajectory $(\tilde{x}, p)$.

Using the Taylor expansion, we have

$$G = \sum_{|\alpha|=3} \frac{1}{\alpha!} \partial_x^\alpha G(t, \cdot; x_0)(x-\tilde{x})^\alpha = \sum_{|\alpha|=3} \frac{1}{\alpha!} \partial_x^\alpha \lambda(\cdot, \cdot)(x-\tilde{x})^\alpha, \quad (3.3.19)$$

which means that $G$ vanishes up to the third order on $x = \tilde{x}$.

We observe that equation (3.3.18) is of nonlinear Ricatti type. In order to avoid a finite time blow-up of $M$, one has to choose the initial condition for $M$ with positive imaginary part [30].

In summary, we obtain evolution equations for the phase components subject to appropriately chosen initial data:

$$\begin{align*}
\dot{\tilde{x}} &= \partial_k \lambda(\tilde{x}, p), \quad \tilde{x}|_{t=0} = x_0, \\
\dot{p} &= -\partial_x \lambda(\tilde{x}, p), \quad p|_{t=0} = \partial_x S_0(x_0), \\
\dot{S} &= 0, \quad S|_{t=0} = S_0(x_0), \\
\dot{M} &= -MK_3 M - K_2 M - MK_2^\top - K_1, \quad M|_{t=0} = \partial_x^2 S_0 + iI. \quad (3.3.20)
\end{align*}$$
Note that $\partial_k \lambda(x, p)$ may not be well defined for $|p| = 0$; for example, if $\lambda = |k|$, then $\partial_k \lambda(x, p) = \frac{p}{|p|}$.

The following result tells that we can construct well defined beams with $p(0; x_0) \neq 0$.

**Lemma 3.3.2.** If $p(0; x_0) \neq 0$, then

$$|p(t; x_0)| \geq |p(0; x_0)|e^{-ct},$$

(3.3.21)

where constant $c$ may depend on $T$ and the data given.

**Proof.** First we show that $\dot{p} \leq c|p|$. Since $\lambda$ is homogeneous in $k$ of degree 1, we have $\lambda(x, k) = |k|\lambda(x, \omega)$, where $\omega = \frac{k}{|k|}$ a directional unit vector. Hence

$$\dot{p} = -\partial_x \lambda(x, p) = -\partial_x \lambda(x, \omega)|p|,$$

which leads to

$$|\dot{p}| \leq \max_{t \leq T, \omega \in S^{n-1}} |\partial_x \lambda(x, \omega)||p| := c|p|.$$

Next, we consider

$$\frac{d}{dt} (|p|^2 e^{2ct}) = (2p \cdot \dot{p} + 2c|p|^2) e^{2ct} \geq (-2c|p|^2 + 2c|p|^2) e^{2ct} = 0.$$

This proves (3.3.21) as claimed. \hfill $\square$

### 3.3.2 Construction of the Gaussian Beam Amplitude

We recall that

$$c_1 = (\partial_t + L(x, \partial_x))v_0(t, x) + i(\partial_t \Phi + L(x, \partial_x \Phi))v_1(t, x),$$

(3.3.22)

where

$$\partial_t \Phi + L(x, \partial_x \Phi) = G(t, x) + L(x, k(t, x)) - \lambda(x, k(t, x)),$$

so that we may use $G = O((x - \tilde{x})^3)$ when applicable. Here and in what follows, we omit the identity matrix against any scalar quantity unless a distinction is needed.

On the ray $x = \tilde{x}(t)$, we require that $c_1 = 0$, that is:

$$(\partial_t + L(\tilde{x}, \partial_x))v_0(t, x)_{|x = \tilde{x}} + i(L(\tilde{x}, p) - \lambda(\tilde{x}, p))v_1(t, \tilde{x}) = 0.$$

(3.3.23)
In order for \( v_1 \) to exist, it is necessary that
\[
\langle (\partial_t + L(\tilde{x}, \partial_x))(a(t, x)b(x, p))|_{x=\tilde{x}}, b(\tilde{x}, p) \rangle_A = 0. \tag{3.3.24}
\]

For \( x \neq \tilde{x}(t) \), we have
\[
c_1 = (\partial_t + L(x, \partial_x))v_0(t, x) + iG(t, x; x_0)v_1 + i(L(x, k(t, x)) - \lambda(x, k(t, x)))v_1^\perp,
\]
where \( v_1^\perp \) contains the orthogonal complement of \( b \), satisfying \( \langle v_1^\perp, b \rangle_A = 0 \).

We choose
\[
v_1^\perp = i(L(x, k(t, x)) - \lambda(x, k(t, x)))^{-1}(\langle (\partial_t + L(x, \partial_x))v_0, b \rangle_A), \tag{3.3.25}
\]
which is well defined since the term in the bracket is perpendicular to \( b \) against matrix \( A \).

Therefore using (3.3.24) we obtain
\[
c_1 = \langle (\partial_t + L(x, \partial_x))a(t, x)b, b \rangle_A + iGv_1, \tag{3.3.26}
\]
where \( v_1 \in \text{span}\{v_1^\perp, b\} \).

**Lemma 3.3.3.** For the first order Gaussian beam construction, \( a(t, x) = a(t; x_0) \) and satisfies the following evolution equation
\[
\dot{a} = a \langle (\partial_t + L(x, \partial_x))a(t, x)b, b \rangle_A |_{x=\tilde{x}}, \tag{3.3.27}
\]
where \( D_x := \partial_x + M(t; x_0)\partial_k \). Moreover,
\[
c_0 = ia(t, x_0)G(t, x; x_0)b(x, k(t, x)), \tag{3.3.28}
\]
\[
c_1 = a(t; x_0)d_1 \cdot (x - \tilde{x})b(x, k(x)) + iv_1G \tag{3.3.29}
\]
where
\[
|d_1| \leq C(1 + |x - \tilde{x}|),
\]
and \( v_1 \in \text{span}\{v_1^\perp, b\} \) with \( v_1^\perp \) defined in (3.3.25), and \( G = O(|x - \tilde{x}|^3) \).

**Proof.** For the first order Gaussian beams, we look for amplitude of form \( a(t, x) = a(t; x_0) \), then (3.3.24) gives
\[
a_t + a \langle (\partial_t + L(x, \partial_x))a(t, x)b, b \rangle_A |_{x=\tilde{x}} = 0. \tag{3.3.30}
\]
Note that $b = b(x, k(t, x))$ with

$$k(t, x) = p(t) + M(t)(x - \tilde{x}(t)). \quad (3.3.31)$$

Let $D_x$ denote $\partial_x$ with only $t$ fixed, then we have

$$D_x = \partial_x + \partial_x k \partial_k = \partial_x + M \partial_k,$$

then

$$L(x, \partial_x)b = L(x, D_x)b(x, k(t, x)).$$

Using $(3.3.31)$ and the ray equation $(3.3.9)$, we obtain

$$\partial_t k(t, x) = -\partial_x \lambda + \dot{M}(x - \tilde{x}) - M \partial_k \lambda,$$

which when evaluated on the ray $x = \tilde{x}$ gives

$$\partial_t k(t, x) = -\partial_x \lambda - M \partial_k \lambda = -D_x \lambda(\tilde{x}(t), p(t)).$$

This gives

$$\partial_t b = \partial_t b \cdot \partial_t k(t, x) = -\partial_k b \cdot D_x \lambda, \quad x = \tilde{x}(t).$$

These together have justified $(3.3.27)$.

Set

$$f(x, k(x)) = \langle \partial_t b + L(x, \partial_x)b, b \rangle_A,$$

then it follows from $(3.3.26)$ and $(3.3.27)$ that

$$c_1 = a \left( f(x, k(x)) - f(\tilde{x}, p) \right) b + iGv_1 \quad (3.3.32)$$

$$= aD_x f(\cdot, \cdot) \cdot (x - \tilde{x})b + iGv_1,$$

where $D_x f(\cdot, \cdot)$ is evaluated at the intermediate value between $x$ and $\tilde{x}$.

From the definition of $f$ we have

$$f = b \cdot A(x) (L(x, D_x)b + \partial_k b \cdot \partial_t k) \quad (3.3.33)$$

$$= b \cdot \left( \sum_{j=1}^n D^j D_x b + A(x) \partial_k b \cdot (-D_x \lambda + \dot{M}(x - \tilde{x})) \right).$$
By the product rule we see that
\[ |D_x f| \leq C(1 + |x - \tilde{x}|) \]
if \(D_x b\) and \(D_x \lambda\) are uniformly bounded for \(i \leq 2\). This bound when inserted into (3.3.32) gives (3.3.28).

In order to complete the estimate for \(c_1\) in (3.3.28), we still need to estimate \(v^\perp_1\).

**Lemma 3.3.4.** Let \(v^\perp_1\) be defined in (3.3.25). If eigenvector \(b(x, k) \in C^1_b\) and eigenvalue \(\lambda\) is simple and assumption (3.2.3) is satisfied, i.e.
\[ \Delta \lambda = \min_{1 \leq i < j \leq m} |\lambda_i - \lambda_j| > 0, \]
then
\[ \sup_{t, x_0} |v^\perp_1| \leq C(1 + |x - \tilde{x}|), \]
where \(C\) depends on Gaussian beam components and \(\Delta \lambda\).

