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GAUSSIAN BEAM FORMULATIONS AND INTERFACE CONDITIONS FOR THE ONE-DIMENSIONAL LINEAR SCHRÖDINGER EQUATION

DONGSHENG YIN* AND CHUNXIONG ZHENG†

Abstract. Gaussian beams are asymptotic solutions of linear wave-like equations in the high frequency regime. This paper is concerned with the beam formulations for the Schrödinger equation and the interface conditions while beams pass through a singular point of the potential function. The equations satisfied by Gaussian beams up to the fourth order are given explicitly. When a Gaussian beam arrives at a singular point of the potential, it typically splits into a reflected wave and a transmitted wave. Under suitable conditions, the reflected wave and/or the transmitted wave will maintain a beam profile. We study the interface conditions which specify the relations between the split waves and the incident Gaussian beam. Numerical tests are presented to validate the beam formulations and interface conditions.

Key words. Gaussian beam, high-order, interface condition, Schrödinger equation

AMS subject classifications. 81Q20, 65M99

1. Introduction. This paper is concerned with the one-dimensional Schrödinger equation of the following form

\[ i\epsilon u_t + \frac{\epsilon^2}{2} u_{xx} = V(x)u. \]  

(1.1)

Here \( \epsilon > 0 \) is the re-scaled Plank constant, and \( V(x) \) is a time-independent potential function. In general, the solution to the Schrödinger equation (1.1) is highly oscillatory when \( \epsilon \) is small. This solution behavior presents a significant numerical difficulty, since for any naive domain-based discretization method, the number of mesh points in each spatial direction should be at least of order \( O(\epsilon^{-1}) \) [22]. This situation is analogous to the well-known pollution effect of high frequencies when dealing with the Helmholtz equation [2]. If the potential is sufficiently smooth, and the wave field is uniformly localized, the time-splitting spectral method studied in [3] seems to be the best among the existing methods. As suggested by the numerical evidences in [3], the spatial meshing strategy is almost of the optimal order \( O(\epsilon^{-1}) \) in each spatial direction. However, this strategy is no longer valid for the Schrödinger equation with non-smooth potentials.

One alternative numerical approach for the Schrödinger equation (1.1) is the classical geometrical optics, or WKB (Wentzel-Kramers-Brillouin) method, which attempts to represent the wave field in the asymptotic form

\[ u(x,t) = A'(x,t) \exp \left( \frac{iS(x,t)}{\epsilon} \right), \quad A' = \sum_{j=0}^{\infty} (-i\epsilon)^j A_j, \]  

(1.2)

where the amplitude \( A_j \) and the phase (real) \( S \) are smooth functions. Substituting (1.2) into the Schrödinger equation (1.1), and equating the different powers of \( \epsilon \) one

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derives a sequence of equations, among which the first two are

\[ S_t + \frac{1}{2} S_x^2 + V(x) = 0, \]
\[ (1.3) \]
\[ A_{0,t} + S_x A_{0,x} + \frac{1}{2} S_{xx} A_0 = 0. \]
\[ (1.4) \]

The phase equation (1.3) is of Hamilton-Jacobi type, which can be solved by the ray tracing method \textit{(the method of characteristic)}. After \( S \) is determined, the first amplitude function \( A_0 \) is then solved along each specific ray, see [20]. Keeping only the first term in the summation term of (1.2), a first order approximation \textit{(w.r.t.} \( \epsilon \)) of the wave field is thus obtained.

Despite the tremendous success in handling various wave propagation problems, the WKB method has its own shortcomings. A serious drawback of this method following the above solution strategy is that in general the solution of the phase equation (1.3) does not exist globally. The asymptotic solution ceases to be valid at caustics where the rays intersect and the amplitude blows up. As a matter of fact, the correct semiclassical solution to the Schrödinger equation (1.1) may develop several phases, which means that the asymptotic solution is actually a summation of functions with the ansatz (1.2). Up to now, many approaches have been proposed to resolve this multi-phased solution and/or their associated physical observables, such as the big ray tracing method [4], wave front method [8], moment method [6, 10, 11, 16], and level set method [5, 17, 18]. The readers are referred to [7, 15] for a thorough review.

