RECOVERY OF HIGH FREQUENCY WAVE FIELDS FROM PHASE SPACE BASED MEASUREMENTS

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ABSTRACT. Computation of high frequency solutions to wave equations is important in many applications, and notoriously difficult in resolving wave oscillations. Gaussian beams are asymptotically valid high frequency solutions concentrated on a single curve through the physical domain, and superposition of Gaussian beams provides a powerful tool to generate more general high frequency solutions to PDEs. An alternative way to compute Gaussian beam components such as phase, amplitude and Hessian of the phase, is to capture them in phase space by solving Liouville type equations on uniform grids. However, the usual Gaussian beam ansatz, once mapped into phase space is no longer an asymptotic solution of the wave equation. In this work we present a recovery theory of high frequency wave fields from phase space based measurements. The construction of these components use essentially the idea of Gaussian beams, that is to allow complex Hessian so that the wave is localized, and globally bounded amplitude and the Hessian can thus be obtained in phase space. We show that a superposition of these ansatz over a moving domain remains an asymptotic solution. Moreover, we prove that the kth order phase space based Gaussian beam superposition converges to the original wave field in L^2 at the rate of $\epsilon^{\frac{k}{2}-\frac{n}{4}}$ in dimension n. Though some calculations are carried out only for linear Schrödinger equations, our results and main arguments apply to more general linear wave equations.

CONTENTS

1. Introduction

In this paper we consider the following equation

$$(1.1) \qquad\qquad P\psi = 0, \quad (x,t) \in \mathbb{R}^n \times \mathbb{R},$$

where $P = -i\epsilon\partial_t + H(x, -i\epsilon\partial_x)$ is a linear differential operator with a real principal symbol $\tau + H(x,p)$, subject to the highly oscillatory initial data

$$(1.2) \qquad\qquad \psi(x,0) = \psi_{in}(x) := A_{in}(x)e^{iS_{in}(x)/\epsilon},$$

where $\psi_{in} \in C_0^\infty(\mathbb{R}^n)$ is a given function. The canonical example is the Schrödinger equation with the Hamiltonian $H(x,p) = \frac{1}{2}|p|^2 + V_{ext}(x)$, where $V_{ext}(x)$ is a given external potential function. The small parameter ϵ represents the fast space and time scale introduced in the equation, as well as the typical wave length of oscillations of the initial data. Propagation of oscillations of wave length ϵ causes mathematical and numerical challenges in solving the problem. Our interest in this article lies in construction of globally valid asymptotic wave fields and analysis of their convergence as well as convergence rates.

Geometric optics, also known as the WKB method or ray-tracing, when applied to model high frequency wave propagation problems such as (1.1) leads to the WKB-type system for both phase and amplitude. The phase is governed by the Hamilton-Jacobi equation

$$(1.3) \qquad\qquad \partial_t S + H(x, \nabla_x S) = 0, \quad x \in \mathbb{R}^n, \ t > 0.$$

This leads to the problem that solving the equation for the phase using the method of characteristics produces singularities which invalidate the approximation. In general, this breakdown occurs when nearby rays intersect resulting in a caustic where geometric optics incorrectly predicts that the amplitude of the solution is infinite. The consideration of these difficulties, beginning with Keller [13], and Maslov [24], lead to the development of the theory of Fourier integral operators, e.g., as given by Hörmander [7].

An alternative approach to the standard WKB method is to seek multi-valued phases, $\{S_i(t,x)\}_{i=1}^K$, to (1.3) corresponding to crossing waves [31]. This is in a sharp contrast to the notion of viscosity solution [3] adopted when (1.3) arises in some other applications. In the last decade considerable amount of work has been done to numerically capture multi-valued phases associated to the WKB system; we refer to review articles [5, 30] and references therein. Recently the level set method has been developed to resolve multi-valuedness of involved quantities in phase space as well as to compute physical observables, e.g. [26, 2, 11, 27, 10, 9, 17, 18, 19, 20, 21]. The key idea, for instance in [2, 17], is to represent characteristic trajectories by common zero sets of some implicit level set functions, and evolve all relevant quantities in phase space, see the review [18]. Another phase space based approach is the use of Wigner transformation [34] to map the underling wave equation into a phase space description, see [16, 23, 22, 31] for its application in the semiclassical limit of Schrödinger equations. These phase space based approaches are extremely useful since they unfold 'caustics'. However, at caustics, neither gives correct prediction for the amplitude.

Yet, superpositions of Gaussian beams (GB) as approximate high frequency solutions are valid at caustics wherever they appear. The existence of such solutions has been known since sometime in the 1960s and these solutions have been used to obtain results on propagation of singularities in PDEs, see [8, 28]. More recently, the Gaussian beam construction has been performed for adiabatic perturbations in magnetic Bloch bands [4]. The individual GB solutions are concentrated on a single ray through space-time. More general solutions that are not necessarily concentrated on a single ray can be obtained from

a superposition of Gaussian beams, we refer to [33] for the construction and convergence analysis in optical wave equations. In geophysical applications, Gaussian beam superpositions have been used to model the seismic wave field [1], for seismic migration [6], as well as to model the atmospheric waves that result from steady airflow over topography [32]. Computation of high frequency waves using Gaussian beams has drawn a growing interest, see e.g. [32, 15, 33, 25, 14, 12]. Particularly efforts have been made to extend Gaussian beam solutions using some phase space based techniques – called Eulerian Gaussian beams in [15].

These motivate us to consider the effectiveness of recovery of wave fields from phase space based measurements using Gaussian beams. Briefly stated, the objective of this article is two fold:

  i) to formulate globally valid asymptotic solutions to (1.1)-(1.2) using phase space based measurements;
  ii) to estimate the error between the exact wave field and the asymptotic ones.

The construction is based on Gaussian beams in physical space, and then mapped into the phase space, in which the Taylor coefficients of phase and amplitude are obtained by solving Liouville type equations. However, the usual Gaussian beam ansatz, once mapped into the phase space, is no longer an asymptotic solution to the wave equation! In this work we prove that a superposition of these ansatz over a moving domain remains an asymptotic solution. To estimate the approximation error we use the well-posedness theory for the Schrödinger equation, from which it follows that the accuracy of the Gaussian beam solution is controlled by the continuous dependence on initial data estimates. Thus, the sources of error in the Gaussian beam solution are the error in approximating the initial data and the error in the numerical solution of Gaussian beam components.

To be specific, our asymptotic solution is expressed as

$$(1.4) \qquad \psi^\epsilon(t,y) = Z(n,\epsilon) \int_{\Omega(t)} \psi_{PGB}(t,y,X)dX,$$

where $X = (x,p)$ denotes variables in phase space $\mathbb{R}^{2n}$, $\Omega(0)$ is the domain where we initialize Gaussian beams form the given data, and $\Omega(t) = X(t,\Omega(0))$ is the image of $\Omega(0)$ under the Hamiltonian flow. Here $\psi_{PGB}(t,y,X)$ is the phase space based Gaussian beam ansatz, and $Z(n,\epsilon)$ is a normalization parameter chosen to match initial data against the Gaussian profile. Our result shows that for the kth order phase space Gaussian beam superposition, the following estimate holds on any bounded time interval, $|t| \leq T$,

$$(1.5) \qquad \|(\psi^\epsilon - \psi)(t,\cdot)\|_{L^2} \lesssim \|(\psi^\epsilon(0,\cdot) - \psi_{in}(\cdot)\|_{L^2} + |\Omega(0)|\epsilon^{\frac{k}{2}-\frac{n}{4}}.$$

Here and in what follows we use $A \lesssim B$ to denote the estimate $A \leq CB$ for a constant C which is independent of ϵ.

For the initial data of the form $\psi_{in} = A_{in}(x)e^{iS_{in}(x)/\epsilon}$ we sample initial Gaussian beams from only the surface $p = \nabla_x S_{in}(x)$. The asymptotic solution is then represented as

$$(1.6) \qquad \psi^\epsilon(t,y) = Z(n,\epsilon) \int_{\Omega(t)} \psi_{PGB}(t,y,X)\delta(w(t,X))dX,$$

where w is obtained from the Liouville equation

$$\partial_t w + H_p \cdot \nabla_x w - H_x \cdot \nabla_p w = 0, \quad w(0,X) = p - \nabla_x S_{in}(x).$$

Out result shows that

$$(1.7) \qquad \|(\psi^\epsilon - \psi)(t,\cdot)\|_{L^2} \lesssim |\operatorname{supp}(A_{in})|\epsilon^{\frac{k}{2}-\frac{n}{4}}.$$

Gaussian beams and geometric optics are closely related in the form of the solution ansatz,

$$\psi(t,x) \sim [A_0(t,x) + \epsilon A_1(t,x) + \cdots + \epsilon^N A_N(t,x)]e^{i\Phi(t,x)/\epsilon},$$

but differ in the assumptions on the phase: the geometric optics method assumes that the phase is a real valued function, while the Gaussian beam construction allows phase to be complex away from its central curve. Each Gaussian beam is constructed from a Taylor expansion of the phase and amplitude functions. The recovery theory presented here can in principle be applied to more general linear wave equations, as long as the wave equation is well-posed.

We now conclude this section by outlining the rest of this paper: in Section 2 we start with Gaussian beam solutions in physical space, and define the phase space based GB ansatz through the Hamiltonian map. Section 3 is devoted to a recovery scheme through superpositions over a moving domain. The total error is shown bounded by an initial error and the evolution error of order $\epsilon^{1/2-n/4}$. Control of initial error is discussed in Section 4, followed by the convergence rate obtained for first order GB solutions. In Section 5, we discuss how to use caustic structure to obtain some better error estimates. Both convergence and convergence rate are obtained for higher order GB solutions in Section 6. In Section 7, we present a level set approach for construction of the phase and their derivatives. Finally in the appendix, we derive phase space equations for all involved Gaussian beam components.