**Proof.** Since eigenvalue \(\lambda\) is simple, then \(L(x, k) - \lambda(x, k)\) is invertible on the orthogonal complement to the eigenvector \(b(x, k)\) associated with \(\lambda(x, k)\) and the following resolvent estimate holds:
\[ ||(L(x, k) - \lambda(x, k))^{-1}|| \leq \frac{1}{\Delta \lambda}. \]
From (3.3.25)
\[ |v^\perp_1| \leq \frac{1}{\Delta \lambda} |(\partial_t + L(x, \partial_x))v_0 - ((\partial_t + L(x, \partial_x))v_0, b)_A b|, \quad (3.3.34) \]
where \(v_0 = a(t; x_0)b(x, k)\) and hence
\[ (\partial_t + L(x, \partial_x))v_0 - ((\partial_t + L(x, \partial_x))v_0, b)_A b = a(\partial_t b - (\partial_t b, b)_A b + L(x, \partial_x)b - (L(x, \partial_x)b, b)_A b). \quad (3.3.35) \]
One can see that
\[ |\partial_t b| = |\partial_t b \partial_t k| \leq |\partial_k b||(|\partial_x \lambda M(x - \tilde{x})| - D_x \lambda(x, k(x)))| \leq C|\partial_k b|(1 + |x - \tilde{x}|). \]
Also
\[ |L(x, \partial_x)b| \leq n \max_{j=1,n} ||D^j||_\infty |\partial_x b| \leq C(n, D^j)|\partial_x b| \]
implies that the right hand side of (3.3.35) is bounded in terms of \(\partial_k b, \partial_x b, \partial_x \lambda\), components of the matrix \(M\) and the initial data which completes the proof of the lemma. \(\square\)
Using the linearity of the hyperbolic system, we are able to construct a Gaussian beam approximation for any fixed $x_0$:

$$u_{GB}^{\varepsilon i}(t, x, x_0) = \left(a_i(t, x_0)b_i(x, \partial_x \Phi_i) + \varepsilon v_1^i(t, x; x_0)\right)e^{i\Phi_i(t, x; x_0)/\varepsilon}. \quad (3.3.36)$$

Approximation (3.3.36) is used as a building block for approximating the solution of the initial value problem. For each $x_0 \in K_0 \subset \mathbb{R}^n$, a compact support of $B_0(x)$, we can construct an approximate solution by the GB superposition:

$$u_{\varepsilon}^i(t, x) = \frac{1}{(2\pi \varepsilon)^{n/2}} \int_{K_0} \sum_{i=1}^{m} u_{GB}^{\varepsilon i}(t, x; x_0) dx_0. \quad (3.3.37)$$

Based on our construction, we have the following residual representation

$$P(u_{\varepsilon}^i) = \frac{1}{(2\pi \varepsilon)^{n/2}} \int_{K_0} \sum_{i=1}^{m} A(x)(\frac{1}{\varepsilon}c_{0i} + c_{1i})e^{i\Phi_i(t, x; x_0)/\varepsilon} dx_0, \quad (3.3.38)$$

where $c_{0i}$ and $c_{1i}$ can be obtained from (3.3.28) and (3.3.29), respectively.

**Remark 3.3.1.** In order to construct $v_1$ in the Gaussian beam amplitude, eigenvalues need to be separated, which is the case when the system is strictly hyperbolic. However, our construction can work for some nonstrictly hyperbolic systems as well, see the example in Chapter 4.

### 3.4 Error Estimate

#### 3.4.1 Initial Error Estimate

The initial condition is approximated as follows:

$$u_{\varepsilon}^0 = \frac{1}{(2\pi \varepsilon)^{n/2}} \int_{K_0} \sum_{i=1}^{m} (a_i(x_0)b_i(x, \partial_x \Phi^0) + \varepsilon v_1^i(0, x; x_0))e^{i\Phi^0/\varepsilon} dx_0. \quad (3.4.1)$$

Here the term $v_1^i(0, x; x_0)$ is defined to be consistent with that in (3.3.25). In other words it is understood to be the limit of $v_1^i(t, x; x_0)$ as $t \to 0$, therefore we have from previous estimate on $v_1$,

$$\max_{x, x_0} \left| \sum_{i=1}^{m} v_1^i(0, x; x_0) \right|^2 \leq C. \quad (3.4.2)$$

In this section we state and prove the initial error estimate result.
Theorem 3.4.1. Let $u_0^*$ be defined in (3.4.1),

$$u_0(x) = \sum_{i=1}^{m} a_i(x) b_i(x, \partial_x S_0(x)) e^{iS_0(x)/\varepsilon}.$$  

Then the energy norm of the difference $u_0 - u_0^*$ satisfies:

$$\|u_0 - u_0^*\|_E \leq C \varepsilon^{1/2},$$  \hspace{0.5cm} (3.4.3)

where the constant $C$ depends on the data given.

We split the proof of the theorem into two parts. Let us define an intermediate quantity:

$$u^*(x) := \frac{1}{(2\pi \varepsilon)^{n/2}} \int_{\mathbb{R}^n} B^*(x; x_0) e^{i\Phi^0(x; x_0)/\varepsilon} dx_0,$$  \hspace{0.5cm} (3.4.4)

where

$$B^*(x; x_0) = \sum_{i=1}^{m} a_i(x_0) b_i(x, \partial_x S_0(x)).$$

Lemma 3.4.1. Let $u^*$ be defined in (3.4.4), $a(x)$ and $b(x, \cdot) \in H^1(\mathbb{R}^n)$, then

$$\|u^* - u_0\|_E \leq C \varepsilon^{1/2},$$  \hspace{0.5cm} (3.4.5)

where $C$ depends on $|A|_{C^1}$, $|b|_{C^1}$, $\|B_0\|_E$, and $\|\partial_x B_0\|_E$.

Proof. First, we rewrite

$$u^* - u_0 = \frac{1}{(2\pi \varepsilon)^{n/2}} \int_{\mathbb{R}^n} (B^*(x; x_0) - B_0(x)) e^{iT_2^{x_0}[S_0]/\varepsilon} e^{-|x-x_0|^2/2\varepsilon} dx_0 + B_0(x) (e^{iT_2^{x_0}[S_0]/\varepsilon} - e^{iS_0/\varepsilon}) e^{-|x-x_0|^2/2\varepsilon} dx_0 = I_1 + I_2,$$

where $T_2^{x_0}[S_0]$ is the second order Taylor polynomial of $S_0$ about $x_0$. Noting that

$$\|u_0 - u^*\|_E \leq \|I_1\|_E + \|I_2\|_E.$$  

We start with $\|I_1\|_E$:

$$\|I_1\|_E^2 = \frac{1}{(2\pi \varepsilon)^n} \int_{\mathbb{R}^n} A(x) \int_{\mathbb{R}^n} (B^* - B_0) e^{iT_2^{x_0}[S_0]/\varepsilon} e^{-|x-x_0|^2/2\varepsilon} dx_0$$

$$\cdot \int_{\mathbb{R}^n} (B^* - B_0) e^{iT_2^{x_0}[S_0]/\varepsilon} e^{-|x-x_0|^2/2\varepsilon} dx_0 dx$$

$$= \frac{1}{(2\pi \varepsilon)^n} \sum_{i=1}^{m} \sum_{l=1}^{m} \int_{\mathbb{R}^n} \int_{\mathbb{R}^n} (a_i(x_0) - a_i(x)) (a_l(x_0') - a_l(x))$$

$$\cdot A(x) b_l(x, \partial_x S_0(x)) \cdot b_i(x, \partial_x S_0(x)) e^{-(|x-x_0|^2+|x-x_0'|^2)/2\varepsilon} dx_0 dx_0' dx.$$
Using the orthogonality of vectors $b_k$ with respect to the matrix $A$ we derive,

$$
\|I_1\|^2_E = \frac{1}{(2\pi \varepsilon)^n} \sum_{i=1}^{m} \int_{\mathbb{R}^n} \left( \int_{\mathbb{R}^n} (a_i(x_0) - a_i(x)) e^{-|x-x_0|^2/2\varepsilon}dx_0 \right)^2 dx
$$

$$
\leq \frac{1}{(2\pi \varepsilon)^n} \sum_{i=1}^{m} \int_{\mathbb{R}^n} \int_{\mathbb{R}^n} |a_i(x_0) - a_i(x)|^2 e^{-|x-x_0|^2/2\varepsilon}dx_0 dx
\leq \frac{1}{(2\pi \varepsilon)^n/2} \sum_{i=1}^{m} \int_{\mathbb{R}^n} \int_{\mathbb{R}^n} |a_i(x_0) - a_i(x)|^2 e^{-|x-x_0|^2/2\varepsilon}dx_0 dx.
$$

Changing variable $\xi = \frac{x_0 - x}{\sqrt{2\varepsilon}}$ and by the mean value theorem, we obtain:

$$
\|I_1\|^2_E = \frac{1}{\pi^{n/2}} \int_{\mathbb{R}^n} \int_{\mathbb{R}^n} \sum_{i=1}^{m} |a_i(x + \sqrt{2\varepsilon} \xi) - a_i(x)|^2 e^{-|\xi|^2}d\xi dx
$$

$$
= \frac{2\varepsilon}{\pi^{n/2}} \int_{\mathbb{R}^n} \int_{\mathbb{R}^n} \sum_{i=1}^{m} |\partial_x a_i(x + \theta \sqrt{2\varepsilon} \xi)|^2 |\xi|^2 e^{-\xi^2} d\xi dx
$$

$$
= n\varepsilon \int_{\mathbb{R}^n} \sum_{i=1}^{m} |\partial_x a_i(x)|^2 dx =: C\varepsilon,
$$

where we have used the Fubini theorem. Here a careful calculation shows that $C$ depends on $\|(B_0, \partial_x B_0)\|^2_E$ and the bound of $A$, $\partial_x A$, $\partial_x b$, $\partial_k b$ and $\partial_x S_0$.

