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 for generating 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. In this work we review and extend recent constructions of asymptotic high frequency wave fields from computations in phase space. We give a new level set method of computing the Hessian and higher derivatives of the phase. 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.

Key words. high frequency waves, Gaussian beams, phase space, level set, superposition

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1. Introduction.

In this paper we consider the equation

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

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

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

where $A_{in} \in C_0^\infty(\mathbb{R}^n)$ and $S_{in} \in C^\infty(\mathbb{R}^n)$. The canonical example is the semiclassical Schrödinger equation with the Hamiltonian $H(x,p) = \frac{1}{2}|p|^2 + V(x)$, where $V(x)$ is a given external potential. The small parameter ϵ represents the fast space and time scale introduced in the equation, as well as the typical wavelength of oscillations of the initial data. Propagation of oscillations of wavelength $O(\epsilon)$ causes mathematical and numerical challenges in solving the problem. In this article we are interested in the construction of globally valid asymptotic wave fields and the analysis of their convergence to the true solutions of the initial value problem.

Geometric optics, also known as the Wentzel–Kramers–Brillouin (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

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

Solving this equation using the method of characteristics can lead to singularities which invalidate the approximation. In general, this breakdown occurs when the density of rays becomes infinite. This corresponds to the formation of 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 and Fedoriuk [24], led to the development of the theory of Fourier integral operators, e.g., as given by Hörmander [7].

A closely related alternative to Fourier integral operators 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 have a history going back to at least the late 1960s. They were initially used to study resonances in lasers [1], and later to obtain results on the propagation of singularities in solutions of PDEs [8, 28]. 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 [2] and [6]. Recent work in this direction includes [32] on "gravity waves," [14] and [12] on the semiclassical Schrödinger equation, and [33] and [25] on acoustic wave equations.

An alternative to the standard WKB method is to use multivalued solutions, $\{S_i(t, x)\}_{i=1}^K$, to (1.3) corresponding to crossing waves [31]. This is in sharp contrast to the notion of viscosity solution [4] adopted when (1.3) arises in other applications. In the last decade a considerable amount of work has been done to capture multivalued phases associated to the WKB system numerically; we refer to review articles [5, 30] and the references therein. Recently the level set method has been developed to resolve multivaluedness of involved quantities in phase space as well as to compute physical observables; see, e.g., [26, 3, 11, 27, 10, 9, 17, 18, 19, 20, 21]. The key idea, for instance in [3, 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 the Wigner transformation [34] to map solutions of the underlying wave equation to functions on phase space. See [16, 22, 23, 31] for the application of the Wigner transformation to the semiclassical Schrödinger equation. These phase space–based approaches are extremely useful since they unfold "caustics." However, at caustics, neither method gives correct prediction for the amplitude. This has led to an effort to combine the accuracy of beam superpositions at caustics with the level set method of computation in phase space. This approach, with attention paid to the accuracy of the resulting approximations, is the subject of this paper.

In this article we have two objectives:

(i) to present the construction of beam superpositions by level set methods;

(ii) to estimate the error between the exact wave field and the asymptotic ones. The construction for (i) is based on Gaussian beams in physical space, but it is carried out by solving inhomogeneous Liouville equations in phase space, as in [15, 14, 12]. The result is no longer a superposition of asymptotic solutions to the wave equation (1.1)! Since it can be written as a superposition of standard Gaussian beams composed with a time-dependent symplectic change of variables, the *superposition over phase space* is still an asymptotic solution, as was pointed out in [15]. Here we consider *superpositions over subdomains* moving with the Hamiltonian flow, and we show directly that they are asymptotic solutions without reference to standard Gaussian beams. For (ii) we use the well-posedness theory for (1.1), i.e., the continuous dependence of solutions of $P\psi = f$ on their initial data and f. Thus, the sources of

error in the Gaussian beam superposition for an initial value problem are the error in approximating the initial data and the error in solving the PDE.