2. Phase space based Gaussian beam Ansatz

2.1. **First order Gaussian beam solutions.** As is well known, the idea underlying Gaussian beams (GB) [29] is to build asymptotic solutions concentrated on a single curve in physical space $(t,x) \in \mathbb{R} \times \mathbb{R}^n$. This means that, given a curve γ parameterized by $x = x(t)$, one makes the Ansatz

$$(2.1) \qquad\qquad \psi^\epsilon(t,x) = A^\epsilon(t,x)e^{i\Phi(t,x)/\epsilon},$$

where $\Phi(t,x(t))$ is real, and $Im\{\Phi(t,x)\} > 0$ for $x \neq x(t)$. The amplitude is allowed to be complex and have an asymptotic expansion in terms of ϵ:

$$A^\epsilon(t,x) = A_0(t,x) + \epsilon A_1(t,x) + \cdots + \epsilon^N A_N(t,x).$$

We wish to build asymptotic solutions to $P\psi(t,x) = 0$, i.e., we want $P\psi^\epsilon = O(\epsilon^2)$. Substituting from (2.1),

$$P\psi^\epsilon = e^{i\Phi(t,x)/\epsilon} [(\partial_t\Phi + H(x,\partial_x\Phi))A_0 + \epsilon(-iLA_0 + (\partial_t\Phi + H(x,\partial_x\Phi))A_1)] + O(\epsilon^2),$$

where L is a linear differential operator, whose form is clear from (2.3) below. The key step in the GB construction is the choice of Φ such that $\partial_t\Phi + H(x,\partial_x\Phi)$ vanishes to high order on γ. The propagation of amplitude can then be determined by $LA_0 = 0$ to make the $O(\epsilon)$ term vanish. We denote $\Phi(t,x)$ on the curve γ by S and the leading amplitude by $A = A_0$. These lead to the standard WKB system

$$(2.2) \qquad\qquad \partial_t S + H(x, \nabla_x S) = 0,$$

$$(2.3) \qquad\qquad \partial_t A + H_p \cdot \nabla_x A = -\frac{A}{2}[Tr(H_{xp}) + Tr(\nabla_x^2 S H_{pp})],$$

where Tr is the usual trace map. We then compute the Taylor series of $\partial_t\Phi + H(x,\Phi_x)$ about $x(t)$ to first and second order to obtain equations for the phase gradient and Hessian

$(u, M) = (\nabla_x \Phi, \nabla_x^2 \Phi)$ as follows

$$(2.4) \qquad \partial_t u + H_p \cdot \nabla_x u = -H_x,$$

$$(2.5) \qquad \partial_t M + H_p \cdot \nabla_x M + H_{xx} + H_{xp}M + MH_{px} + MH_{pp}M = 0.$$

It is shown in [28] that the above construction is only possible if $(x(t), p(t))$, where $p(t) = \nabla_x \Phi(t, x(t))$, is a (null) bi-characteristic curve, which is consistent with the characteristic system for the Hamilton-Jacobi equation (2.2).

$$(2.6) \qquad \frac{d}{dt}x = H_p, \quad x(0) = x_0,$$

$$(2.7) \qquad \frac{d}{dt}p = -H_x, \quad p(0) = p_0,$$

where $(x, p) = (x, p)(t; x_0, p_0)$. From here on we denote the phase space variable as $X = (x, p)$ and $X_0 = (x_0, p_0)$. Then the Hamiltonian dynamics can be expressed as

$$(2.8) \qquad \frac{d}{dt}X(t, X_0) = V(X(t, X_0)), \quad X(0, X_0) = X_0.$$

The phase velocity $V = (H_p, -H_x)$ is divergence free, i.e. $div_X(V) = 0$. On this curve $X = X(t, X_0)$, Gaussian beam components of the first order such as the phase $S(t; X_0)$, the Hessian $M(t; X_0)$ as well as the amplitude $A(t; X_0)$, are obtained by solving the following system of ODEs

$$(2.9) \qquad \frac{d}{dt}S(t; X_0) = p \cdot H_p - H(x, p), \quad S(0; X_0) = S_{\text{in}}(x_0),$$

$$(2.10) \qquad \frac{d}{dt}M(t; X_0) + H_{xx} + H_{xp}M + MH_{px} + MH_{pp}M = 0, \quad M(0; X_0) = M_{\text{in}}(X_0),$$

$$(2.11) \qquad \frac{d}{dt}A(t; X_0) = -\frac{A}{2}\left[Tr[H_{xp}] + Tr[MH_{pp}]\right], \quad A(0; X_0) = A_{\text{in}}(x_0).$$

The essential idea behind the GB method is to choose some complex Hessian M_{in} initially so that M remains bounded for all time, and its imaginary part is positive definite. This way the amplitude $A(t; X_0)$ is ensured to be also globally bounded from solving (2.11).

With these components in place, the Gaussian beam phase is constructed as

$$\Phi(t, y; X_0) = S(t; X_0) + p(t, X_0)(y - x(t, X_0)) + \frac{1}{2}(y - x(t, X_0))^\top M(t; X_0)(y - x(t, X_0)),$$

where $p(t, X_0) = \nabla_x \Phi(t, x(t, X_0))$. The leading order of the amplitude is taken as

$$A(t, y; X_0) = A(t; X_0).$$

The above construction ensures that the following GB Ansatz is an approximate solution

$$\psi_{GB}(t, y; X_0) = A(t; X_0) \exp\left(\frac{i}{\epsilon}\Phi(t, y; X_0)\right).$$

The requirement that $Im(M)$ be positive definite ensures that the asymptotic solution is concentrated on $y = x(t, X_0)$, see e.g. [28].

2.2. Phase space based Gaussian beam ansatz.
If we regard X_0 to be the Lagrangian particle marker, then the map

$$(2.12) \qquad X = X(t, X_0)$$

serves as a particle trajectory mapping: an initial domain $\Omega \in R^{2n}$ in phase space evolves in time to

$$(2.13) \qquad X(t, \Omega) = \{X(t, X_0), \quad X_0 \in \Omega\},$$

with the vector $V = (H_p, -H_x)$ tangent to the particle trajectory in phase space. Since the velocity field is divergent-free, the elementary properties of $X(t, X_0)$ tells that $Vol(X(t, \Omega)) = Vol(\Omega) = |\Omega|$ and

$$det\left(\frac{\partial X(t, X_0)}{\partial X_0}\right) = 1.$$

In other words the map is volume-preserving and invertible.

The phase space based Gaussian beam ansatz is thus obtained by changing X_0 to X through this particle-trajectory map:

$$(2.14) \qquad \psi_{PGB}(t, y, X) = \tilde{A}(t, X) \exp\left(\frac{i}{\epsilon}\tilde{\Phi}(t, y, X)\right),$$

where

$$(2.15) \qquad \tilde{\Phi}(t, y, X) = \tilde{S}(t, X) + p \cdot (y - x) + \frac{1}{2}(y - x)^\top \tilde{M}(t, X)(y - x).$$

To derive the corresponding dynamics for $(\tilde{S}, \tilde{M}, \tilde{A})$ we need the following fact.

Lemma 2.1. (Operator lifting) *Let the phase representative of $w(t; X_0)$ be $\tilde{w}(t, X)$ in the sense that $w(t; X_0) = \tilde{w}(t, X(t, X_0))$ for any $t > 0$, then*

$$\frac{d}{dt}w(t; X_0) = \mathcal{L}\tilde{w}(t, X),$$

where $\mathcal{L}$ is the usual Liouville operator defined by

$$(2.16) \qquad \mathcal{L} := \partial_t + V \cdot \nabla_X.$$

Proof. Taking differentiation of

$$w(t; X_0) \equiv w(t, X(t, X_0)), \quad \forall t > 0$$

in time, we obtain

$$\frac{d}{dt}w(t; X_0) = \partial_t w + \frac{d}{dt}X(t, X_0) \cdot \nabla_X w = \partial_t w + V \cdot \nabla_X w.$$

$\square$

Changing the time derivative $\frac{d}{dt}$ to the Liouville operator $\mathcal{L}$ in the Lagrangian formulation of equations for (S, M, A) in (2.9)-(2.11), we obtain PDEs for $(\tilde{S}, \tilde{M}, \tilde{A})$ in phase space.

$$(2.17) \qquad \mathcal{L}(\tilde{S}) = p \cdot H_p - H(x, p), \quad \tilde{S}(0, X) = S_{\text{in}}(x),$$

$$(2.18) \qquad \mathcal{L}(\tilde{M}) + H_{xx} + H_{xp}\tilde{M} + \tilde{M}H_{px} + \tilde{M}H_{pp}\tilde{M} = 0, \quad \tilde{M}(0, X) = M_{\text{in}}(X),$$

$$(2.19) \qquad \mathcal{L}(\tilde{A}) = -\frac{\tilde{A}}{2}\left[Tr[H_{xp}] + Tr[\tilde{M}H_{pp}]\right], \quad \tilde{A}(0, X) = A_{\text{in}}(X).$$

We point out that though $\psi_{GB}(t, y; X_0)$ is an asymptotic solution to the wave equation, $\psi_{PGB}(t, y, X)$ is usually not. But we shall show that its integral over the moving domain $X(t, \Omega(0))$ remains an asymptotic solution of the wave equation. It is this remarkable feature that allows us to globally recover the original wave field from only some phase space based measurements!