We continue with $\|I_2\|_E$.

$$
\|I_2\|^2_E = \frac{1}{(2\pi \varepsilon)^n} \int_{\mathbb{R}^n} A(x) \int_{\mathbb{R}^n} B_0(x) (e^{i T_2^0 [S_0]/\varepsilon} - e^{i S_0/\varepsilon}) e^{-|x-x_0|^2/2\varepsilon} dx_0 
\cdot \int_{\mathbb{R}^n} B_0(x) (e^{i T_2^0 [S_0]/\varepsilon} - e^{i S_0/\varepsilon}) e^{-|x-x_0|^2/2\varepsilon} dx_0 dx
$$

$$
= \frac{1}{(2\pi \varepsilon)^n} \int_{\mathbb{R}^n} \int_{\mathbb{R}^n} \sum_{i=1}^{m} |a_i(x)|^2 \left( \int_{\mathbb{R}^n} (e^{i T_2^0 [S_0]/\varepsilon} - e^{i S_0/\varepsilon}) e^{-|x-x_0|^2/2\varepsilon} dx_0 \right)^2 dx.
$$

Simplifying $e^{i T_2^0 [S_0]/\varepsilon} - e^{i S_0/\varepsilon}$ and using the H"older inequality, we obtain:

$$
\|I_2\|^2_E \leq \frac{1}{(2\pi \varepsilon)^n} \int_{\mathbb{R}^n} \int_{\mathbb{R}^n} \sum_{i=1}^{m} |a_i(x)|^2 \left( \frac{|R_2^0 [S_0]|}{\varepsilon} \right)^2 e^{-|x-x_0|^2/2\varepsilon} dx_0 \int_{\mathbb{R}^n} e^{-|x-x_0|^2/2\varepsilon} dx_0 dx
$$

$$
\leq \frac{C}{(2\pi \varepsilon)^n/2} \int_{\mathbb{R}^n} \int_{\mathbb{R}^n} \sum_{i=1}^{m} |a_i(x)|^2 \frac{|x-x_0|^6}{\varepsilon^2} e^{-|x-x_0|^2/2\varepsilon} dx_0 dx_0 dx,
$$

where we have used the Taylor remainder so that $|R_2^0 [S_0]| \leq C |x - x_0|^3$ with $C$ depending on $|S_0|_C^3$. Making the same change of variables as in the previous step, we have:

$$
\|I_2\|^2_E \leq C \varepsilon \int_{\mathbb{R}^n} \int_{\mathbb{R}^n} \sum_{i=1}^{m} |a_i(x)|^2 |\xi|^6 e^{-|\xi|^2} d\xi dx
\leq C \|B_0\|^2_E \varepsilon.
$$
Hence,
\[ \|u_0 - u^*\|_E^2 \leq C\varepsilon \]
as needed.

**Lemma 3.4.2.** Let \( u_0^\varepsilon \) be defined in (3.4.1) and \( u^* \) in (3.4.4). Then
\[ \|u_0^\varepsilon - u^*\|_E \leq C\varepsilon^{1/2}, \quad (3.4.6) \]
where \( C \) depends on the matrix \( A \) and \( \partial_k b \) but is independent of \( \varepsilon \).

**Proof.** From (3.4.1),
\[ u_0^\varepsilon = \frac{1}{(2\pi \varepsilon)^{n/2}} \int_{K_0} \sum_{i=1}^m (a_i(x_0)b_i(x, \partial_x \Phi^0(x; x_0)) + \varepsilon v_1^i(0, x; x_0)) e^{i\Phi^0(x; x_0)/\varepsilon} dx_0. \]
Then
\[ \|u^* - u_0^\varepsilon\|_E^2 = \frac{1}{(2\pi \varepsilon)^n} \int_{\mathbb{R}^n} A(x) \left( \int_{\mathbb{R}^n} \sum_{i=1}^m a_i(x_0)b_i(x, \partial_x S_0(x)) e^{i\Phi^0(x;x_0)/\varepsilon} dx_0 \right. \]
\[ - \left. \left( \int_{K_0} \sum_{i=1}^m a_i(x_0)b_i(x, \partial_x S_0(x)) e^{i\Phi^0(x;x_0)/\varepsilon} dx_0 \right) \cdot \left( \int_{K_0} \sum_{i=1}^m a_i(x_0)b_i(x, \partial_x \Phi^0(x; x_0)) + \varepsilon v_1^i(0, x; x_0)) e^{i\Phi^0(x;x_0)/\varepsilon} dx_0 \right) dx. \]
Set
\[ K_i = b_i(x, \partial_x S_0(x)) - b_i(x, \partial_x \Phi^0(x; x_0)). \]
Using the fact that
\[ |\partial_x S_0(x) - \partial_x \Phi^0(x; x_0)| = |\partial_x S_0(x) - \partial_x S_0(x_0) - \partial_x^2 S_0(x_0)(x - x_0) - iI(x - x_0)| \]
\[ \leq |x - x_0|(1 + C|x - x_0|), \]
where \( C \) depends on \(|S_0|_{C^3}\), we obtain
\[ |K_i| \leq \tilde{C}|x - x_0|(1 + |x - x_0|), \]
where \( \tilde{C} = C \max \|\partial_k b_i(x, \cdot)\| \leq C\|b\|_{C^1}. \)
Using that each \(a_i(x_0) = 0\) on \(\mathbb{R}^n \setminus K_0\) together with the boundedness of the matrix \(A\), we obtain:

\[
\|u^* - u_0^\varepsilon\|^2_E \leq \frac{C}{(2\pi\varepsilon)^n} \int_{\mathbb{R}^n} \left| \int_{K_0} \sum_{i=1}^m a_i(x_0)(K_i - \varepsilon v_1^i(0, x; x_0)) e^{i\Phi_0(x; x_0)/\varepsilon} \, dx \right|^2 \, dx \\
\leq \frac{C}{(2\pi\varepsilon)^n} \int_{\mathbb{R}^n} \left( \int_{K_0} \sum_{i=1}^m |a_i(x_0)(K_i - \varepsilon v_1^i(0, x; x_0))| e^{-|x-x_0|^2/2\varepsilon} \, dx \right)^2 \, dx.
\]

By the Hölder inequality,

\[
\|u^* - u_0^\varepsilon\|^2_E \leq \frac{C}{(2\pi\varepsilon)^n} \int_{\mathbb{R}^n} \int_{K_0} \left( \sum_{i=1}^m |a_i(x_0)(K_i - \varepsilon v_1^i(0, x; x_0))| \right)^2 e^{-|x-x_0|^2/2\varepsilon} \, dx_0 \, dx \\
\leq \frac{C}{(2\pi\varepsilon)^{n/2}} \int_{\mathbb{R}^n} \int_{K_0} \left( \sum_{i=1}^m |a_i(x_0)(K_i - \varepsilon v_1^i(0, x; x_0))| \right)^2 e^{-|x-x_0|^2/2\varepsilon} \, dx_0 \, dx.
\]

Going further,

\[
\|u^* - u_0^\varepsilon\|^2_E \leq C\varepsilon^{-n/2} \left( \int_{\mathbb{R}^n} \int_{K_0} \sum_{i=1}^m |a_i(x_0)|^2 |K_i|^2 e^{-|x-x_0|^2/2\varepsilon} \, dx_0 \, dx \right) \\
+ \varepsilon^2 \int_{\mathbb{R}^n} \int_{K_0} \left( \sum_{i=1}^m |v_1^i(0, x; x_0)| \right)^2 e^{-|x-x_0|^2/2\varepsilon} \, dx_0 \, dx \\
= I_1 + I_2.
\]