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 from 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 need a superposition over an n-dimensional submanifold of phase space. 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

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

Our result shows that

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

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 Gaussian beam 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 Gaussian beam 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 Gaussian beam solutions in section 6. In section 7, we present a new 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 [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

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

where $\Phi(t, x(t))$ is real, and $\text{Im}\{\Phi(t, x)\} > 0$ 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 Gaussian beam construction is the choice of Φ such that $\partial_t \Phi + H(x, \partial_x \Phi)$ vanishes to high order on γ. We are going to choose Φ so that $\text{Im}\{\Phi\} \geq cd(x, \gamma)^2$. Note that

$$d(x, \gamma)^r e^{-cd(x,\gamma)^2/\epsilon} = O(\epsilon^{r/2}).$$

So we need to have $\partial_t \Phi + H(x, \partial_x \Phi) = O(d(x, \gamma)^4)$. 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

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

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

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 possible only if $(x(t), p(t))$, where $p(t) = \nabla_x \Phi(t, x(t))$, is a (null) bicharacteristic 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., $\text{div}_X(v) = 0$. 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) $\quad \dfrac{d}{dt}S(t; X_0) = p \cdot H_p - H(x, p), \quad S(0; X_0) = S_{\text{in}}(x_0),$

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

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

The essential idea behind the Gaussian beam 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 by solving (2.11).

With these components in place, the Gaussian beam phase is constructed as
(2.12)
$$\Phi(t, y; X_0) = S(t; X_0) + p(t, X_0) \cdot (y - x(t, X_0)) + \frac{1}{2}(y - x(t, X_0)) \cdot M(t; X_0)(y - x(t, X_0)),$$

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 Gaussian beam 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 $\text{Im}(M)$ 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

(2.13) $$X = X(t, X_0)$$

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

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

with the vector $v = (H_p, -H_x)$ tangent to the particle trajectory in phase space. Since the velocity field is divergence-free, the elementary properties of $X(t, X_0)$ tell us that $\text{Vol}(X(t, \Omega)) = \text{Vol}(\Omega) = |\Omega|$ 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:

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

where

$$\tilde{\Phi}(t, y, X) = \tilde{S}(t, X) + p \cdot (y - x) + \frac{1}{2}(y - x) \cdot \tilde{M}(t, X)(y - x). \tag{2.16}$$

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

$$\mathcal{L} := \partial_t + v \cdot \nabla_X. \tag{2.17}$$

Proof. Taking differentiation of

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

in time, we obtain

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

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 the PDEs for $(\tilde{S}, \tilde{M}, \tilde{A})$ in phase space:

$$\mathcal{L}(\tilde{S}) = p \cdot H_p - H(x, p), \quad \tilde{S}(0, X) = S_{\text{in}}(x), \tag{2.18}$$

$$\mathcal{L}(\tilde{M}) + H_{xx} + H_{xp}\tilde{M} + \tilde{M}H_{px} + \tilde{M}H_{pp}\tilde{M} = 0, \quad \tilde{M}(0, X) = M_{\text{in}}(X), \tag{2.19}$$

$$\mathcal{L}(\tilde{A}) = -\frac{\tilde{A}}{2}\left[\text{Tr}[H_{xp}] + \text{Tr}[\tilde{M}H_{pp}]\right], \quad \tilde{A}(0, X) = A_{\text{in}}(X). \tag{2.20}$$

A method for solving the equation for $\tilde{M}$ based on Riccati equations was given by Leung and Qian (see [14, formulas (56)–(57)]). Jin, Wu, and Yang have an alternative way of computing $\tilde{M}$ based on complex level set functions (see [12, formulas (3.5)–(3.16)]). We give yet another method of constructing $\tilde{M}$, as well as the higher derivatives of the phase by level set methods, in section 7. 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,

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

where

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

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

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

In this description, $X = (x, p)$ is a fixed point in phase space (independent of t) and the phase function for ψ_{PGB} is given by (2.16). As remarked earlier, since the map is time dependent, the above phase space–based Gaussian beam 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 requires only 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 $\mathrm{Im}(\tilde{\Phi}(t, y, X)) \geq c|y - x|^2$, $c > 0$, and the Lebesgue 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