3. Recovery of wave fields by superposition

Since the wave equation we consider is linear, the high frequency wave field ψ at (t, y) in physical space is expected to be generated by a superposition of neighboring Gaussian beams

$$(3.1) \qquad \psi^\epsilon(t, y) = Z(n, \epsilon) \int_{\Omega(0)} \psi_{GB}(t, y; X_0) dX_0,$$

where

$$\Omega(0) = \{X_0, \quad x_0 \in \operatorname{supp}(A_{\text{in}}), \quad p_0 \in \operatorname{range}(\partial_x S_{\text{in}}(x))\}$$

is an open domain in phase space from which we construct initial Gaussian beams from the given data. The normalization parameter $Z(n, \epsilon)$ is determined by matching the initial data $\psi_0(y)$ so that

$$\|\psi_0(\cdot) - \psi^\epsilon(0, \cdot)\| \to 0, \quad \epsilon \to 0.$$

By invoking the volume preserving map $X = X(t, X_0)$ and its inverse $X_0 = X_0(t, X)$, we obtain a phase space based Gaussian beam ansatz

$$\psi_{PGB}(t, y, X) := \psi_{GB}(t, y; X_0(t, X)).$$

As remarked earlier, since the map is time dependent, the above phase space based GB ansatz is no longer an asymptotic solution of the wave equation. We note that their superposition over the moving domain $X(t, \Omega(0))$ remains a correct asymptotic solution.

$$(3.2) \qquad \psi^\epsilon(t, y) = Z(n, \epsilon) \int_{\Omega(t)} \psi_{PGB}(t, y, X) dX,$$

where

$$\Omega(t) = X(t, \Omega(0)).$$

This can be seen directly by using change of variables to go back to the Lagrangian superposition (3.1).

In what follows we will construct ψ_{PGB} without reference to ψ_{GB}. While we could still recover ψ_{GB} from ψ_{PGB} by coordinate transformations, we can check directly that superpositions of ψ_{PGB} are asymptotic solutions. This only requires the following two lemmas.

Lemma 3.1. *For any smooth $f(t, X)$ and divergence-free velocity field V, one has*

$$(3.3) \qquad \frac{d}{dt} \int_{X(t, \Omega)} f(t, X) dX = \int_{X(t, \Omega)} [\partial_t f + \nabla_X \cdot (fV)] dX.$$

Our estimates are consequences of the following elementary lemma.

Lemma 3.2. *Assume that $Im(\tilde{\Phi}(t, y, X)) \geq c|y - x|^2$, $c > 0$, and the Lebeque measure of the initial domain $|\Omega(0)|$ is bounded. Let $B(t, y, X)$ be a smooth function, satisfying*

$$|B| \leq C|y - x|^k, \quad k > 0.$$

Then we have

$$\left\| \int_{\Omega(t)} B(t, y, X) e^{i\tilde{\Phi}(t, y, X)/\epsilon} dX \right\|_{L_y^2} \lesssim |\Omega(0)| \epsilon^{\frac{k}{2} + \frac{n}{4}}.$$

Proof. Using Minkowski's integral inequality we have

$$\left\| \int_{\Omega(t)} B(t,y,X)e^{i\tilde{\Phi}(t,y,X)/\epsilon}dX \right\|_{L_y^2} \leq \left(\int_y \left| \int_{\Omega(t)} |B|e^{-Im(\tilde{\Phi})/\epsilon}dX \right|^2 dy \right)^{1/2}$$

$$\leq \int_{\Omega(t)} \left(\int_y |B|^2 e^{-2Im(\tilde{\Phi})/\epsilon}dy \right)^{1/2} dX$$

$$\leq C \int_{\Omega(t)} \left(\int_y |y-x|^{2k} e^{-2c|y-x|^2/\epsilon}dy \right)^{1/2} dX,$$

continuing the estimate with the stretched coordinates $y - x = \epsilon^{1/2}y'$, and changing from y to y' in the integral

$$\leq C \int_{\Omega(t)} \epsilon^{\frac{k}{2}+\frac{n}{4}} \left(\int_{y'} |y'|^{2k} e^{-2c|y'|^2}dy' \right)^{1/2} dX$$

$$= C|\Omega(t)|\epsilon^{\frac{k}{2}+\frac{n}{4}} \left(\int_y |y|^{2k} e^{-2c|y|^2}dy \right)^{1/2},$$

which when using $|\Omega(t)| = |\Omega(0)|$ proves the result. $\square$

The normalization parameter needs to be chosen to match the initial data. For example, if initially $Im(M_{\mathrm{in}}) = \beta I$, $\beta > 0$, then we need to arrange to match the initial data against $\exp(-\beta|x-y|^2/\epsilon)$. That accounts for

$$(3.4) \qquad Z(n,\epsilon) = \left(\int_y e^{-y^\top Im(M_{\mathrm{in}})y/(2\epsilon)}dy \right)^{-1} = \left(\frac{\beta}{2\pi\epsilon} \right)^{n/2} \sim \epsilon^{-n/2}$$

in dimension n. Taking the Schrödinger equation as an example, we obtain the following.

Theorem 3.3. *Let P be the linear Schrödinger wave operator of the form $P = -i\epsilon\partial_t + H(y, -i\epsilon\partial_y)$, where $H(y,p) = \frac{|p|^2}{2} + V_{ext}(y)$, and ψ^ϵ is defined in (3.2) with $Im(\tilde{M})$ being positive definite, and $Z(n,\epsilon) \sim \epsilon^{-n/2}$, then ψ^ϵ is an asymptotic solution and satisfies*

$$(3.5) \qquad \|P[\psi^\epsilon](t,\cdot)\|_{L_y^2} \lesssim |\Omega(0)|\epsilon^{\frac{3}{2}-\frac{n}{4}}.$$

Proof. We apply the operator P to both sides of (3.2) to obtain

$$Z^{-1}P[\psi^\epsilon] = (-i\epsilon\partial_t + H(y,-i\epsilon\partial_y)) \int_{\Omega(t)} \psi_{PGB}(t,y,X)dX$$

$$(3.6) \qquad = \int_{\Omega(t)} [P[\psi_{PGB}] - i\epsilon\nabla_X \cdot (V\psi_{PGB}))] dX.$$

By a straightforward calculation it follows

$$P[\psi_{PGB}] = -i\epsilon\partial_t \tilde{A}(t,X)e^{i\tilde{\Phi}(t,y,X)/\epsilon} + \tilde{A}P[e^{i\tilde{\Phi}(t,y,X)/\epsilon}]$$

$$= e^{i\tilde{\Phi}(t,y,X)/\epsilon} \left[\tilde{A}[\partial_t\tilde{\Phi} + H(y,\partial_y\tilde{\Phi})] - i\epsilon \left(\partial_t\tilde{A} + \frac{\tilde{A}}{2}Tr[\partial_y^2\tilde{\Phi}] \right) \right].$$

The transport term in the integrand gives

$$-i\epsilon\nabla_X \cdot (V\psi_{PGB}) = e^{i\tilde{\Phi}(t,y,X)/\epsilon} \left[-i\epsilon V \cdot \nabla_X\tilde{A} + \tilde{A}V \cdot \nabla_X\tilde{\Phi} \right].$$

Putting together we have
(3.7)
$$[P - i\epsilon \nabla_X \cdot V](\psi_{PGB}) = e^{i\tilde{\Phi}(t,y,X)/\epsilon} \left[\tilde{A}[\mathcal{L}[\tilde{\Phi}] + H(y, \partial_y \tilde{\Phi})] - i\epsilon \left(\mathcal{L}[\tilde{A}] + \frac{\tilde{A}}{2} Tr[\partial_y^2 \tilde{\Phi}] \right) \right].$$

Using $\partial_y^2 \Phi = \tilde{M}(t, X)$ and that $\tilde{A}$ solves (2.19), we see that $O(\epsilon)$ term vanishes. From (2.15) it follows that

$$\mathcal{L}[\tilde{\Phi}] = \mathcal{L}[\tilde{S}] - |p|^2 - \partial_x V_{ext} \cdot (y - x) + \frac{1}{2}(y - x)^\top \mathcal{L}[\tilde{M}](y - x) - p^\top \tilde{M}(y - x)$$

and

$$H(y, \partial_y \tilde{\Phi}) = V_{ext}(y) + \frac{1}{2}|p + \tilde{M}(y - x)|^2.$$

This when using equation (2.17) for $\tilde{S}$ gives
(3.8)
$$\mathcal{L}[\tilde{\Phi}] + H(y, \partial_y \tilde{\Phi}) = V_{ext}(y) - V_{ext}(x) - \partial_x V_{ext}(y - x) + \frac{1}{2}(y - x)^\top \partial_x^2 V_{ext}(y - x) = O(|y - x|^3).$$

Consequently, using the above lemma with $k = 3$,

$$\|P[\psi^\epsilon](t, \cdot)\|_{L_y^2} \lesssim Z(n, \epsilon)|\Omega(0)|\epsilon^{\frac{3}{2} + \frac{n}{4}},$$

which with (3.4) leads to the desired estimate. $\qquad\square$

Remark 3.1. The extra term in the integral in (3.6) gives an alternate way of seeing that the phase space super-position is an accurate solution of the PDE. Of course, it integrates to zero when the support of the beam superposition does not touch the boundary of the integration domain, but it makes it possible to verify the accuracy without going back to the Lagrangian super-position.

We now obtain the following estimate.

Theorem 3.4. *Given $T > 0$, and let ψ be the solution of the Schrödinger equation subject to the initial data ψ_0, and ψ^ϵ be the approximation defined in (3.2) with $Im(M_{in})$ being positive definite, and $|\Omega(0)| < \infty$. Then there exists $\epsilon_0 > 0$, a normalization parameter $Z(n, \epsilon) \sim \epsilon^{-n/2}$, and a constant C such that for all $\epsilon \in (0, \epsilon_0)$*

$$\|(\psi^\epsilon - \psi)(t, \cdot)\|_{L^2} \leq \|\psi^\epsilon(0, \cdot) - \psi_{in}(\cdot)\|_{L^2} + C|\Omega(0)|\epsilon^{\frac{1}{2} - \frac{n}{4}}$$

for $t \in [0, T]$.

Proof. Let $e := \psi^\epsilon - \psi$, then from $P[\psi] = 0$ it follows

$$P[e] = P[\psi^\epsilon] - P[\psi] = P[\psi^\epsilon].$$

A calculation of $\int_{R^n} [e\overline{P[e]} - \bar{e}P[e]]dy$ leads to

$$\epsilon \frac{d}{dt} \int_y |e|^2 dy = \int_y Im(e\overline{P[\psi^\epsilon]})dy.$$

Integration over $[0, t]$ gives

$$(3.9) \qquad \|e(t, \cdot)\|_{L_y^2} \leq \|e(0, \cdot)\|_{L_y^2} + \frac{1}{\epsilon} \int_0^t \|P[\psi^\epsilon](\tau, \cdot)\|_{L^2} d\tau, \quad t \in [0, T].$$

This when combined with the estimate for $P[\psi^\epsilon]$ in (3.5) gives the result as desired. $\qquad\square$

Remark 3.2. The approximation error comes from two sources: initial error and the evolution error. To improve accuracy one has to enhance the accuracy for both. The evolution accuracy can be improved by obtaining more phase space based measurements such as higher order derivatives of phase and amplitude, which will be sketched in §5.