Applying the change of variable for fixed \(x_0\)

\[
\xi = \frac{x-x_0}{\sqrt{2\varepsilon}}, \quad dx = \sqrt{2\varepsilon} \, d\xi
\]

we have \(|K_i| \leq C(\sqrt{\varepsilon} |\xi| + \varepsilon |\xi|^2)\), hence

\[
I_1 \leq C \int_{\mathbb{R}^n} \int_{K_0} \sum_{i=1}^m |a_i(x_0)|^2 (\varepsilon |\xi|^2 + \varepsilon^2 |\xi|^4) e^{-|\xi|^2} \, d\xi \, dx_0 \\
\leq C \varepsilon \|B_0\|^2_E.
\]

As for \(I_2\), using (3.4.2) we have

\[
I_2 \leq \varepsilon^2 \max_{x,x_0} \left| \sum_{i=1}^m v_1^i(0, x; x_0) \right|^2 \\
\leq C \varepsilon^2,
\]

which produces an additional rate of convergence. Therefore, we recover the needed order of convergence for \(\|u^* - u_0^\varepsilon\|_E\).

\[\square\]

Combining both lemmas and using the triangle inequality we finish the proof of Theorem 3.4.1.
3.4.2 Evolution Error Estimate

From the residual representation (3.3.38) we have

$$\|P(u^\varepsilon)\| \leq \sum_{i=1}^{m} (\|I_{0i}\| + \|I_{1i}\|),$$

where

$$I_{li} := \frac{\varepsilon^{l-1}}{(2\pi \varepsilon)^{n/2}} \int_{K_0} A(x)c_{li}e^{i\Phi_i/\varepsilon} \, dx_0$$

is vector-valued. Since the estimate for each wave field is similar, we thus omit the index $i$ using only $I_l(t, x; x_0)$ in the sequel.

Let $'$ denote quantities defined on the ray radiating from $x'_0$ such as $\tilde{x}'$, $c'_l$ and $\Phi'$. Then we can represent the $L^2$ norm of $I_l$ by

$$\|I_l\|^2 = \int_{\mathbb{R}^n} I_l(t, x; x_0) \cdot \overline{I_l(t, x; x'_0)} \, dx$$

$$= \int_{\mathbb{R}^n} \int_{K_0} \int_{K_0} J_l(t, x, x_0, x'_0) dx_0 dx'_0 dx,$$

where

$$J_l = \frac{\varepsilon^{-n+2l-2}}{(2\pi)^n} A(x)c_l(t, x; x_0) \cdot \overline{A(x)c_l(t, x, x'_0)} e^{i\psi(t, x; x_0, x'_0)/\varepsilon}$$

with

$$\psi(t, x, x_0, x'_0) = \Phi(t, x; x_0) - \overline{\Phi(t, x; x'_0)}.$$

The rest of this section is to establish the following

$$\left| \int_{\mathbb{R}^n} \int_{K_0} \int_{K_0} J_l dx_0 dx'_0 dx \right| \leq C\varepsilon.$$

With this estimate we have $\|I_l\| \leq C\varepsilon^{1/2}$, leading to the desired estimate

$$\|P(u^\varepsilon)\| \leq C\varepsilon^{1/2},$$

which when combined with the initial error obtained in Theorem 3.4.1 and the wellposedness inequality (3.2.12) gives the main result (3.2.11) stated in Theorem 3.2.1.

In order to estimate (3.4.9), we note that

$$\Im \psi = \Im \Phi + \Im \Phi' \geq \frac{\delta}{2} (|x - \tilde{x}|^2 + |x - \tilde{x}'|^2),$$
hence
\[ |J_l| \leq C \varepsilon^{-n+2l-2} |c_l(t, x; x_0)| \cdot |c_l(t, x, x'_0)| e^{-\frac{4}{\pi} (|x - \tilde{x}|^2 + |x - \tilde{x}'|^2)}, \]  
(3.4.10)

with \( C = (2\pi)^{-n} |A|^{\frac{2}{\infty}}, \) and \( l = 0, 1. \)

Let \( \rho_j(x, x_0, x'_0) \in C^\infty \) be a partition of unity such that
\[
\rho_2 = \begin{cases} 
1, & |x - \tilde{x}| \leq \eta \cap |x - \tilde{x}'| \leq \eta, \\
0, & |x - \tilde{x}| \geq 2\eta \cup |x - \tilde{x}'| \geq 2\eta, 
\end{cases}
\]  
(3.4.11)

and \( \rho_1 + \rho_2 = 1. \) Moreover, let
\[ J^1_l = \rho_1 J_l(t, x, x_0, x'_0), \quad J^2_l = \rho_2 J_l(t, x, x_0, x'_0), \]

so that \( J_l(t, x, x_0, x'_0) = J^1_l + J^2_l. \)

We first estimate \( c_0: \) using \((3.3.11)\) with \((3.3.13)\) and \((3.3.9)\), we have
\[ G(t, x; x_0) = \lambda(x, k) - \lambda(\tilde{x}, p) - \partial_x \lambda(\tilde{x}, p) \cdot (x - \tilde{x}) \]
\[ - \partial_k \lambda(\tilde{x}, p) M(x - \tilde{x}) + \frac{1}{2} (x - \tilde{x})^\top \cdot \hat{M}(x - \tilde{x}), \]  
(3.4.12)

with \( \hat{M} = -\partial^2_x \lambda(\tilde{x}, p). \) Also from \((3.3.14)\) and \( k = p + M(x - \tilde{x}), \) we thus obtain
\[ |c_0| = |aGb| \leq C(1 + |x - \tilde{x}|^2), \quad |x - \tilde{x}| \geq 2\eta, \]  
(3.4.13)
\[ |c_0| = |aGb| \leq C|x - \tilde{x}|^3, \quad |x - \tilde{x}| \leq 2\eta, \]  
(3.4.14)

provided \( \eta \) is sufficiently small.

As for \( c_1, \) if \( |x - \tilde{x}| \geq 2\eta, \) we use \((3.3.32)\) of the form
\[ c_1 = a(f(x, k(x)) - f(\tilde{x}, p))b + iGv_1. \]

Note that both \((3.3.33)\) and Lemma 3.3.4 imply that \( |f| + |v_1| \leq C(1 + |x - \tilde{x}|), \) hence
\[ |c_1| \leq C(1 + |x - \tilde{x}|)(1 + |x - \tilde{x}|^2), \quad |x - \tilde{x}| \geq 2\eta, \]  
(3.4.15)
\[ |c_1| \leq C|x - \tilde{x}|, \quad |x - \tilde{x}| \leq 2\eta, \]  
(3.4.16)

where we have used \((3.3.29)\) and Lemma 3.3.4 to infer \((3.4.16)\).
3.4.3 Estimate of $J_l^1$

Denote

\[ s = |x - \tilde{x}|, \quad s' = |x - \tilde{x}'|, \]

then from \((3.4.7)\) using \((3.4.13)\) and \((3.4.15)\) it follows that

\[ |J_l^1| \leq C \rho_1 \varepsilon^{-n+2l-2} (1 + s)(1 + s^2) (1 + s') (1 + (s')^2) e^{-\frac{4}{\pi}(s^2 + (s')^2)}. \]

Using the estimate

\[ s^p e^{-as^2} \leq \left( \frac{p}{a} \right)^{p/2} a^{-p/2} e^{-as^2/2}, \quad (3.4.17) \]

with \( a = \frac{\delta}{\varepsilon} \), we have

\[ (1 + s)(1 + s^2) e^{-\frac{4}{\pi}s^2} \leq C (1 + \varepsilon^{1/2} + \varepsilon^1 + \varepsilon^{3/2}) e^{-\frac{4}{\pi}s^2} \leq 4C e^{-\frac{4}{\pi}s^2}. \]

Hence

\[ |J_l^1| \leq C \varepsilon^{-n+2l-2} e^{-\frac{4}{\pi}(s^2 + (s')^2)} \leq C \varepsilon^{-n+2l-2} e^{-\frac{4}{\pi}s^2} e^{-\frac{n^2\delta}{\varepsilon}} , \]

where we have assumed \( s' > 2\eta \) due to the definition of \( \rho_1 \), we thus obtain an exponential decay

\[ \left| \int_{\mathbb{R}^n} \int_{K_0} J_l^1 dx_0 dx_0' dx \right| \leq C \varepsilon^{2l-2-\frac{n}{2}} |K_0|^2 e^{-\frac{n^2\delta}{\varepsilon}} \leq C \varepsilon^m \quad \forall m. \]

3.4.4 Estimate of $J_l^2$.

For \( |x - \tilde{x}| \leq \eta \), both \((3.4.14)\) and \((3.4.16)\) imply that \( |c_l| \leq C |x - \tilde{x}|^{3-2l} \), then from \((3.4.10)\) it follows that

\[
\int_{\mathbb{R}^n} |J_l^2| dx \leq C \varepsilon^{-n+2l-2} \int_{\mathbb{R}^n} |c_l(t, x, x_0)| \cdot |c_l(t, x, x_0')| e^{-\frac{4}{\pi} |(x - \tilde{x})^2 + |x - \tilde{x}'|^2|} dx \\
\leq C \varepsilon^{-n+2l-2} \int_{\mathbb{R}^n} |x - \tilde{x}|^{3-2l} |x - \tilde{x}'|^{3-2l} e^{-\frac{4}{\pi} |(x - \tilde{x})^2 + |x - \tilde{x}'|^2|} dx \\
\leq C \varepsilon^{-n+1} \int_{\mathbb{R}^n} e^{-\frac{4}{\pi} |(x - \tilde{x})^2 + |x - \tilde{x}'|^2|} dx.
\]