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

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

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

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 $\text{Im}(M_{\text{in}}) = \beta I$, $\beta > 0$, then we need to arrange to match the initial data against $\exp(-\beta|x - y|^2/\epsilon)$. That accounts for

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

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 $H(y, p) = \frac{|p|^2}{2} + V(y)$, and ψ^ϵ is defined in (3.2) with $\text{Im}(\tilde{M})$ being positive definite, and $Z(n, \epsilon) \sim \epsilon^{-n/2}$. If $A_{\text{in}} \in C_0^2(\mathbb{R}^n)$, $S_{\text{in}} \in C^3(\mathbb{R}^n)$, and $V \in C_b^3(\mathbb{R}^n)$, 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

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

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

By a straightforward calculation it follows that

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

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

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 everything together, we have
(3.7)

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

Using $\partial_y^2\Phi = \tilde{M}(t, X)$ and that $\tilde{A}$ is a globally bounded solution to (2.20), we see that the $O(\epsilon)$ term vanishes. From (2.16) it follows that $\partial_y\tilde{\Phi} = p + \tilde{M}(y - x)$,

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

and

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

From (2.18) we have $\mathcal{L}[\tilde{S}] = |p|^2 - H(x, p)$, and (2.19) yields $\mathcal{L}[\tilde{M}] = -\partial_x^2 V(x) - \tilde{M}^2$. These together lead to
(3.8)
$$\mathcal{L}[\tilde{\Phi}] + H(y, \partial_y \tilde{\Phi}) = V(y) - V(x) - \partial_x V(x) \cdot (y - x) - \frac{1}{2}(y - x) \cdot \partial_x^2 V(x)(y - x) = O(|y - x|^3).$$

Here the difference between $V(y)$ and its Taylor expansion about x is evaluated, and the estimate is ensured by the assumption $V \in C_b^3(\mathbb{R}^3)$. Consequently, using Lemma 3.2 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 divergence term in the integral in (3.6) gives an alternative way of seeing that the phase space superposition is an accurate solution of the PDE. It integrates to zero when the support of the beam superposition does not touch the boundary of the integration domain, and hence we verify the accuracy without going back to the Lagrangian superposition.

We now obtain the following estimate.

THEOREM 3.4. *Given $T > 0$, let ψ be the solution of the Schrödinger equation subject to the initial data ψ_0, let ψ^ϵ be the approximation defined in (3.2) with $\text{Im}(M_{\text{in}})$ being positive definite, and let $|\Omega(0)| < \infty$. If $A_{\text{in}} \in C_0^1(\mathbb{R}^n)$, $S_{\text{in}} \in C^3(\mathbb{R}^n)$, and $V \in C_b^3(\mathbb{R}^n)$, then there exists a normalization parameter $Z(n, \epsilon) \sim \epsilon^{-n/2}$ and a constant C such that*

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

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

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

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

A calculation of $\int_{R^n} [e\overline{P[e]} - \bar{e}P[e]]dy = i\epsilon \int_y |e|^2 dy$ leads to

$$\epsilon \frac{d}{dt} \int_y |e(t, y)|^2 dy = 2 \int_y \text{Im}(e\overline{P[\psi^\epsilon]})dy \leq 2\|e(t, \cdot)\|_{L^2} \cdot \|P[\psi^\epsilon](t, \cdot)\|_{L^2}.$$

Hence $\frac{d}{dt}\|e(t, \cdot)\|_{L^2} \leq \frac{1}{\epsilon}\|P[\psi^\epsilon](t, \cdot)\|_{L^2}$. Integration of this inequality over $[0, t]$ gives

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

When combined with the estimate for $P[\psi^\epsilon]$ in (3.5), this gives the desired result. $\quad\square$

Remark 3.2. The approximation error comes from two sources: initial error and 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 section 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