Remark 3.3. In phase space the tracking of the beam propagation is lost in the Gaussian beam ansatz, but has been recorded through the moving domain $\Omega(t)$, which can be traced back to $\Omega(0)$.

4. Control of the initial error

Let $K(x,\tau) = \frac{1}{(4\pi\tau)^{n/2}}e^{-\frac{|x|^2}{4\tau}}$ be the usual heat kernel, satisfying $\lim_{\tau\downarrow 0}K(x,\tau) = \delta(x)$ as distributions on $\mathbb{R}^n$. Then

$$\int_x K(x-y,\tau)dx = 1, \quad \forall \tau > 0, \ y \in \mathbb{R}^n.$$

For highly oscillatory initial data we have

$$\psi_{\text{in}}(y) = A_{\text{in}}(y)e^{iS_{\text{in}}(y)/\epsilon} = \int_x A_{\text{in}}(y)e^{iS_{\text{in}}(y)/\epsilon}K\left(x-y,\frac{\epsilon}{2}\right)dx.$$

Both the phase and amplitude in the integrand can be approximated by their Taylor expansion when $|x-y|$ is small, say $|x-y| < \epsilon^{1/3}$, and the integral will then be $O(\exp(-c/\epsilon^{1/3}))$ with some $c < \frac{1}{2}$ outside this neighborhood. Let $T_j^x[f](y)$ denote the jth order Taylor polynomial of f about x at the point y. Then

(4.1) $$\psi_{\text{in}}(y) \sim \int_x A_{\text{in}}(x)e^{\frac{i}{\epsilon}\left[T_2^x[S_{\text{in}}](y)\right]}K\left(x-y,\frac{\epsilon}{2}\right)dx,$$

which tends to ψ_{in} as $\epsilon \to 0$.

Indeed, the approximate accuracy is ensured by the following result by Tanushev [33].

Lemma 4.1. *Let* $S_{\text{in}} \in C^\infty(R^n)$ *be a real-valued function, and* $A_{\text{in}} \in C_0^\infty(R^n)$, *and* $\rho \in C_0^\infty(R^n)$ *be such that* $\rho \geq 0$, $\rho \equiv 1$ *in a ball of radius* $\delta > 0$ *about the origin. Define,*

$$\psi_{\text{in}}(y) = A_{\text{in}}(y)e^{iS_{\text{in}}(y)/\epsilon},$$

$$v(y;x) = \rho(y-x)T_j^x[A_{\text{in}}](y)e^{\frac{i}{\epsilon}\left[T_{j+2}^x[S_{\text{in}}](y)\right]}K\left(x-y,\frac{\epsilon}{2}\right).$$

Then

$$\left\|\psi_{\text{in}}(\cdot) - \int_{supp(A_{\text{in}})} v(\cdot;x)dx\right\|_{L^2} \lesssim \epsilon^{\frac{j+1}{2}}.$$

Remark 4.1. We note that for the case $j = 0$ the cutoff function ρ is unnecessary, and it can be shown the initial approximation error remains of order $\epsilon^{1/2}$. However, a cutoff function is certainly important when one is building beams of higher accuracy because the higher order terms in the Taylor expansion of the phase can change the sign of its imaginary part when one does not stay close to the central ray, see §5.

We take the above approximation in (4.1) as initial data for $\psi^\epsilon(0,y)$ and rewrite it as follows

(4.2) $$\psi^\epsilon(0,y) = Z(n,\epsilon)\int_{\Omega(0)}\psi_{PGB}(0,y,X)\delta(p - \nabla_x S_{\text{in}}(x))dX, \quad Z(n,\epsilon) = \frac{1}{(2\pi\epsilon)^{n/2}}$$

with $\tilde{A}_{\text{in}} = A_{\text{in}}(x)$, $\tilde{S}_{\text{in}}(X) = S_{\text{in}}(x)$ and $\tilde{M}_{\text{in}}(X) = \partial_x^2 S_{\text{in}}(x) + iI$. The above lemma ensures that

$$(4.3) \qquad \|\psi_{\text{in}}(\cdot) - \psi^\epsilon(0, \cdot)\|_{L^2} \lesssim \epsilon^{1/2}.$$

In order to track the deformation of the surface $p - \nabla_x S_{\text{in}}(x) = 0$ as time evolves, we introduce a function $w = w(t, X)$ such that

$$(4.4) \qquad \mathcal{L}[w] = 0, \quad w(0, X) = p - \nabla_x S_{\text{in}}(x).$$

For smooth Hamiltonian $H(x, p)$, w remains smooth once it is initially so. A modified approximation is defined as

$$(4.5) \qquad \psi^\epsilon(t, y) := Z(n, \epsilon) \int_{\Omega(t)} \psi_{PGB}(t, y, X)\delta(w(t, X))dX,$$

which has taken care of the Dirac delta function in (4.2). We then have the following theorem.

Theorem 4.2. *If assumptions of Theorem 3.3 are met, then ψ^ϵ defined in (4.5) is also an asymptotic solution, satisfying*

$$(4.6) \qquad \|P[\psi^\epsilon](t, \cdot)]\|_{L^2} \lesssim |\text{supp}(A_{in})|\epsilon^{\frac{3}{2} - \frac{n}{4}}.$$

Proof. Using the volume-preserving map of $X = X(t, X_0)$ and $w(t, X(t, X_0)) = w(0, X_0)$, we have

$$\psi^\epsilon(t, y) = Z(n, \epsilon) \int_{\Omega(0)} \psi_{PGB}(t, y, X(t, X_0))\delta(w(t, X(t, X_0)))dX_0$$

$$= Z(n, \epsilon) \int_{\Omega(0)} \psi_{GB}(t, y; X_0)\delta(w(0, X_0))dX_0$$

$$= Z(n, \epsilon) \int_{\Omega(0)} \psi_{GB}(t, y; X_0)\delta(p_0 - \nabla_x S_{\text{in}}(x_0))dX_0$$

$$(4.7) \qquad = Z(n, \epsilon) \int_{\text{supp}(A_{\text{in}})} A(t; x_0)G(t, y; x_0)e^{i\Phi(t, y; x_0)/\epsilon}dx_0.$$

Here for simplicity we use only x_0 in the integrand instead of $X_0 = (x_0, \nabla_x S_{in}(x_0))$. We now repeat the similar estimate to that in the proof of Lemma 3.2 with $k = 3$ to obtain

$$(4.8) \qquad \left\|\int_{\text{supp}(A_{\text{in}})} A(t; x_0)G(t, y; x_0)e^{i\Phi(t, y; x_0)/\epsilon}dx_0\right\|_{L_y^2} \lesssim |\text{supp}(A_{\text{in}})|\epsilon^{\frac{3}{2} + \frac{n}{4}}.$$

Hence

$$\|P[\psi^\epsilon](t, \cdot)\|_{L^2} \lesssim Z(n, \epsilon)|\text{supp}(A_{\text{in}})|\epsilon^{\frac{3}{2} + \frac{n}{4}}$$

which with (3.4) leads to the desired estimate. $\qquad \square$

Plugging estimates (4.3) and (4.6) into (3.9) we arrive at our main result.

Theorem 4.3. *Given $T > 0$, and let ψ be the solution of the Schrödinger equation subject to the initial data $\psi_{\text{in}} = A_{\text{in}}e^{iS_{\text{in}}(x)/\epsilon}$, and ψ^ϵ be the first order approximation defined in (4.5) with initial data satisfying $\tilde{S}_{\text{in}}(X) = S_{\text{in}}(x)$, $\tilde{M}_{\text{in}}(X) = \partial_x^2 S_{\text{in}}(x) + iI$, and $\tilde{A}_{\text{in}}(X) = A_{\text{in}}(x)$ with $|supp(A_{\text{in}})| < \infty$. Then there exists $\epsilon_0 > 0$, a normalization parameter $Z(n, \epsilon)$, and a constant C such that for all $\epsilon \in (0, \epsilon_0)$*

$$\|(\psi^\epsilon - \psi)(t, \cdot)\|_{L^2} \lesssim |\text{supp}(A_{\text{in}})|\epsilon^{\frac{1}{2} - \frac{n}{4}}$$

for $t \in [0, T]$.

Remark 4.2. The exponent $1/2$ reflects the accuracy of the Gaussian beam in solving the PDE. It will increase when one uses more accurate beams. The exponent $-\frac{n}{4}$ indicates the blow-up rate for the worst possible case due to caustics. Of course, if nature of the caustic were a priori known, it would be possible to obtain a better convergence rate by taking the caustic structure into account.