Using the identity

\[ |x - \tilde{x}|^2 + |x - \tilde{x}'|^2 = 2 \left| x - \frac{\tilde{x} + \tilde{x}'}{2} \right|^2 + \frac{1}{2} |\tilde{x} - \tilde{x}'|^2, \quad (3.4.18) \]

we obtain

\[ \int_{\mathbb{R}^n} |J_l^2| dx \leq C \varepsilon^{-n+1} \int_{\mathbb{R}^n} e^{-\frac{4}{\pi} \frac{3}{2} \left| x - \frac{\tilde{x} + \tilde{x}'}{2} \right|^2} dx e^{-\frac{4}{\pi}|\tilde{x} - \tilde{x}'|^2}. \]
Hence,
\[
\left| \int_{\mathbb{R}^n} \int_{K_0} \int_{K_0} J_l^2 dx_0 dx_0' dx \right| \leq C \varepsilon^{-\frac{n}{2}+1} \int_{K_0} \int_{K_0} e^{-\frac{\delta}{8\varepsilon} |x-x'|^2} dx_0 dx_0'.
\] (3.4.19)

In order to obtain (3.4.9), we need to recover an extra \( \varepsilon \frac{n}{2} \) from the integral on the right hand side, which is difficult when \( |\tilde{x} - \tilde{x}'| \) is small.

Following [23], we split the set \( K_0 \times K_0 \) into
\[
D_1(t, \theta) = \left\{ (x_0, x_0') : |\tilde{x} - \tilde{x}'| \geq \theta |x_0 - x_0'| \right\},
\]
which corresponds to the non-caustic region of the solution, and the set associated with the caustic region
\[
D_2(t, \theta) = \left\{ (x_0, x_0') : |\tilde{x} - \tilde{x}'| < \theta |x_0 - x_0'| \right\}.
\]
For the former we have
\[
\int_{D_1} e^{-\frac{\delta}{8\varepsilon} |x-x'|^2} dx_0 dx_0' \leq \int_{D_1} e^{-\frac{\delta s}{8\varepsilon} |x_0 - x_0'|^2} dx_0 dx_0'.
\]
Changing to spherical coordinates, we obtain
\[
\int_{D_1} e^{-\frac{\delta s}{8\varepsilon} |x_0 - x_0'|^2} dx_0 dx_0' \leq C \int_0^\infty s^{n-1} e^{-\frac{\delta s}{8\varepsilon} s^2} ds \\
\leq C \varepsilon^{-\frac{n-1}{2}} \int_0^\infty e^{-\frac{\delta s}{8\varepsilon} s^2} ds \leq C \varepsilon^{\frac{n}{2}}
\]
as needed.

To estimate \( J_l^2 \) restricted on \( D_2 \), we need the following result on phase estimate.

**Lemma 3.4.3. (Phase estimate)** For \((x_0, x_0') \in D_2\), it holds
\[
|\nabla_x \psi(t, x, x_0, x_0')| \geq C(\theta, \eta)|x_0 - x_0'|,
\] (3.4.20)

where \( C(\theta, \eta) \) is independent of \( x \) and positive if \( \theta \) and \( \eta \) are sufficiently small.

The proof of this result is due to [23], where the non-squeezing lemma is crucial. Since all requirements for the non-squeezing argument are satisfied by the construction of Gaussian beam solutions in present work, we therefore omit details of the proof.

To continue, we note that the phase estimate ensures that for \((x_0, x_0') \in D_2, x_0 \neq x_0', \nabla_x \psi(t, x, x_0, x_0') \neq 0\). Therefore, in order to estimate \( J_l^2_{|D_2} \) we shall use the following non-stationary phase lemma.
Lemma 3.4.4. (Non-stationary phase lemma) Suppose that \( u(x, \xi) \in C_0^\infty(\Omega \times Z) \) where \( \Omega \) and \( Z \) are compact sets and \( \psi(x; \xi) \in C^\infty(O) \) for some open neighborhood \( O \) of \( \Omega \times Z \). If \( \partial_x \psi \) never vanishes in \( O \), then for any \( K = 0, 1, \ldots \),

\[
\left| \int_\Omega u(x; \xi) e^{i\psi(x; \xi)/\varepsilon} \, dx \right| \leq C_K \varepsilon^K \sum_{|\beta| = 1}^K \int_\Omega \left| \frac{\partial^\beta_x u(x; \xi)}{\partial_x \psi(x; \xi)} \right|^{2K-|\beta|} e^{-\varepsilon \psi(x; \xi)/\varepsilon} \, dx,
\]

where \( C_K \) is a constant independent of \( \xi \).

Using the non-stationary lemma, (3.4.7), (3.4.10) and the lower bound for \( \psi \) in (3.4.20), we obtain for \((x_0, x'_0) \in D_2,\)

\[
\left| \int_{\mathbb{R}^n} J_2^2 \, dx \right| \leq C \varepsilon^{K-n+2l-2} \int_{\mathbb{R}^n} \sum_{|\beta| = 1}^K \frac{|L_\beta^l|}{\inf_x |\partial_x \psi|^{2K-|\beta|}} e^{-\frac{\varepsilon}{2\pi} ((|x-x'|^2+|x-x'|^2)}} \, dx
\]

\[
\leq C \sum_{|\beta| = 1}^K \frac{\varepsilon^{K-n+2l-2}}{\inf_x |\partial_x \psi|^{2K-|\beta|}} \int_{\mathbb{R}^n} |L_\beta^l| e^{-\frac{\varepsilon}{2\pi} ((|x-x'|^2+|x-x'|^2)}} \, dx,
\]

where we have used the notation

\[
L_\beta^l := \partial_x^\beta [\rho_2 A(x) c_l(t, x, x_0) \cdot A(x) c_l(t, x, x_0')].
\]

We claim the following estimate for \( L_\beta^l,\)

\[
|L_\beta^l| \leq C \sum_{|\beta_1| + |\beta_2| = |\beta|} |x - \tilde{x}|^{(3-2l-|\beta_1|)} |x - \tilde{x}'|^{(3-2l-|\beta_2|)}.
\]  

(3.4.21)

Therefore,

\[
\left| \int_{\mathbb{R}^n} J_2^2 \, dx \right| \leq C \sum_{|\beta| = 1}^K \frac{\varepsilon^{K-n+2l-2}}{\inf_x |\partial_x \psi|^{2K-|\beta|}} \int_{\mathbb{R}^n} \sum_{|\beta_1| + |\beta_2| = |\beta|} |x - \tilde{x}|^{(3-2l-|\beta_1|)} |x - \tilde{x}'|^{(3-2l-|\beta_2|)} \, dx
\]

\[
\times e^{-\frac{\varepsilon}{2\pi} ((|x-x'|^2+|x-x'|^2)}} \, dx
\]

\[
\leq C \sum_{|\beta| = 1}^K \frac{\varepsilon^{K-n-|\beta|/2+1}}{\inf_x |\partial_x \psi|^{2K-|\beta|}} \int_{\mathbb{R}^n} e^{-\frac{\varepsilon}{2\pi} ((|x-x'|^2+|x-x'|^2)}} \, dx
\]

Using (3.4.18) we have

\[
\left| \int_{\mathbb{R}^n} J_2^2 \, dx \right| \leq C \sum_{|\beta| = 1}^K \frac{\varepsilon^{K-n-|\beta|/2+1}}{\inf_x |\partial_x \psi|^{2K-|\beta|}} \int_{\mathbb{R}^n} e^{-\frac{\varepsilon}{2\pi} \left(2|x-x'| + |x-x'|^2 \right)^2 + \frac{1}{2} |x-x'|^2}} \, dx
\]

\[
\leq C \sum_{|\beta| = 1}^K \frac{\varepsilon^{K-n/2-|\beta|/2+1}}{\inf_x |\partial_x \psi|^{2K-|\beta|}} e^{-\frac{\varepsilon}{2\pi} |\tilde{x}-\tilde{x}'|^2}}.
\]
Hence,
\[ \left| \int_{\mathbb{R}^n} \int_{D_2} J_1^2 \, dx_0 \, dx' \right| \leq C \varepsilon^{1 - \frac{n}{2}} \int_{D_2} e^{-\frac{\delta}{\varepsilon} |x - x'|^2} \frac{1}{\inf_{|\beta| = 1} |\partial_x \psi / \sqrt{\varepsilon}|^{2K - |\beta|}} \, dx_0 \, dx'. \]