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

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 $S_{\text{in}} \in C^{k+2}(\mathbb{R}^n)$ be a real-valued function, let $A_{\text{in}} \in C_0^k(\mathbb{R}^n)$, and let $\rho \in C_0^k(\mathbb{R}^n)$ be such that $\rho \geq 0$, $\rho \equiv 1$ in a ball of radius $\delta > 0$ about the origin. Define*

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

$$v(y; x) = \rho(y - x)T_{k-1}^x[A_{\text{in}}](y)e^{\frac{i}{\epsilon}\left[T_{k+1}^x[S_{\text{in}}](y)\right]}K\left(x - y, \frac{\epsilon}{2}\right).$$

Then

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

Remark 4.1. We note that for the case $k = 1$ the cutoff function ρ is unnecessary, and it can be shown that 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 section 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 $\tilde{A}_{\mathrm{in}} = A_{\mathrm{in}}(x)$, $\tilde{S}_{\mathrm{in}}(X) = S_{\mathrm{in}}(x)$, and $\tilde{M}_{\mathrm{in}}(X) = \partial_x^2 S_{\mathrm{in}}(x) + iI$. The above lemma ensures that

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

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

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

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*

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

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

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

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

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

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

Here for simplicity we use only x_0 in the integrand instead of $X_0 = (x_0, \nabla_x S_{in}(x_0))$. According to the Gaussian beam construction, the $\psi_{GB}(t, y; x_0)$ are asymptotic solutions for each x_0, and thus superpositions of them in x_0 are asymptotic solutions. It remains to verify the claimed estimate. First we see that

$$(4.7) \qquad P[\psi^\epsilon(t, y)] = Z(n, \epsilon) \int_{\mathrm{supp}\{A_{\mathrm{in}}\}} P[\psi_{GB}(t, y; x_0)] dx_0$$

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

Here $G(t, y; x_0) = \tilde{G}(t, y, X(t, x_0, \nabla_x S_{in}(x_0)))$, which from (3.8) has the estimate

$$\tilde{G}(t, y, X) := \mathcal{L}[\tilde{\Phi}] + H(y, \partial_y \tilde{\Phi}) = O(|y - x|^3).$$

We now repeat an estimate similar to that in the proof of Lemma 3.2 with $k = 3$, to obtain

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

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. $\square$

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

THEOREM 4.3. *Given $T > 0$, 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 let 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 $|\text{supp}(A_{\text{in}})| < \infty$. If $A_{\text{in}} \in C_0^1(\mathbb{R}^n)$, $S_{\text{in}} \in C^3(\mathbb{R}^n)$, and $V \in C_b^3(\mathbb{R}^n)$, then there exist a normalization parameter $Z(n,\epsilon)$ and a constant C such that*

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

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 the 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

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

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 the left-hand side of (4.8). So for simplicity

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

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

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

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

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.

5.2. An example with remarkable accuracy. 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

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

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

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

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

$$\psi(t, y) = \frac{1}{(2\pi i\epsilon t)^{n/2}} \int_{x_0} \psi_{\text{in}}(x_0) \exp\left(\frac{i}{2\epsilon t}|y - x_0|^2\right) dx_0.$$

Evaluating at $t = 1$, we have

$$\psi(1, y) = \frac{1}{(2\pi i\epsilon)^{n/2}} \int_{x_0} g(x_0)e^{-iy\cdot x_0/\epsilon}dx_0 e^{i|y|^2/(2\epsilon)} = c\epsilon^{-n/2}\hat{g}(y/\epsilon)e^{i|y|^2/(2\epsilon)},$$

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

$$\hat{g}(\xi) = \frac{1}{(2\pi)^{n/2}} \int g(x_0)e^{-ix_0\cdot\xi}dx_0.$$

It is easy to verify that

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

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

We now build a superposition of Gaussian beams approximation for the solution of the same problem. For the Gaussian beam superposition, the phase defined by (2.12) is

$$\Phi(t, y; x_0) = (t - 1)\frac{|x_0|^2}{2} - y \cdot x_0 + |x_0|^2(1 - t) + \frac{\beta i - 1}{1 + (\beta i - 1)t}\frac{|y - x_0(1 - t)|^2}{2}.$$