5. A CLOSER LOOK AT CAUSTICS

5.1. **Schur's lemma.** Instead of using the Minkowski inequality we shall use Schur's lemma to see how caustic structure may be used to obtain a better estimate. Recall Schur's Lemma: If $[Tf](y) = \int K(x,y)f(x)dx$ and

$$\sup_x \int_y |K(x,y)|dy = C_1, \ \sup_y \int_x |K(x,y)|dx = C_2,$$

then

$$\|Tf\|_{L^2} \leq \sqrt{C_1 C_2}\|f\|_{L^2}.$$

Proof. We have by Schwartz

$$|[Tf](y)|^2 \leq \left(\int |K(x,y)||f(x)|dx\right)^2 \leq \int |K(x,y)|dx \int |K(x,y)||f(x)|^2 dx$$

$$\leq C_2 \int |K(x,y)||f(x)|^2 dx.$$

So integrating both sides in y and taking the square root gives the result. $\square$

We now apply Schur's lemma to left hand side of (4.8). So for simplicity

$$[Tf](y) = \int_{\mathrm{supp}(A_{\mathrm{in}})} A(t;x_0)G(t,y;x_0)e^{i\Phi(t,y;x_0)/\epsilon}dx_0,$$

where the imaginary part of $\Phi(t,y;x_0)$ is bounded below by cI and for convenience we will assume that $|G| \leq |y - x(t,x_0)|^k$. Then one can apply Schur's lemma with

$$C_1 = \sup_{x_0} \int_y |y - x(t,x_0)|^k e^{-(c/\epsilon)|y-x(t,x_0)|^2} dy = \epsilon^{\frac{k}{2}+\frac{n}{2}} \int_z |z|^k e^{-c|z|^2} dz, \quad \text{and}$$

$$C_2(t,\epsilon) = \sup_y \int_{x_0} |y - x(t,x_0)|^k e^{-(c/\epsilon)|y-x(t,x_0)|^2} dx_0.$$

In general one does not know what $C_2(t,\epsilon)$ will be. As long as A has compact support C_2 will be at least bounded by $c\epsilon^{k/2}$. Thus the error in L^2 norm will be bounded by $c\epsilon^{k/2+n/4}$, as shown in (4.8) with the Minkowski inequality. Note that the worst case for the wave equation, $\partial_t^2\psi - \Delta\psi = 0$, occurs when $x(t,x_0) = x_0(1 - t/|x_0|)$. In that case $C_2 = c\epsilon^{k/2+(1+n)/4}$, yielding a better rate.

5.2. **An example with remarkable accuracy.** Here below we illustrate that a better convergence rate can also be obtained for the Schrödinger equation with quadratic potential and quadratic phase. We consider the solution of

$$i\epsilon\partial_t\psi = -\frac{\epsilon^2}{2}\Delta\psi, \quad x \in \mathbb{R}^n,$$

with the initial data $\psi(0,x) = \exp(-i|x|^2/(2\epsilon))$, then

$$\psi(t,x) = (1-t)^{-n/2}\exp\left(-\frac{i|x|^2}{2\epsilon(1-t)}\right).$$

This solution becomes a multiple of the δ-function at $t = 1$. This suggested solving the free Schrödinger equation with initial data $\psi(x, 0) = g(x) \exp\left(-i|x|^2/(2\epsilon)\right)$ where $g \in C^\infty(\mathbb{R}^n)$ and evaluating the solution at $t = 1$. Using Fourier transform one may express the solution as

$$\psi(t, x) = \frac{1}{(2\pi i \epsilon t)^{n/2}} \int_y \psi_0(y) \exp\left(\frac{i}{2\epsilon t}|x - y|^2\right) dy.$$

Evaluating at $t = 1$, we have

$$\psi(1, x) = \frac{1}{(2\pi i \epsilon)^{n/2}} \int_y g(y) e^{-ix \cdot y/\epsilon} dy \, e^{i|x|^2/(2\epsilon)} = c\epsilon^{-n/2} \hat{g}(x/\epsilon) e^{i|x|^2/(2\epsilon)},$$

where $c = e^{-\pi n i/4}$ and $\hat{g}$ is the Fourier transform of g, defined by

$$\hat{g}(\xi) = \frac{1}{(2\pi)^{n/2}} \int g(x) e^{-ix \cdot \xi} dx.$$

It is easy to verify that

$$\|\psi(1, \cdot)\|_{L^2} = \|\psi(0, \cdot)\|_{L^2}.$$

As $\epsilon \to 0$, $\psi(1, x)$ diverges (pointwise) like $\epsilon^{-n/2}$ near $x = 0$, but goes rapidly to zero away from $x = 0$.

We now build a superposition of Gaussian beams approximation for the solution of the same problem. For the Gaussian beam superposition, the phase is obtained as

$$\Phi(t, x; y) = (t - 1)\frac{|y|^2}{2} - x \cdot y + |y|^2(1 - t) + \frac{\beta i - 1}{1 + (\beta i - 1)t}\frac{|x - y(1 - t)|^2}{2}.$$

Note that we have chosen $\beta > 0$ for the initial beam width. For the amplitude we get

$$(1 + (\beta i - 1)t)^{n/2} A(t, y(1 - t)) = A(0, y) = g(y).$$

So, setting $x(t; y) = (1 - t)y$, we obtain

$$A(t, x(t; y)) = (1 + (\beta i - 1)t)^{-n/2} g(y).$$

If we do the superposition with the normalization, we end up with

$$\psi^\epsilon(t, x) = \left(\frac{\beta}{2\pi\epsilon}\right)^{n/2} \int_y [1 + (\beta i - 1)t]^{-n/2} g(y) e^{i\Phi(t, x; y)/\epsilon} dy.$$

If we evaluate that at $t = 1$, it becomes

$$\psi^\epsilon(1, x) = \left(\frac{\beta}{2\pi\epsilon}\right)^{n/2} \int_y [\beta i]^{-n/2} g(y) e^{\frac{i}{\epsilon}[-x \cdot y + \frac{\beta i - 1}{\beta i}\frac{|x|^2}{2}]} dy$$

$$= c\epsilon^{-n/2} \hat{g}(x/\epsilon) e^{(\beta i - 1)|x|^2/(2\beta\epsilon)}$$

$$= \psi(1, x) e^{-|x|^2/(2\beta\epsilon)}.$$

This shows that at the caustic $x = 0$, both become the same. We can see the error $\psi(1, x)\left(1 - e^{-|x|^2/(2\beta\epsilon)}\right)$ when measured in L^2-norm:

$$\|\psi^\epsilon(1, \cdot) - \psi(1, \cdot)\|_{L^2}^2 = \epsilon^{-n} \int |\hat{g}\left(\frac{x}{\epsilon}\right)|^2 \left(1 - e^{-|x|^2/(2\beta\epsilon)}\right)^2 dx$$

$$= \int |\hat{g}(z)|^2 \left(1 - e^{-\epsilon|z|^2/(2\beta)}\right)^2 dz.$$

That implies that
(a) For any $g \in L^2$ the Gaussian beam approximation converges to the true solution (at $t = 1$), but there is no uniform estimate on the difference in terms of the L^2-norm of g (an

example of strong but not uniform convergence).

(b) If $\int |\hat{g}(z)|^2(1+|z|^2)^2 dz < \infty$, i.e. if $g \in H^2$, then the norm of the difference is $O(\epsilon)$.

Actually in the current example, it can be verified that the evolution error is zero, so the initial error should propagate in time. If we look at the initial error of the Gaussian beam approximation, we have

$$\|\psi^\epsilon(0,\cdot) - \psi(0,\cdot)\|_{L^2}^2 = \int_x \left| \left(\frac{\beta}{2\pi\epsilon}\right)^{n/2} \int_y g(y) e^{-\frac{\beta}{2\epsilon}|x-y|^2} dy - g(x) \right|^2 dx$$

$$= \left(\frac{\beta}{2\pi\epsilon}\right)^n \int_x \left| \int_y (g(y) - g(x)) e^{-\frac{\beta}{2\epsilon}|x-y|^2} dy \right|^2 dx.$$

Set $K(x) = \left(\frac{\beta}{2\pi\epsilon}\right)^{n/2} e^{-\frac{\beta}{2\epsilon}|x|^2}$, a direct integration shows that $\hat{K} = (2\pi)^{-n/2} e^{-\epsilon|\xi|^2/(2\beta)}$. If we apply Parseval's theorem, we obtain

$$\|\psi^\epsilon(0,\cdot) - \psi(0,\cdot)\|_{L^2}^2 = \|\hat{g} - (2\pi)^{n/2}\hat{g} \cdot \hat{K}\|_{L^2}^2$$

(5.1)
$$= \int |\hat{g}(z)|^2 \left(1 - e^{-\epsilon|z|^2/(2\beta)}\right)^2 dz,$$

which is the same error as that evaluated at $t = 1$. We point out that for the initial phase of general form, the initial error is still $O(\epsilon^{1/2})$ unless an higher order expansion of the phase is used.

There are two conclusions that one can draw from the preceding.

Theorem 5.1. *Under assumptions of Theorem 4.3 and assume that the potential is a quadratic function. Then for $t \in [0,T]$ and $\epsilon \in (0,\epsilon_0)$ we have*

- *If S_{in} is a quadratic function and $A_{\text{in}} \in H^2$*

$$\|(\psi^\epsilon - \psi)(t,\cdot)\|_{L^2} \lesssim \epsilon.$$

- *If $S_{\text{in}} \in C^\infty$ and $A_{\text{in}} \in C_0^\infty$*

$$\|(\psi^\epsilon - \psi)(t,\cdot)\|_{L^2} \lesssim \epsilon^{1/2}.$$

Proof. It follows from (3.8) that for quadratic potentials

$$P[\psi^\epsilon] = 0.$$

Then the total error is governed by the initial error only. For quadratic potentials and $A_{\text{in}} \in H^2(\mathbb{R}^n)$ we obtain the $O(\epsilon)$ error as shown in (5.1). For the general phase function the claim follows from Lemma 4.1 with $j = 0$. $\qquad\square$

6. HIGHER ORDER APPROXIMATIONS

The accuracy of the phase space based Gaussian beam superposition also depends on accuracy of the individual Gaussian beam ansatz. If we refer the above construction as a first order GB solution, then the kth order GB solution should involve terms up to $(k+1)^{th}$ order for the phase, and $(k-1-2l)^{th}$ order for the lth amplitude A_l for $l = 0, \cdots, \left[\frac{k-1}{2}\right]$. The equations for these phase and amplitude Taylor coefficients can be derived by letting the leading order ones to hold on γ along with several of their derivatives (see the Appendix).