The last estimate together with (3.4.19) yields:
\[
\left| \int J_1^2 \, dx_0 \right| \leq C \varepsilon^{1 - \frac{n}{2}} \int_{D_2} e^{-\frac{\delta}{\varepsilon} |x - x'|^2} \min \left[ 1, \sum_{|\beta| = 1} \frac{1}{\inf_{|\beta| = 1} |\partial_x \psi / \sqrt{\varepsilon}|^{2K - |\beta|}} \right] \, dx_0 \, dx'.
\]
\[
\leq C \varepsilon^{1 - \frac{n}{2}} \int_{K_0} e^{-\frac{\delta}{\varepsilon} |x - x'|^2} \sum_{|\beta| = 1} \frac{1}{1 + \inf_{|\beta| = 1} |\partial_x \psi / \sqrt{\varepsilon}|^{2K - |\beta|}} \, dx_0 \, dx'.
\]
\[
\leq C \varepsilon^{1 - \frac{n}{2}} \int_{K_0} \left( \frac{1}{1 + \varepsilon^{n+1}} \right) \, dx_0 \, dx'.
\]

Taking \( K = n + 1 \) and changing variable \( \xi = \frac{x_0 - x'}{\sqrt{\varepsilon}} \), we compute
\[
\left| \int J_1^2 \, dx_0 \right| \leq C \varepsilon^{1 - \frac{n}{2}} \int_{K_0} \frac{1}{1 + (|x_0 - x'|/\sqrt{\varepsilon})^{n+1}} \, dx_0 \, dx'.
\]
\[
\leq C \varepsilon \int_0^\infty \frac{1}{1 + \xi^{n+1}} \, d\xi = C \varepsilon.
\]

which gives (3.4.9) when restricted to the caustic region. This completes the proof of (3.4.9), except the claim (3.4.21), which we show now.

We assume smoothness and boundedness of any component contributing to
\[
\partial_x^\beta \{ \rho_2 A(x)c_1(t, x, x_0) + \overline{A}(x)c_1(t, x, x_0') \}.
\]

Note that the typical term in \( L_2^\beta \) has form \( \partial_x^\beta \{ \rho_2 A(x)b \cdot \overline{A}(x) \overline{b} g g/(x - \bar{x})^\alpha (x - \bar{x}')^\alpha \} \), where \( g \) is a third order partial derivative of \( \lambda \) and \( \alpha \) is a multiindex, \( |\alpha| = 3 \). For the sake of brevity, we denote
\[
h := \rho_2 A(x)b \cdot \overline{A}(x) \overline{b} g g/(x - \bar{x}).
\]

Hence
\[
|L_2^\beta| \leq C \left| \partial_x^\beta [h(x - \bar{x})^\alpha (x - \bar{x}')^\alpha] \right| = C \left| \sum_{|\beta_1| + |\beta_2| = |\beta|} \partial_x^\beta \psi \partial_x^\beta \psi \right| \left| (x - \bar{x})^\alpha (x - \bar{x}')^\alpha \right|.
\]
\[
= C \left| \sum_{|\beta_1| + |\beta_2| = |\beta|} \partial_x^\beta \psi \sum_{|\beta_2| + |\beta_3| = |\beta_2|} \frac{1}{(\alpha - \beta_21 + (x - \bar{x})^\alpha (x - \bar{x}')^\alpha.}
\]
In the “worst” case, i.e., when $|\beta_1| = 0$ we obtain the lowest power of $(x - \tilde{x})(x - \tilde{x}')$ and since $x$ is near the ray, then the higher order terms are controlled by lower order terms, and (3.4.21) is satisfied for $l = 0$.

As for $l = 1$ case, we use (3.3.32) to only take care of the lower order term,

$$|L_1^1| \leq C \left| \partial^3_x [\rho_2 A(x) a D_x f(\cdot, \cdot) \cdot (x - \tilde{x})b \cdot A(x) a D_x f(\cdot, \cdot) \cdot (x - \tilde{x}') \tilde{b}] \right|,$$

so that (3.4.21) follows for $l = 1$ too.

**3.5 Extensions to More General Initial Phase**

Our GB construction and the error estimates have been carried out for the case that $\partial_x S_0(x) \neq 0$, $\forall x \in \mathbb{R}^n$. In this section, we show that this restriction can be relaxed so that a stronger result as stated in Corollary 3.2.1 can be proved.

Set $\sigma = \{ x, \ |\partial_x S_0(x)| = 0 \}$. Since $\sigma$ has measure zero, i.e., $\mu(\sigma) = 0$, then set $\sigma$ can be covered by a union of open sets $\Sigma$ such that

$$\mu(\Sigma) \leq \epsilon^n$$

for any $\epsilon > 0$. For each $x_0 \in K_0 \setminus \Sigma$, we can construct a single Gaussian beam as illustrated in section 2. The superposition of there beams expressed by

$$u^\varepsilon(t, x) = \frac{1}{(2\pi \varepsilon)^{n/2}} \int_{K_0 \setminus \Sigma} \sum_{i=1}^m (a_i(x_0)b_k(x_0, \partial_x \Phi_i) + \varepsilon v_i^1(t, x; x_0)) e^{i\Phi_i(t, x; x_0)/\varepsilon} dx_0$$

(3.5.1)

can thus be used as our approximate solution. The initial Gaussian beam approximation then takes the form

$$u^0_\varepsilon = \frac{1}{(2\pi \varepsilon)^{n/2}} \int_{K_0 \setminus \Sigma} \sum_{i=1}^m (a_i(x_0)b_k(x_0, \partial_x S_0(x)) + \varepsilon v_i^1(0, x; x_0)) e^{i\Phi_i^0(x; x_0)/\varepsilon} dx_0,$$

(3.5.2)

which approximates the given initial data

$$u_0(x) = \sum_{i=1}^m a_k(x)b_i(x, \partial_x S_0(x)) e^{iS_0(x)/\varepsilon}.$$

We are now ready to prove Corollary 3.2.1. The wellposedness estimate

$$\| u - u^\varepsilon \|_E \leq \| u_0 - u^0_\varepsilon \|_E + \int_0^T \| P[u^\varepsilon] \|_{L^2} dt$$

again tells that we need to bound both initial and evolution error. Since the exclusion of set $\Sigma$ from set $K_0$ will not affect the estimate of $\|P(u^\varepsilon)\|$, hence we have

$$\|P(u^\varepsilon)\| \leq C\varepsilon^{1/2}.$$  

To bound the initial error, we can use the same technique as in the proof of Theorem 3.4.1. That is, we use the triangle inequality

$$\|u_0 - u_0^\varepsilon\|_E \leq \|u_0 - u^*\|_E + \|u^* - u_0^\varepsilon\|_E,$$  

(3.5.3)

where $u^*$ is introduced in (3.4.4),

$$u^* := \frac{1}{(2\pi\varepsilon)^n/2} \int_{\mathbb{R}^n} \sum_{i=1}^{m} a_i(x_0) b_i(x, \partial_x S_0(x)) e^{i\Phi(x;0)/\varepsilon} \, dx_0.$$  

(3.5.4)

It was shown in Lemma 3.4.1 that $\|u_0 - u^*\|_E \leq C\varepsilon^{1/2}$.

We next estimate $\|u^* - u_0^\varepsilon\|_E$. Using the fact that $a_i(x_0) = 0$ on $\mathbb{R}^n \setminus K_0$, and for constant $C$ depending on $\|A\|_{L^\infty}$ we have

$$\|u^* - u_0^\varepsilon\|_E^2 \leq \frac{C}{(2\pi\varepsilon)^n} \int_{\mathbb{R}^n} \int_{K_0} \sum_{i=1}^{m} a_i(x_0) b_i(x, \partial_x S_0(x)) e^{i\Phi(x;0)/\varepsilon} \, dx_0 \left| \int_{K_0 \setminus \Sigma} \sum_{i=1}^{m} (a_i(x_0) b_i(x, \partial_x S_0(x)) - b_i(x, \partial_x \Phi^0)) \right|^2 \, dx$$

$$- \frac{C}{(2\pi\varepsilon)^n} \int_{\mathbb{R}^n} \int_{K_0 \setminus \Sigma} \sum_{i=1}^{m} (a_i(x_0) b_i(x, \partial_x S_0(x)) - b_i(x, \partial_x \Phi^0)) \, dx_0 \right|^2 \, dx$$

$$+ \frac{C}{(2\pi\varepsilon)^n} \int_{\mathbb{R}^n} \int_{\Sigma} \sum_{i=1}^{m} a_i(x_0) b_i(x, \partial_x S_0(x)) + \varepsilon v_1^i(0, x; x_0)) e^{i\Phi(x;0)/\varepsilon} \, dx_0 \, dx \leq I_1 + I_2.$$  

For $I_1$ we can repeat the proof of Lemma 3.4.2 to obtain the same result. For $I_2$, we proceed to obtain

$$I_2 \leq C\varepsilon^{-n} \int_{\mathbb{R}^n} \int_{\Sigma} \left| \sum_{i=1}^{m} (a_i(x_0) b_i(x, \partial_x S_0(x)) + \varepsilon v_1^i(0, x; x_0)) e^{i\Phi(x;0)/\varepsilon} \right|^2 \, dx_0 \, dx \leq C \varepsilon^n,$$
where, as before, we have used Hölder inequality and the Fubini theorem. All these estimates when inserted into (3.5.3) yield the desired initial error \( \|u_0 - u_0^\varepsilon\|_E \leq C\varepsilon^{\frac{1}{2}}. \)
CHAPTER 4. APPLICATIONS