Here we are using the ray $(x, p) = (x_0(1-t), -x_0)$ obtained from (2.8); $S = \frac{|x_0|^2}{2}(t-1)$ obtained by solving (2.9) with $S_{\text{in}} = -|x_0|^2/2$; and $M = \frac{\beta i-1}{1+(\beta i-1)t}I$ from solving (2.10)

with $M_{\text{in}} = (\beta i - 1)I$. Note that we have chosen $\beta > 0$ for the initial beam width. For the amplitude we get

$$(1 + (\beta i - 1)t)^{n/2} A(t, x_0(1 - t)) = A(0, x_0) = g(x_0).$$

So, setting $y(t; x_0) = (1 - t)x_0$, we obtain

$$A(t, y(t; x_0)) = (1 + (\beta i - 1)t)^{-n/2} g(x_0).$$

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

$$\psi^\epsilon(t, y) = \left(\frac{\beta}{2\pi\epsilon}\right)^{n/2} \int_{x_0} [1 + (\beta i - 1)t]^{-n/2} g(x_0) e^{i\Phi(t, y; x_0)/\epsilon} dx_0.$$

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

$$\psi^\epsilon(1, y) = \left(\frac{\beta}{2\pi\epsilon}\right)^{n/2} \int_{x_0} [\beta i]^{-n/2} g(x_0) e^{\frac{i}{\epsilon}[-y \cdot x_0 + \frac{\beta i - 1}{\beta i} \frac{|y|^2}{2}]} dx_0$$

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

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

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

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

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

That implies the following:

(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

$$\|\psi^\epsilon(0, \cdot) - \psi(0, \cdot)\|_{L^2}^2 = \int_y \left|\left(\frac{\beta}{2\pi\epsilon}\right)^{n/2} \int_{x_0} g(x_0) e^{-\frac{\beta}{2\epsilon}|y - x_0|^2} dx_0 - g(y)\right|^2 dy$$

$$= \left(\frac{\beta}{2\pi\epsilon}\right)^n \int_y \left|\int_{x_0} (g(x_0) - g(y)) e^{-\frac{\beta}{2\epsilon}|y - x_0|^2} dx_0\right|^2 dy.$$

Set $K(y) = (\frac{\beta}{2\pi\epsilon})^{n/2} e^{-\frac{\beta}{2\epsilon}|y|^2}$. 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 a higher order expansion of the phase is used.

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

THEOREM 5.1. *Under the assumptions of Theorem 4.3 and the assumption that the potential is a quadratic function, then for $t \in [0, T]$ we have the following:*

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

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

- *If $S_{\mathrm{in}} \in C^3$ and $A_{\mathrm{in}} \in C_0^1$,*

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

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 $A_{\mathrm{in}} \in H^2(\mathbb{R}^n)$ we obtain the $O(\epsilon)$ error as shown in (5.1). For the general phase function the claim follows from Lemma 4.1 with $k = 1$.   ∎

6. Higher order approximations. The accuracy of the phase space–based Gaussian beam superposition also depends on accuracy of the individual Gaussian beam ansatz. Gaussian beams can be constructed to satisfy the Schrödinger equation modulo errors of order ϵ^N, for arbitrary N, by computing higher order terms in the spatial Taylor series for the phase and amplitude about the central ray. If we refer to the construction in previous sections as the first order Gaussian beam solution, then a kth order Gaussian beam solution will include the Taylor series up to $(k+1)$th order for the phase, and $(k - 1 - 2l)$th order for the lth amplitude A_l for $l = 0, \ldots, \left[\frac{k-1}{2}\right]$.