Let $X = X(t; X_0)$, with $x = x(t; X_0)$, denote the characteristic path at time $t > 0$, which originates from X_0. Following [33] we define the kth order Gaussian beams as follows

$$\psi_{kGB}(t, y; X_0) = \rho(y - x) \left[\sum_{l=0}^{\lfloor \frac{k-1}{2} \rfloor} \epsilon^l T^x_{k-1-2l}[A_l](y) \right] \exp\left(\frac{i}{\epsilon} T^x_{k+1}[\Phi](y) \right),$$

where $T^x_k[f](y)$ is the kth order Taylor polynomial of f about x evaluated at y, and ρ is a cut-off function such that on its support the Taylor expansion of Φ still has a positive imaginary part.

By invoking the volume preserving map $X = X(t, X_0)$ and its inverse map denoted by $X_0 = X_0(t, X)$, we obtain a phase space based k^{th} order Gaussian beam Ansatz

$$\psi_{kPGB}(t, y, X) := \psi_{kGB}(t, y; X_0(t, X)).$$

Beyond the first order GB components, all Taylor coefficients $\partial_y^\alpha \Phi$ for $|\alpha| \geq 3$ in phase space are replaced by $m_\alpha(t, X)$, satisfying a linear equation (8.1) in phase space; and Taylor coefficients $\partial_y^\alpha A_l$ for $|\alpha| \geq 1$ in the amplitude are replaced by $\tilde{A}_{l,\alpha}$, which can be obtained recursively from solving transport equations in phase space, see the appendix for details.

Proceeding as previously, we form the superpositions.

(6.1) $$\psi_k^\epsilon(t, y) = Z(n, \epsilon) \int_{\Omega(t)} \psi_{kPGB}(t, y, X)\delta(w(t, X))dX,$$

where $\Omega(t) = X(t, \Omega(0))$, and $w(t, X)$ is the solution of the Liouville equation subject to $w(0, X) = p - \nabla_x S_{\text{in}}(x)$.

This gives a kth order asymptotic solution of the wave equation. More precisely, we have the following theorem.

Theorem 6.1. *Let P be the linear Schrödinger wave operator of the form $P = -i\epsilon\partial_t + H(y, -i\epsilon\partial_y)$, where $H(y, p) = \frac{|p|^2}{2} + V_{ext}(y)$, and ψ^ϵ is defined in (6.1) with $Im(M_{\text{in}}) = I$ and $Z(n, \epsilon) = (2\pi\epsilon)^{-n/2}$, then ψ_k^ϵ is an asymptotic solution and satisfies*

(6.2) $$\|P[\psi_k^\epsilon](t, \cdot)\|_{L_y^2} \lesssim |\text{supp}(A_{\text{in}})|\epsilon^{\frac{k}{2}+1-\frac{n}{4}}.$$

Proof. Using the volume-preserving map of $X = X(t, X_0)$ and $w(t, X(t, X_0)) = w(0, X_0)$, we have

$$\psi_k^\epsilon(t, y) = Z(n, \epsilon) \int_{\Omega(0)} \psi_{kPGB}(t, y, X(t, X_0))\delta(w(t, X(t, X_0)))dX_0$$

$$= Z(n, \epsilon) \int_{\Omega(0)} \psi_{kGB}(t, y; X_0)\delta(w(0, X_0))dX_0$$

$$= Z(n, \epsilon) \int_{\Omega(0)} \psi_{kGB}(t, y; X_0)\delta(p_0 - \nabla_x S_{\text{in}}(x_0))dX_0$$

$$= Z(n, \epsilon) \int_{\text{supp}\{A_{\text{in}}\}} \psi_{kGB}(t, y; x_0)dx_0.$$

According to the GB construction sketched in the appendix, $\psi_{kGB}(t, y; x_0)$ are asymptotic solutions for each x_0, so will be their superpositions $\psi_k^\epsilon(t, y)$. It remains to verify (6.2). First we see that

$$P[\psi_k^\epsilon(t, y)] = Z(n, \epsilon) \int_{\text{supp}\{A_{\text{in}}\}} P[\psi_{kGB}(t, y; x_0)]dx_0.$$

Using (8.3) in the appendix with A replaced by $\rho(y-x)\left[\sum_{l=0}^{\lfloor\frac{k-1}{2}\rfloor}\epsilon^l T_{k-1-2l}^x[A_l](y)\right]$ and Φ by $T_{k+1}^x[\Phi](y)$, we have

$$c_0(t,y) = [\partial_t T_{k+1}^x[\Phi](y) + H(y, \nabla_y T_{k+1}^x[\Phi](y))]\rho(y-x)T_{k-1}^x[A_0](y).$$

Using $T_{k+1}^x[\Phi](y) = \Phi(y) + R_{k+1}^x[\Phi](y)$, here R_{k+1}^x denotes the remainder of the Taylor expansion, and $G(t,y) = \partial_t\Phi + H(y, \nabla_y\Phi) = O(|y-x|^{k+2})$ we can see that

$$|c_0(t,y)| \leq C|y-x|^{k+2}.$$

Also using the construction for A_l and their derivatives in the appendix, we are able to show

$$|c_l(t,y)| \leq C|y-x|^{k+2-2l},$$

where we have used the fact that differentiation of ρ vanishes in a neighborhood of x. The use of the cut-off function ensures that we can always choose a small neighborhood of $x(t;x_0)$ so that

$$Im(T_{k+1}^x[\Phi](y)) \geq c|y-x|^2.$$

Consequently, using Minkowski's integral inequality,

$$Z^{-1}\|P[\psi_k^\epsilon(t,\cdot)]\|_{L^2} \leq \left(\int_y \left|\int_{\text{supp}(A_{\text{in}})} e^{-Im(T_{k+1}^x[\Phi](y))/\epsilon}|c_0 + c_1\epsilon + \cdots|\,dx_0\right|^2 dy\right)^{1/2}$$

$$\leq \int_{\text{supp}(A_{\text{in}})}\left(\int_y e^{-2c|y-x(t,x_0)|^2/\epsilon}|c_0 + c_1\epsilon + \cdots|^2\,dy\right)^{1/2} dx_0$$

$$\leq C\int_{\text{supp}(A_{\text{in}})}\left(\int_y e^{-2c|y-x(t,x_0)|^2/\epsilon}\sum_{l=0}^{\lfloor\frac{k-1}{2}\rfloor}|y-x(t,x_0)|^{2(k+2-2l)}\epsilon^{2l}dy\right)^{1/2} dx_0.$$

If we introduce the stretched coordinates $y - x(t;x_0) = \epsilon^{1/2}y'$, and changing from y to y' in the integral, we see that the new integrand is bounded by

$$\epsilon^{k+2+\frac{n}{2}}|y'|^{2(k+2-2l)}\exp\left(-2c|y'|^2\right).$$

Thus $\|P[\psi_k^\epsilon(t,\cdot)]\|_{L^2}$ is bounded by $Z(n,\epsilon)|\text{supp}(A_{\text{in}})|\epsilon^{\frac{k}{2}+1+\frac{n}{4}}$. The desired estimate then follows. □

In order to obtain an estimate of $\|(\psi_k^\epsilon - \psi)(t,\cdot)\|$ for any $t \leq T$, all that remains to verify is that the superposition (6.1) accurately approximates the initial data. For $t = 0$, the approximation is as follows

$$\psi_k^\epsilon(0,y) = Z(n,\epsilon)\int_{\Omega(0)}\psi_{kPGB}(0,y,X)\delta(w(0,X))dX$$

$$= Z(n,\epsilon)\int_{\Omega(0)}\psi_{kGB}(0,y,X_0)\delta(p_0 - \nabla_x S_{\text{in}}(x_0)))dX_0$$

$$= Z(n,\epsilon)\int_{\text{supp}A_{\text{in}}}\psi_{kGB}(0,y,x_0,\nabla_x S_{\text{in}}(x_0))dx_0,$$

where

$$\psi_{kGB}(0,y,x,\nabla_x S_{\text{in}}(x)) = \rho(y-x)\left[T_{k-1}^x[A_{\text{in}}](y)\right]\exp\left(\frac{i}{\epsilon}T_{k+1}^x[S_{\text{in}}](y)\right)e^{-i|y-x|^2/(2\epsilon)},$$

where we have taken $A_0 = A_{\text{in}}$ and $A_l = 0$ for $l \geq 1$, $\partial_x^\alpha \Phi(0, x) = \partial_x^\alpha S_{\text{in}}(x)(\alpha \neq 2)$, and $\partial_x^2 \Phi(0, x) = \partial_x^2 S_{\text{in}}(x) + iI$. From Lemma 4.1 we have that

$$\|\psi_{\text{in}} - \psi^\epsilon(0, \cdot)\|_{L^2} \lesssim \epsilon^{\frac{k}{2}}.$$

Thus our main result for k^{th} order phase space GB superposition is as follows.

Theorem 6.2. *Given $T > 0$, and let ψ be the solution of the Schrödinger equation subject to the initial data $\psi_{\text{in}} = A_{\text{in}} e^{iS_{\text{in}}(x)/\epsilon}$, and ψ^ϵ be the kth order approximation defined in (6.1) with initial data chosen as described above with $|supp(A_{\text{in}})| < \infty$. Then there exists $\epsilon_0 > 0$, a normalization parameter $Z(n, \epsilon) \sim \epsilon^{-n/2}$, and a constant C such that for all $\epsilon \in (0, \epsilon_0)$*

$$\|(\psi^\epsilon - \psi)(t, \cdot)\|_{L^2} \lesssim |supp(A_{\text{in}})| \epsilon^{\frac{k}{2} - \frac{n}{4}}$$

for $t \in [0, T]$.

7. Computing Taylor coefficients of the phase via level set functions

We now turn to construction of the phase space ingredients required for the approximation. In order to identify a bi-characteristic curve in phase space, we introduce a vector-valued level set function $\phi \in \mathbb{R}^{2n}$ so that the interaction of zeros of each component uniquely defines the target curve. In other words, we assume that

$$\Gamma = \{(t, X), \ \phi(t, X) = \phi(0, X_0)\}$$

contains the bi-characteristic curve starting from $X_0 = (x_0, p_0)$ for any $t > 0$, then ϕ must satisfy

$$\phi(t, X(t, X_0)) \equiv \phi(0, X_0).$$

This is equivalent to the following Liouville equation

$$(7.1) \qquad\qquad \mathcal{L}[\phi(t, X)] = 0,$$

where $\mathcal{L} := \partial_t + V \cdot \nabla_X$ is the Liouville operator. The initial data can be simply taken as

$$(7.2) \qquad\qquad \phi(0, X) = X - X_0.$$

Then the curve Γ is globally determined by the zero set of a vector level set function $\phi = (\phi_1, \phi_2)^\top$.