4.1 Strongly Hyperbolic Systems

In this section, we consider a case of strongly but not strictly symmetric hyperbolic systems. Such systems are common in applications, such as acoustic wave equations and Maxwell equations. We recall that our construction is based on the spectral decomposition of the hyperbolic system, and hence applies to the strongly hyperbolic system which also has a complete orthonormal basis formed by its eigenvectors. On the other hand, the specifics of the Gaussian beam amplitude construction imposes additional requirements to ensure the desired accuracy of the asymptotic solution. In the case when $\lambda(x,k)$ is an eigenvalue of the dispersion matrix $L(x,k)$ defined in (3.2.1) with multiplicity $l$, $l > 1$ and $b_1, \ldots, b_l$ are the correspondent eigenvectors, chosen to be orthonormal with respect to matrix $A$, the difficulty occurs in equations (3.3.26-3.3.23). One can conclude that the solvability condition for $v_1$ has the following form:

$$\langle (\partial_t + L(\tilde{x}, \partial_x)(a_\alpha b_\alpha), b_\beta) |_{x=\tilde{x}} = 0, \quad 1 \leq \alpha, \beta \leq l \rangle$$

(4.1.1)

or equivalently,

$$\langle \partial_t b_\alpha + L(\tilde{x}, \partial_x)b_\alpha, b_\beta \rangle |_{x=\tilde{x}} = 0, \quad 1 \leq \alpha \neq \beta \leq l.$$  

(4.1.2)

In the following subsection, we consider a system of acoustic equations which is an example for strongly hyperbolic symmetric systems. The fact that the repeating eigenvalues are zeros, simplifies our construction.
4.2 Acoustic Waves

We formulate a Gaussian beam approach for the acoustic wave equations:

\[
\begin{align*}
\rho(x) \partial_t v + \partial_x p &= 0, \\
\kappa(x) \partial_t p + \partial_x \cdot v &= 0,
\end{align*}
\]

(4.2.1)

where \( \rho(x) \) is density, \( \kappa(x) \) is compressibility, both \( \rho(x) \) and \( \kappa(x) \) are smooth and positive functions, we require that

\[
\min_x (\rho(x), \kappa(x)) \geq \gamma > 0.
\]

for some \( \gamma \).

Vector-valued function \( v(x) = (v_1(x), v_2(x), v_3(x)) \) denotes velocity and scalar-valued function \( p(x) \) denotes pressure, \( x \in \mathbb{R}^3, u = (v, p) \in \mathbb{R}^4 \).

We consider a quite general high frequency initial condition:

\[
u(0, x) = B_0(x) e^{i S_0(x) / \varepsilon},\]

with \( B_0 \) and \( S_0 \) being smooth and bounded functions, \( B_0 \) is compactly supported.

Using the notation we introduced in (3.1.1), we have the following notations for the symmetric matrices:

\[
A(x) = \begin{pmatrix}
\rho(x) & 0 & 0 & 0 \\
0 & \rho(x) & 0 & 0 \\
0 & 0 & \rho(x) & 0 \\
0 & 0 & 0 & \kappa(x)
\end{pmatrix},
\]

\[
D^1 = \begin{pmatrix}
0 & 0 & 0 & 1 \\
0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 \\
1 & 0 & 0 & 0
\end{pmatrix},
\]

\[
D^2 = \begin{pmatrix}
0 & 0 & 0 & 0 \\
0 & 0 & 0 & 1 \\
0 & 0 & 0 & 0 \\
0 & 1 & 0 & 0
\end{pmatrix},
\]
\[
D^3 = \begin{pmatrix}
0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 \\
0 & 0 & 0 & 1 \\
0 & 0 & 1 & 0 \\
\end{pmatrix}.
\]

Hence the dispersive matrix \(L(x, k)\) from (3.2.1) has the following form:

\[
L(x, k) = \begin{pmatrix}
0 & 0 & 0 & \frac{k_1}{\rho(x)} \\
0 & 0 & 0 & \frac{k_2}{\rho(x)} \\
0 & 0 & 0 & \frac{k_3}{\rho(x)} \\
\frac{k_1}{\kappa(x)} & \frac{k_2}{\kappa(x)} & \frac{k_3}{\kappa(x)} & 0 \\
\end{pmatrix},
\]

(4.2.2)

which is symmetric with respect to the inner product \(\langle \cdot, \cdot \rangle_A\).

Solving the eigenvalue problem

\[
L(x, k)b(x, k) = \lambda(x, k)b(x, k)
\]

we find:

\[
\lambda_{1,2} = 0, \quad \lambda_{3,4} = \pm \frac{|k|}{\sqrt{\kappa(x) \rho(x)}}.
\]

The associated normalized eigenvectors are as follows:

\[
b_1 = \frac{1}{\sqrt{\rho(x)(k_1^2 + k_2^2)}}(k_2, -k_1, 0, 0),
\]

\[
b_2 = \frac{1}{|k| \sqrt{\rho(x)(k_1^2 + k_2^2)}}(k_1 k_3, k_2 k_3, -k_1^2 - k_2^2, 0),
\]

\[
b_3 = \frac{1}{|k|} \left( \frac{k_1}{\sqrt{2 \rho(x)}}, \frac{k_2}{\sqrt{2 \rho(x)}}, \frac{k_3}{\sqrt{2 \rho(x)}}, \frac{|k|}{\sqrt{2 \kappa(x)}} \right),
\]

\[
b_4 = \frac{1}{|k|} \left( -\frac{k_1}{\sqrt{2 \rho(x)}}, -\frac{k_2}{\sqrt{2 \rho(x)}}, -\frac{k_3}{\sqrt{2 \rho(x)}}, \frac{|k|}{\sqrt{2 \kappa(x)}} \right).
\]

We start with \(\lambda = 0\), noting that the geometric optics ansatz

\[
u^\varepsilon(t, x) = A(t, x)e^{\Phi(t, x)/\varepsilon}
\]

does not produce Hamilton-Jacobi equation and hence there is no caustics occur. In a word, equation

\[
\Phi_t(t, x) + \lambda(x, k) = 0
\]
degenerates to
\[ \Phi_t(t, x) = 0, \]
and hence we choose the initial phase \( S_0(x) \) as the phase for the asymptotic solution.
\[ \Phi(t, x) := S_0(x). \]

Equations for the amplitudes \( a_1 \) and \( a_2 \) are the following transport equations:
\[ (\partial_t + L(x, \partial_x)) (a_{\alpha}(t, x) b_{\alpha}(x, \partial_x S_0)) = 0, \quad \alpha = 1, 2, \]
thus we observe that unlike the first order Gaussian beam amplitudes, the geometric optics amplitudes actually depend on \( x \).

The initial conditions for the amplitudes can be obtained from the initial data in the following way:
\[ a_{\alpha}(0, x) = \langle B_0(x), b_{\alpha}(x, \partial_x) \rangle_A, \quad \alpha = 1, 2, \]
which concludes the asymptotic construction for \( \lambda = 0 \).

As for the nonzero eigenvalues, we use Gaussian beam method as for the strictly hyperbolic systems case. Computing the evolution equations for the GB phase components for \( \lambda_3 = c(x)|p| \), where
\[ c(x) = \frac{|p|}{\sqrt{\kappa(x)p(x)}}, \]
we obtain:
\[
\begin{align*}
\dot{x} &= \frac{p}{|p|\sqrt{\kappa(\tilde{x})p(\tilde{x})}}, \quad \dot{\tilde{x}}|_{t=0} = x_0, \\
\dot{p} &= \frac{|p|\partial_x(\kappa(\tilde{x})p(\tilde{x}))}{2(\kappa(\tilde{x})p(\tilde{x}))^{\frac{3}{2}}}, \quad p|_{t=0} = \partial_x S_0(x_0), \\
\dot{S} &= 0, \quad S|_{t=0} = S_0(x_0), \\
M &= -M\partial_p^2 \frac{|p|}{\sqrt{\kappa(\tilde{x})p(\tilde{x})}} M - \partial_{xx}^2 \frac{|p|}{\sqrt{\kappa(\tilde{x})p(\tilde{x})}} M - \partial_{x}^2 \frac{|p|}{\sqrt{\kappa(\tilde{x})p(\tilde{x})}}, \\
M|_{t=0} &= \partial_x^2 S_0 + iI.
\end{align*}
\]
As for the amplitude equation, we start with formula (3.3.27) and show that it can be simplified in case of eigenvectors \( b_3 \) and \( b_4 \). We will show detailed calculations for \( b_3 \) below. First we compute
the partial derivatives \( \frac{\partial b_3}{\partial k_j}, \ j = 1, 2, 3 \).