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

$$(6.1) \quad \psi_{kGB}(t, y; X_0) = \rho(y - x(t, X_0)) \left[\sum_{l=0}^{\lfloor \frac{k-1}{2} \rfloor} \epsilon^l A_l(t, y; X_0) \right] \exp\left(\frac{i}{\epsilon} \Phi(t, y; X_0) \right),$$

where ρ is a cutoff function such that on its support Φ still has a positive imaginary part. The phase is determined as

$$\Phi(t, y; X_0) = \sum_{|\alpha| \leq k+1} \frac{1}{\alpha!} (y - x(t, X_0))^\alpha \partial_y^\alpha \Phi(t, x(t, X_0)),$$

where $\partial_y \Phi(t, x(t, X_0)) = p(t, X_0)$, $\Phi(t, x(t, X_0)) = S(t, X_0)$ from (2.9), and $\partial_y^2 \Phi(t, x(t, X_0)) = M(t, X_0)$ from (2.10). For $3 \leq |\alpha| \leq k+1$, $\partial_y^\alpha \Phi(t, x(t, X_0))$ are permutable families. The amplitude is given by

$$A_l(t, y; X_0) = \sum_{|\alpha| \leq k-1-2l} \frac{1}{\alpha!} (y - x(t, X_0))^\alpha \partial_x^\alpha A_l(t, x(t, X_0)).$$

The equations for these phase and amplitude Taylor coefficients are derived recursively, starting with the phase and then progressing through the amplitudes. At each

stage (phase function, leading amplitude, next amplitude, etc.) one has to derive the Taylor series up to sufficiently high order before passing to the next function in the expansion (see the appendix).

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 kth order Gaussian beam ansatz

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

Beyond the first order Gaussian beam 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 by solving transport equations in phase space; see the appendix for details.

Proceeding as previously, we form the superpositions:

$$(6.2) \qquad \psi_k^\epsilon(t, y) = Z(n, \epsilon) \int_{\Omega(t)} \psi_{kPGB}(t, y, X) \delta(w(t, X)) dX,$$

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

This gives a kth order asymptotic solution of the Schrödinger 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 $H(y, p) = \frac{|p|^2}{2} + (y)$, and ψ^ϵ is defined in (6.2) with $\mathrm{Im}(M_{in}) = I$ and $Z(n, \epsilon) = (2\pi\epsilon)^{-n/2}$. If $A_{in} \in C_0^k(\mathbb{R}^n)$, $S_{in} \in C^{k+2}(\mathbb{R}^n)$, and $V \in C_b^{k+2}(\mathbb{R}^n)$, then ψ_k^ϵ is an asymptotic solution and satisfies*

$$(6.3) \qquad \|P[\psi_k^\epsilon](t, \cdot)\|_{L_y^2} \lesssim |\mathrm{supp}(A_{in})| \epsilon^{\frac{k}{2}+1-\frac{n}{4}}.$$

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

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

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

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

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

According to the Gaussian beam construction sketched in the appendix, $\psi_{kGB}(t, y; x_0)$ are asymptotic solutions for each x_0, and thus $\psi_k^\epsilon(t, y)$ is an asymptotic solution. It remains to verify (6.3). First we see that

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

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 $T_{k+1}^x[\Phi](y) = \Phi(y) + R_{k+1}^x[\Phi](y)$, where 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 cutoff function ensures that we can always choose a small neighborhood of $x(t; x_0)$ so that

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

Consequently, using Minkowski's integral inequality,

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

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

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

If we introduce the stretched coordinates $y - x(t; x_0) = \epsilon^{1/2} y'$ and change 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 $Z(n, \epsilon)|\mathrm{supp}(A_{\mathrm{in}})|\epsilon^{\frac{k}{2}+1+\frac{n}{4}}$. The desired estimate then follows. $\quad\square$

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 (6.2) accurately approximates the initial data. For $t = 0$, the approximation is as follows:

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

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

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

where

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

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 kth order phase space Gaussian beam superposition is as follows.