For the construction, $\tilde{S}$ can be solved from (2.17), we are then left to determine $\tilde{M}$, followed by solving (2.19) to obtain $\tilde{A}$. Note that equation (2.18) is nonlinear in $\tilde{M}$, the solution might not exist for all $t > 0$. The heart of the GB method is to choose complex initial data so that a global solution is guaranteed and satisfies two requirements [28]:
i) $\tilde{M} = \tilde{M}^T$,
ii) $Im(\tilde{M})$ must be positive definite for all $t > 0$.

7.1. **Evaluation of the Hessian.** We now show this can be done via the obtained level set functions $\phi \in \mathbb{R}^{2n}$.

Theorem 7.1. *Let $\phi = (\phi_1, \phi_2)^\top$ with $\phi_i \in \mathbb{R}^n$ be the global solution of (7.1) with the initial condition (7.2). We have*
a) $\mathcal{L}(k_1\phi_1 + k_2\phi_2) = 0$ for any $k_1, k_2 \in \mathbb{C}$.
b) Set $g := k_1\phi_1 + k_2\phi_2$. If $Im(\bar{k}_1 k_2) \neq 0$, then g_p is invertible for all $t > 0$.
c) If $M_{\text{in}} = -g_x(g_p)^{-1}|_{t=0}$, then $\tilde{M} = -g_x(g_p)^{-1}$ for all $t > 0$,
d) M satisfies (2.18) and i). If $Im(k_1/k_2) < 0$, then $\tilde{M}$ satisfies ii) too.

Proof. a) This follows by noting that the Liouville operator is linear and all its coefficients are real.

b) By taking the gradients ∇_x and ∇_p of the Liouville equation $\mathcal{L}(g) = 0$, respectively, we obtain the following equations

(7.3)
$$\mathcal{L}(g_x) = H_{xx}g_p - H_{xp}g_x,$$

(7.4)
$$\mathcal{L}(g_p) = H_{px}g_p - H_{pp}g_x.$$

The equation is understood to be satisfied by each matrix. Let $B = \overline{g_p}^T g_x - \overline{g_x}^T g_p$ be a complex matrix, and I an identity matrix, a direct verification shows that

$$\mathcal{L}(B) = \mathcal{L}(\overline{g_p}^T g_x) - \mathcal{L}(\overline{g_x}^T g_p)$$
$$= \overline{\mathcal{L}(g_p)}^T g_x + \overline{g_p}^T \mathcal{L}(g_x) - \overline{\mathcal{L}(g_x)}^T g_p + \overline{g_x}^T \mathcal{L}(g_p)$$
$$= 0.$$

Observe that $B(0, X) = -2iIm(\bar{k}_1 k_2)I$ is a constant matrix. Thus for any $t > 0$,

$$B(t, X(t, X_0)) = B(0, X_0) = -2iIm(\bar{k}_1 k_2)I.$$

The condition $Im(\bar{k}_1 k_2) \neq 0$ ensures that g_p must be invertible for all $t > 0$. Otherwise there would be a nonzero vector c such that $g_p c = 0$, hence $\bar{c}^\top B c = \overline{(g_p c)}^\top g_x c = 0$, leading to a contradiction.

c) Set $Q = g_x + \tilde{M}g_p$. A calculation using (2.18), (7.3) and (7.4) gives

$$\mathcal{L}[Q] = \mathcal{L}(g_x) + \mathcal{L}(\tilde{M}g_p) = -(H_{xp} + \tilde{M}H_{pp})Q.$$

If $M_{\text{in}} = -g_x(g_p)^{-1}$ initially, then $Q(0, X) = 0$ for all $X \in \mathbb{R}^{2n}$. Thus we have

$$Q(t, X) = g_x + \tilde{M}g_p \equiv 0.$$

This gives

$$\tilde{M} = -g_x(g_p)^{-1}$$

for all $t > 0$ since g_p is invertible.

d. i) Initially $M_{\text{in}} = -\frac{k_1}{k_2}I = M_{\text{in}}^T$. Since $\tilde{M}^T$ also satisfies equation (2.18), hence $\tilde{M} = \tilde{M}^T$.

ii) With the definition of B, we have

$$B = -\overline{g_p}^T \tilde{M}g_p + \overline{g_p}^T \overline{\tilde{M}}g_p = -2iIm[\overline{g_p}^T \tilde{M}g_p].$$

Initially we have $g_p = k_2 I$. This together with $B(t, X) = B(0, X_0)$ along Γ gives $Im[\overline{g_p}^T \tilde{M}g_p] = |k_2|^2 Im[M_{\text{in}}]$. Note that $Im[M_{\text{in}}]$ is positive definite, hence $Im[\tilde{M}]$ remains positive definite for all $t > 0$. □

Remark 7.1. The formula $M = -\phi_x(\phi_p)^{-1}$, first derived in [10], plays an important role in [10] in deriving the equation

$$\mathcal{L}[f] = 0$$

for the quantity $f(t, X) = |\tilde{A}(t, X)|^2 \det(\phi_p)$, which remains globally bounded even when ϕ_p becomes singular. We note that a complex level set function was used in [12] to obtain a globally bounded Hessian.

Remark 7.2. Since the Liouville equation is geometric and homogeneous, for each fixed X_0, the shift X_0 in the level set function can be simply ignored, and be added back whenever it is needed. In other words, we can take initial data $\phi(0, X) = X$, then the curve Γ can be represented as X_0 level set:

$$\Gamma = \{X, \quad \phi(t, X) = X_0\}.$$

Remark 7.3. If we follow this construction, the initial data for $\tilde{M}_{\mathrm{in}}$ then depends on how we initialize the level set function ϕ. If we take $k_1 = \beta > 0$ and $k_2 = i$, then $g = \beta\phi_1 + i\phi_2$. If $(\phi_1, \phi_2)(x, X) = (x, p)$, then $\tilde{M}_{\mathrm{in}} = i\beta I$. If p_0 is restricted to be the phase gradient at x_0 initially, then the initial level set function can be chosen as $(\phi_1, \phi_2)(0, X) = (x, p - \nabla_x S_{\mathrm{in}}(x))$, this leads to $\tilde{M}_{\mathrm{in}} = \partial_x^2 S_{\mathrm{in}}(x) + i\beta I$. In this case ϕ_2 is the function $w(t, X)$ from (4.4).

7.2. **Evaluation of higher order derivatives of the phase.** Let $G(t, y) = \partial_t \Phi + H(y, \nabla_y \Phi)$. If one wants to have $G(t, y)$ vanish to a higher order than two on γ, it is necessary to obtain higher order derivatives of Φ. In the appendix we derive a system of linear equations for $m_\alpha(t, X) = \partial_y^\alpha \Phi(t, x(t, X_0))$ on γ. We now show that this again can be done through the vector-valued level set function ϕ.

Differentiating $\phi_l(t, x, \nabla_x \Phi) = 0$, $l = 1, 2$, to order of $r \geq 3$ we obtain

$$\sum_{j=1}^{n} \partial_{p_j} \phi_l \partial_{y_j}(\partial_y^\alpha \Phi) + \sum_{|\beta|=r} c_{l\alpha\beta} \partial_y^\beta \Phi + d_{l\alpha} = 0$$

for all multi-indices α of length r. Let $g = k_1 \phi_1 + k_2 \phi_2$, again using the invertibility of g_p we can obtain

$$\nabla_x(m_\alpha) = -(g_p)^{-1} \left[\sum_{|\eta|=r} c_{\alpha\eta} m_\eta(t, X) + d_\alpha \right].$$

We do this recursively, since the coefficients $c_{\alpha,\eta} = (c_{1\alpha,\eta}, \cdots, c_{n\alpha,\eta})^\top$ and $d_\alpha = (d_{1\alpha}, \cdots d_{n\alpha})^\top$ depend on all the partials up to order $r - 1$. Since g_p is invertible, the obtained derivatives remain bounded for all $t > 0$.

8. Appendix

In this appendix we follow [29] to determine higher order derivatives of phase and amplitude on γ, and further derive phase space equations they satisfy. From $\partial_y^\alpha G = 0$ on γ with $|\alpha| \geq 3$, we obtain

$$\partial_t(\partial_y^\alpha \Phi) + H_p \cdot \nabla_x(\partial_y^\alpha \Phi) + \sum_{|\eta|=|\alpha|} c_{\alpha,\eta} \partial_x^\eta \Phi + d_\alpha = 0,$$

where $c_{\alpha,\eta}$ and d_α depends on $\partial_y^\kappa \Phi$ for $|\kappa| < |\alpha|$. Using the Hamiltonian equations $\frac{d}{dt}x = H_p$ we obtain

$$\frac{d}{dt}(\partial_y^\alpha \Phi(t, x(t, X_0); X_0) + \sum_{|\eta|=|\alpha|} c_{\alpha,\eta} \partial_x^\eta \Phi(t, x(t, X_0); X_0) + d_\alpha = 0$$

on $(t, x(t, X_0))$. Following Lemma 2.1 we obtain a linear system of Liouville type PDEs for partial derivatives $m_\alpha(t, X)$ of a fixed order:

$$\mathcal{L}[m_\alpha] + \sum_{|\eta|=|\alpha|} c_{\alpha,\eta} m_\eta + d_\alpha = 0. \tag{8.1}$$

We solve the system (8.1) starting from $|\alpha| = 3$, then $|\alpha| = 4$ and so on until $|\alpha| = k + 1$ for k^{th} order GB solutions. Since equations are linear, we have solutions defined for all $t > 0$. This construction ensures that

$$G(t, y) = O(|y - x|^{k+2}). \tag{8.2}$$

To determine the Taylor series of $A_l, l = 0, \cdots, N$ on γ, one proceeds as follows. Define the coefficients $c_j(t, y)$ by

$$(8.3) \qquad P[A(t,y)e^{i\Phi(t,y)/\epsilon}] = \left(\sum_{j=0}^{N+2} c_j(t,y)\epsilon^j \right) e^{i\Phi/\epsilon}, \quad A = \sum_{j=0}^{N} A_j \epsilon^j.$$

Then, with $P = -i\epsilon\partial_t + H(y, -i\epsilon\partial_y)$, we obtain

$$c_0(t,y) = G(t,y)A_0,$$
$$c_1(t,y) = -iLA_0 + G(t,y)A_1$$
$$c_{l+1}(t,y) = -iLA_l + G(t,y)A_{l+1} + g_l, \quad l = 1, \cdots N+1,$$

where L is a linear differential operator with coefficients depending on Φ,

$$L = \partial_t + H_p \cdot \nabla_y + \frac{1}{2}\left[tr(H_{yp}) + tr(MH_{pp}(y, \Phi_y)) \right],$$

and $g_l = -\frac{1}{2}\Delta_y A_{l-1}$.