\[
\frac{\partial b_3}{\partial k_1} = \frac{1}{|k|^3 \sqrt{2 \rho(x)}} (k_2^2 + k_3^2, -k_1 k_2, -k_1 k_3, 0),
\]
\[
\frac{\partial b_3}{\partial k_2} = \frac{1}{|k|^3 \sqrt{2 \rho(x)}} (-k_1 k_2, k_1^2 + k_3^2, -k_2 k_3, 0),
\]
\[
\frac{\partial b_3}{\partial k_3} = \frac{1}{|k|^3 \sqrt{2 \rho(x)}} (-k_1 k_3, -k_2 k_3, k_1^2 + k_2^2, 0).
\]

Now we observe that

\[
\left\langle \frac{\partial b_3}{\partial k_j}, b_3 \right\rangle_A = 0, \quad j = 1, 2, 3, \tag{4.2.4}
\]

which simplifies our construction. Since then the amplitude equation (3.3.27) can be rewritten as follows:

\[
\dot{a} = -a \sum_{j=1}^{n} \left\langle A^{-1}(x) D^j \left( \frac{\partial b_3}{\partial x_j} + \sum_{i=1}^{n} M_{ji} \frac{\partial b_3}{\partial k_i} \right), b_3 \right\rangle_A
\]
\[
= -a \sum_{j=1}^{n} \left\langle D^j \left( \frac{\partial b_3}{\partial x_j} + \sum_{i=1}^{n} M_{ji} \frac{\partial b_3}{\partial k_i} \right), b_3 \right\rangle_A,
\]

which can be simplified further. Eventually, the amplitude equation corresponding to \( \lambda_3 \) has the following form:

\[
\dot{a} = \frac{a}{2 |p| \sqrt{\rho(x_0) \kappa(x_0)}} \left( \frac{\partial_x \kappa(x_0) \cdot p}{2 \kappa(x_0)} + \frac{\partial_x \rho(x_0) \cdot p}{2 \rho(x_0)} + \frac{1}{|p|^2} (2(M_{12} p_1 p_2 + M_{13} p_1 p_3 + M_{23} p_2 p_3)
\]
\[
- (M_{11}(p_2^2 + p_3^2) + M_{22}(p_1^2 + p_3^2) + M_{33}(p_1^2 + p_2^2))) \right).
\]

The evolution equations for the GB components corresponding to \( \lambda_4 \) are the same as for \( \lambda_3 \) up to ”-” sign. As for the amplitude equation, we see that

\[
\frac{\partial b_4}{\partial k_j} = -\frac{\partial b_3}{\partial k_j}, \quad j = 1, 2, 3
\]

and since then

\[
\left\langle \frac{\partial b_4}{\partial k_j}, b_4 \right\rangle_A = 0, \quad j = 1, 2, 3. \tag{4.2.5}
\]

The amplitude equation corresponding to \( \lambda_4 \) has the following form:

\[
\dot{a} = \frac{a}{2 |p| \sqrt{\rho(x_0) \kappa(x_0)}} \left( \frac{\partial_x \kappa(x_0) \cdot p}{2 \kappa(x_0)} - \frac{\partial_x \rho(x_0) \cdot p}{2 \rho(x_0)} - \frac{1}{|p|^2} (2(M_{12} p_1 p_2 + M_{13} p_1 p_3 + M_{23} p_2 p_3)
\]
\[
- (M_{11}(p_2^2 + p_3^2) + M_{22}(p_1^2 + p_3^2) + M_{33}(p_1^2 + p_2^2))) \right).
\]
The Gaussian beam superposition for acoustic waves has the following form:

\[ u^\varepsilon(t, x) = (a_1(t, x)b_1(x, \partial_x S_0(x)) + a_2(t, x)b_2(x, \partial_x S_0(x))) e^{iS_0(x)/\varepsilon} \]
\[ + \frac{1}{(2\pi\varepsilon)^{3/2}} \int_{K_0} u^\varepsilon_{GB}(t, x; x_0) + u^\varepsilon_{GB}(t, x; x_0) dx_0, \]

where

\[ u^\varepsilon_{GB}(t, x; x_0) = (a_i(t; x_0)b_i(x, \partial_x \Phi_i(t, x; x_0)) + \varepsilon v^i_1(t, x; x_0)) e^{i\Phi_i(t; x_0)/\varepsilon}, \quad i = 3, 4, \]

which combines both geometric optics and Gaussian beam terms. This completes the construction of the asymptotic solution of the acoustic waves.
CHAPTER 5. SUMMARY AND DISCUSSION

5.1 General Conclusion

In this thesis, we have studied error estimates for the Gaussian beam superposition method applied to the Schrödinger equation with periodic potentials and strictly symmetric hyperbolic systems, both subject to highly oscillatory initial data. We obtain optimal error estimates for first order Gaussian beams, using similar techniques for both problems.

As for the Schrödinger equation, the main challenge is the band structure of the solution, which leads to the theory of Bloch waves. The problem is studied in the case with strictly separated energy bands, which allows construction of smooth asymptotic solutions. In this project, the following results were obtained:

- Gaussian beam superposition in the two-scale formulation;
- Initial error estimate;
- Evolution error estimate;
- Validation of the two-scale results for the original problem.

Limitation: these results relies on the assumption of the finite number of energy bands.

Our results can be used in practice by approximating a given high frequency initial data by finite number of bands within certain accuracy. An open question in our Gaussian beam theory is to deal with infinite number of bands. Also we need energy band separation condition (in the quantum physics literature it is called forbidden ranges for energy bands). This condition implies analyticity of Bloch functions, which is needed in order to construct Gaussian beam solutions.

In the strictly hyperbolic systems case, we obtained the following results:

- Asymptotic solution via superposition of Gaussian beams;
• Initial error estimate;

• Evolution error estimate;

• Extension of the result to the general phase with vanishing phase gradient on a set of measure zero.

The construction of the asymptotic approach using Gaussian beams for hyperbolic systems is a new result itself. The existence of the orthogonal basis formed by eigenvectors of the symmetric hyperbolic system is a key condition which makes this construction possible. Several ideas developed in the previous works by Liu, Ralston, et al are used for the proofs of the error bounds. We can construct asymptotic solutions for any highly oscillatory initial data, since the data can always be decomposed into a sum of finite number of eigenvectors. The strict separation of the eigenvalues is needed for construction of the Gaussian beam amplitudes. In order to extend our result to more general hyperbolic systems, we need to check whether additional conditions need do be imposed, which is discussed in Chapter 4.

For both problems, the evolution error is accumulating in time and hence it is practical to consider a time period \([0, T]\) with \(T\) sufficiently less than \(\varepsilon^{-1/2}\). It would be interesting to generalize the results to global in time error estimates, although this appears to be difficult and there might be a need to modify the approximation so that terms contributing to evolution error are decaying in time at a certain rate.

### 5.2 Future Work

There are several directions of the future research for both projects. One immediate extension of our results is estimates for higher order Gaussian beam approximations. This should be the next step in our investigation. Some other possible extensions are listed below.

For the Schrödinger equation, we are dealing with the two-scale approach. This approach is a powerful tool in dealing with high frequency problems. It is a simplest case of a problem with many high frequency scales. Thus, it is worth to consider more general multiscale problems. Another extension of our work is the study of the case of the infinite representation of the initial data. In order to succeed in this extension, a deeper understanding of Bloch bands and energy bands
is needed. In particular, whether there exist uniform bounds for derivatives of energy bands and Bloch functions.

As for the strictly hyperbolic systems, so far we have considered only a relatively simple setting and in the future work we may attack more general hyperbolic systems. This can be a system with non-constant coefficients, a nonhomogeneous system, a system with high frequency coefficients and others. The more advanced goal is to understand more realistic models, for example, the system of Maxwell equations; so far the repeating eigenvalues and divergence free condition appear to be the new difficulty in constructing accurate Gaussian beam approximations.

Another challenge for practical applications of Gaussian beams is the time decay of the phase Hessian $M$ and thus, after some time the beam becomes “flat”, unless some reinitialization of the beams is implemented. One approach of remedy is to consider a "frozen" Gaussian beam with no $M$ involved. Frozen Gaussian beam approach gives the first order convergence, yet a higher computational cost.

The other direction for the future work is to continue to study Bloch bands and energy bands. This topic is important for applications in quantum chemistry and the study of solids with periodic structures. For instance, in experiments, the energy bands are crossing or touching each other, which in theory affects analyticity properties of band functions. Therefore, there is a need to study this topic in greater depth in order to make the Gaussian beam theory more applicable to real processes. Problems involving almost periodic and quasi periodic structures or materials with mixed structure and some random terms involved are also important, this is another possible direction of extension of our results.

The development of efficient computational methods for Gaussian beams is also one of topics for the future study. Another possible direction is the study of high frequency boundary value problems, since this has a lot of applications in geophysics. In particular, the decomposition of the multi-scale high frequency data from the boundary into Gaussian beams, which are used to construct an asymptotic solution, is worth further investigation. A problem involving obstacles is also challenging in the study of high frequency wave propagations.

In the long run, we are interested in the study of nonlinear high frequency problems, for example, nonlinear Schrödinger equations. Since the possibility to construct the superposition of Gaussian
beams is based on the linearity of the equation, some new ideas need to be developed.