THEOREM 6.2. *Given $T > 0$, let ψ be the solution of the Schrödinger equation with $V \in C_b^{k+2}(\mathbb{R}^n)$, subject to the initial data $\psi_{\text{in}} = A_{\text{in}} e^{iS_{\text{in}}(x)/\epsilon}$ with $A_{\text{in}} \in C_0^k(\mathbb{R}^n)$ and $S_{\text{in}} \in C^{k+2}(\mathbb{R}^n)$, and let ψ^ϵ be the kth order approximation defined in (6.2) with initial data chosen as described above with $|\text{supp}(A_{\text{in}})| < \infty$. Then there exists a normalization parameter $Z(n, \epsilon) \sim \epsilon^{-n/2}$ and a constant C such that*

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

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 bicharacteristic 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 bicharacteristic 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 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 (2.18); we are then left to determine $\tilde{M}$, followed by solving (2.20) to obtain $\tilde{A}$. Note that (2.19) is nonlinear in $\tilde{M}$, and the solution might not exist for all $t > 0$. The heart of the Gaussian beam 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) $\text{Im}(\tilde{M})$ must be positive definite for all $t > 0$.

7.1. Evaluation of the Hessian. We now show that 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 the following:*

(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* $\mathrm{Im}(\bar{k}_1 k_2) \neq 0$, *then* g_p *is invertible for all* $t > 0$.

(c) *If* $M_{\mathrm{in}} = -g_x(g_p)^{-1}|_{t=0}$, *then* $\tilde{M} = -g_x(g_p)^{-1}$ *for all* $t > 0$.

(d) M *satisfies* (2.19) *and* (i). *If* $\mathrm{Im}(k_1/k_2) < 0$, *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:

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

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

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

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

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

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

The condition $\mathrm{Im}(\bar{k}_1 k_2) \neq 0$ 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 (2.19), (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 $M_{\mathrm{in}} = -g_x(g_p)^{-1}$ 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 $M_{\mathrm{in}} = -\frac{k_1}{k_2}I = M_{\mathrm{in}}^T$. Since $\tilde{M}^T$ also satisfies (2.19), 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 $\mathrm{Im}[\overline{g_p}^T \tilde{M}g_p] = |k_2|^2 \mathrm{Im}[M_{\mathrm{in}}]$. Note that $\mathrm{Im}[M_{\mathrm{in}}]$ is positive definite; hence $\mathrm{Im}[\tilde{M}]$ remains positive definite for all $t > 0$. $\qquad\square$

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 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 $\tilde{M}_{\text{in}}$ 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 $\tilde{M}_{\text{in}} = i\beta I$. If p_0 is restricted to be the phase gradient at x_0 initially, then the initial level set function can be chosen as $(\phi_1, \phi_2)(0, X) = (x, p - \nabla_x S_{\text{in}}(x))$. This leads to $\tilde{M}_{\text{in}} = \partial_x^2 S_{\text{in}}(x) + i\beta I$. 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 an 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. Letting $g = k_1\phi_1 + k_2\phi_2$, 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 $c_{\alpha,\eta} = (c_{1\alpha,\eta}, \ldots, c_{n\alpha,\eta})^\top$ and $d_\alpha = (d_{1\alpha}, \ldots, d_{n\alpha})^\top$ 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 we 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:

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

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

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

To determine the Taylor series of $A_l, l = 0, \ldots, N$, 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

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

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

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

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 kth order Gaussian beam approximation is determined by the relation

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

In other words, $N = \lfloor \frac{k-1}{2} \rfloor + 1$. Actually, given that $G(t, y)$ 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 $2 > k + 1 - 2N \ge 0$.

Thus for kth order Gaussian beam solutions, it is necessary to compute $\partial_y^\alpha A_l$ for $|\alpha| \le k - 1 - 2l$:

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

$$L(\partial_y^\alpha A_l) + \sum_{|\eta|<|\alpha|} \binom{\alpha}{\eta} \partial_y^{\alpha-\eta} L(\partial_y^\eta A_l) - \frac{i}{2}\Delta_y \partial_y^\alpha A_{l-1} \Big|_\gamma = 0,$$

$$|\alpha| \le k - 1 - 2l, \ l = 1, \ldots, \left\lfloor \frac{k-1}{2} \right\rfloor.$$

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

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

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

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