Thus to make $P[\psi^\epsilon] = O(\epsilon^K)$ for a given $K \in \mathbb{Z}$, we now only need to make c_j vanish on γ to sufficiently high order. To do so we can solve the equations $LA_l + ig_l = 0$ recursively starting with $l = 0$ ($g_0 = 0$), and solve it to arbitrarily high order by solving the linear transport equations for the partial derivatives of A_l that one gets by differentiating the above equations. From the above procedure we see that the number of terms, N, in the solution ansatz for k^{th} order GB approximation is determined by the following relation

$$\frac{k-1}{2} < N \leq \frac{k+1}{2}$$

In other words, $N = \lfloor \frac{k-1}{2} \rfloor + 1$. Actually, given $G(t,y)$ vanishes to order $k+1$ on γ, we can choose the Taylor series of A_0 on γ up to order $k-1$ so that c_1 vanishes to order $k-1$ on γ. Passing to the higher order equations $c_{l+1} = 0$, we see that we can choose A_l so that c_{l+1} vanishes on γ to order $k+1-2(l+1)$. Thus we need $2 > k+1-2N \geq 0$.

Thus for k^{th} order GB solutions, it is necessary to compute $\partial_y^\alpha A_l$ for $|\alpha| \leq k-1-2l$:

$$L(\partial_y^\alpha A_0) + \sum_{|\eta|<|\alpha|} \binom{\alpha}{\eta} \partial_y^{\alpha-\eta} L(\partial_y^\eta A_0)\Big|_\gamma = 0, \quad |\alpha| \leq k-1,$$

$$L(\partial_y^\alpha A_l) + \sum_{|\eta|<|\alpha|} \binom{\alpha}{\eta} \partial_y^{\alpha-\eta} L(\partial_y^\eta A_l) - \frac{i}{2}\Delta_y \partial_y^\alpha A_{l-1}\Big|_\gamma = 0, \quad |\alpha| \leq k-1-2l, l = 1, \cdots \left\lfloor \frac{k-1}{2} \right\rfloor.$$

Lifting the operator into the phase space, we can obtain $\tilde{A}_l(t, X)$ recursively by solving

$$\mathcal{L}[\tilde{A}_l] = -\frac{\tilde{A}_l}{2}\left[tr(H_{yp}) + tr(\tilde{M}(t,X)H_{pp}(y,p)) \right] - \tilde{g}_l,$$

where $\mathcal{L}$ is the Liouville operator. Same lifting can be applied to all involved derivatives of the amplitude A_l for $l = 0, \cdots \lfloor \frac{k-1}{2} \rfloor$. This completes the construction for all involved Taylor coefficients of both phase and amplitude.

Acknowledgments

References

[1] V. Červený, M. Popov, and I. Pšenčík. Computation of wave fields in inhomeneous media – gaussian beam approach. *Geophysics J. R. Astr. Soc.*, 70:109–128, 1982.

[2] L.-T. Cheng, H. Liu, and S. Osher. Computational high-frequency wave propagation using the level set method, with applications to the semi-classical limit of Schrödinger equations. *Comm. Math. Sci.*, 1(3):593–621, 2003.

[3] M. Crandall and P.-L. Lions. Viscosity solutions of Hamilton-Jacobi equations. *Trans. Amer. Math. Soc.*, 277(1):1–42, 1983.

[4] M. Dimassi, J.-C. Guillot, and J. Ralston. Gaussian beam construction for adiabatic perturbations. *Math. Phys. Anal. Geometry*, 9:187–201, 2006.

[5] B. Engquist and O. Runborg. Computational high frequency wave propagation. In *Acta numerica, 2003*, volume 12 of *Acta Numer.*, pages 181–266. Cambridge Univ. Press, Cambridge, 2003.

[6] N. Hill. Prestack gaussian-beam depth migration. *Geophysics*, 66(4):1240–1250, 2001.

[7] L. Hörmander. Fourier integral operator, I. *Acta. Math.*, 127:79–83, 1971.

[8] L. Hörmander. On the existence and the regularity of solutions of linear pseudo-differential equations. *Enseign Math.*, XVII:99–163, 1971.

[9] S. Jin, H. Liu, S. Osher, and R. Tsai. Computing multi-valued physical observables for the high frequency limit of symmetric hyperbolic systems. *J. Comput. Phys.*, 210(2):497–518, 2005.

[10] S. Jin, H. Liu, S. Osher, and Y.-H. R. Tsai. Computing multivalued physical observables for the semiclassical limit of the Schrödinger equation. *J. Comput. Phys.*, 205(1):222–241, 2005.

[11] S. Jin and S. Osher. A level set method for the computation of multivalued solutions to quasi-linear hyperbolic PDEs and Hamilton-Jacobi equations. *Commun. Math. Sci.*, 1(3):575–591, 2003.

[12] S. Jin, H. Wu, and X. Yang. Gaussian beam methods for the Schröodinger equation in the semi-classical regime: Lagrangian and Eulerian formulations. *preprint*.

[13] J. Keller. Corrected bohr-sommerfeld quantum conditions for non-seperable systems. *Ann. of Physics*, 4:180–188, 1958.

[14] S. Leung and J. Qian. Eulerian Gaussian beams for Schrödinger equations in the semi-classical regime. *preprint*.

[15] S. Leung, J. Qian, and R. Burridge. Eulerian gaussian beams for highfrequency wave propagation. *Geophysics*, 72(5):61–76, 2007.

[16] P.-L. Lions and T. Paul. Sur les measures de Wigner. *Rev. Mat. Iberoamericana*, 9:553–618, 1993.

[17] H. Liu, L.-T. Cheng, and S. Osher. A level set framework for capturing multi-valued solutions of nonlinear first-order equations. *J. Sci. Comput.*, 29(3):353–373, 2006.

[18] H. Liu, S. Osher, and Y.-H. R. Tsai. Multi-valued solution and level set methods in computational high frequency wave propagation. *Comm. Compu. Phys.*, 1(5):765–804, 2006.

[19] H. Liu and Z. Wang. A field space based level set method for computing multi-valued solutions to Euler-Poisson equations. *J. Comput. Phys.*, 225:591–614, 2007.

[20] H. Liu and Z. Wang. Superposition of multi-valued solutions in high frequency wave dynamics. *J. Sci. Comput.*, 35(2-3):192–218, 2008.

[21] H. Liu and Z. Wang. A Bloch band based level set method for computing the semiclassical limit of Schrödinger equations. *to appear in JCP*, 2009.

[22] P. Markowich, P. Pietra, and C. Pohl. Weak limits of finite difference schemes of Schrödinger-type equations. *Pybbl. Ian.*, 1035:1–57, 1997.

[23] P. A. Markowich, N. J. Mauser, and F. Poupaud. A Wigner-function approach to (semi)classical limits: electrons in a periodic potential. *J. Math. Phys.*, 35(3):1066–1094, 1994.

[24] V. P. Maslov and M. V. Fedoriuk. *Semiclassical approximation in quantum mechanics*, volume 7 of *Mathematical Physics and Applied Mathematics*. D. Reidel Publishing Co., Dordrecht, 1981. Translated from the Russian by J. Niederle and J. Tolar, Contemporary Mathematics, 5.

[25] M. Motamed and O. Runborg. A wave front-based gaussian beam method for computing high frequency waves. *preprint*.

[26] S. Osher, L.-T. Cheng, M. Kang, H. Shim, and Y.-H. Tsai. Geometric optics in a phase-space-based level set and Eulerian framework. *J. Comput. Phys.*, 179(2):622–648, 2002.

[27] J. Qian and S. Leung. A level set based Eulerian method for paraxial multivalued traveltimes. *J. Comput. Phys.*, 197(2):711–736, 2004.

[28] J. Ralston. Gaussian beams and the propagation of singularities. *Studies in PDEs*, 23:206–248, 1982.

[29] J. Ralston. Gaussian beams. *Notes on Gasussian beams*, available at http://www.math.ucla.edu/ ralston/pub/Gaussnotes.pdf, 2005.

[30] O. Runborg. Mathematical models and numerical methods for high frequency waves. *Commun. Comput. Phys.*, 2(5):827–880, 2007.
[31] C. Sparber, P. Markowich, and N. J. Mauser. Multivalued geometrical optics: Wigner functions versus WKB-methods. *Asymptotic Analysis*, 33:153–187, 2003.
[32] N. Tanushev, J. Qian, and J. Ralston. Mountain waves and gaussian beams. *SIAM Multiscale Modeling and Simulation*, 6:688–709, 2007.
[33] N. M. Tanushev. Superpositions and higher order gaussian beams. *Commun. Math. Sci.*, 6(2):449–475, 2008.
[34] E. P. Wigner. On the quantum correction for thermodynamic equilibrium. *Phys. Rev.*, 40:749–759, 1932.

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