The Gaussian beam approach [12, 24, 25] based on the local ray tracing is another alternative numerical method. The basic idea is to decompose the whole wave field into a summation of local asymptotic solutions with beam-like profile, each of which is called a Gaussian beam. Unlike the classical WKB solution, the Gaussian beam has a complex-valued phase in general, though it becomes real at the beam center, which is exactly a single ray. Gaussian beams can be determined by a set of beam parameters. This is a remarkable advantage for representing a wave field, especially from the numerical point of view. Another highlight of Gaussian beam approach compared with those methods mentioned in the last paragraph is its capability of resolving the wave field even at caustics [25]. This advantage is very important in many applications, for example, in seismic imaging [13, 14].

In the last several years, some important developments have been made on the Gaussian beam approach. Among them, we mention the papers by Leung-Qian [21] and Jin-Wu-Yang [19], which proposed the Gaussian beam based Eulerian formulation for the Schrödinger equation with smooth potentials. Faou and Lubich [9] constructed a poisson integrator for Gaussian beam. Tanushev [27] studied the Gaussian beam decomposition method and made a rigorous error analysis. More recently, a sophisticated decomposition algorithm was proposed by Tanushev, Engquist and Tsai [28] to simulate the solution of high frequency hyperbolic wave equation. Zheng [29] applied the Gaussian beam approach for the boundary value Helmholtz problem. Robert [26] proved the uniformly convergence of the Gaussian beam method with respect to \( \epsilon \) by using the semiclassical Fourier integral operator theory.

In this paper, we construct high-order (up to fourth-order) Gaussian beams to the Schrödinger equation (1.1) in the semi-classical regime. Though the general procedure has been proposed in [25] for wave-like equations, we deduce the beam formulations explicitly for the specific equation. We also deduce interface conditions of a Gaussian beam at the singular points of the potential, which is a fundamental issue when
applying Gaussian beam approach to the Schrödinger equation with piecewise smooth potentials. When a beam propagates to a singular point, it typically splits into a reflected wave and a transmitted wave. The transmitted wave could be either traveling or evanescent, depending on the magnitude of the potential jump. Interface conditions thus specify the ways how these two split waves relate to the original propagating Gaussian beam. We will show through numerical tests that high-order Gaussian beams and high-order interface conditions have a great advantage over the lower-order ones.

This paper is organized as follows. In section 2, we explicitly present the formulations satisfied by the Gaussian beam asymptotic solutions to the Schrödinger equation. A simple Taylor-expansion method is proposed to prevent the contamination of high order phase terms on the Gaussian profiles. In section 3, based on the impedance analysis for the one-way wave modes, we derive interface conditions which specify the relations between the split waves and the propagating Gaussian beam at a singular point of the potential. An algorithm is proposed to compute the transmitted evanescent wave. This issue is important since the evanescent wave is not beam-like, and the beam ansatz is no longer valid. In section 4, we present some numerical examples to test the accuracy of different order Gaussian beams and different order interface conditions.

2. Gaussian beams. The classical semiclassical approximation presents asymptotic traveling wave solutions for the Schrödinger equation (1.1) with the form of WKB series

\[ u(x, t) = \exp \left\{ \frac{\imath S(x, t)}{\epsilon} \right\} \sum_{k=0}^{\infty} \left( \frac{\epsilon}{i} \right)^k A_k(x, t), \]

(2.1)

where \( S \) is the real phase function. Substituting (2.1) into the Schrödinger equation (1.1) and equating the different powers of \( \epsilon \) gives

\[ S_t + \frac{1}{2} S_x^2 + V(x) = 0, \]

(2.2)

\[ A_k - 1, t + S_x A_k - 1, x + \frac{1}{2} S_{xx} A_k - 1 + \frac{1}{2} A_{k-2,xx} = 0, \quad k \geq 1. \]

(2.3)

Here we have made the convention \( A_{-1} \equiv 0 \). The eikonal equation (2.2) is of the Hamilton-Jacobi type. By solving the ray tracing ODEs

\[ \frac{dx}{dt} = p, \quad \frac{dp}{dt} = -V'(x) \]

(2.4)

with the initial conditions

\[ x(x_0, 0) = x_0, \quad p(x_0, 0) = S_x(x_0, 0), \]

the phase function can be determined as

\[ S(x(x_0, t), t) = S(x_0, 0) + \int_0^t \left( \frac{p^2(x_0, \tau)}{2} - V(x(x_0, \tau)) \right) d\tau. \]

The amplitude function \( A_k \) is then derived by solving the transport equation (2.3) along each specific ray.
A drawback of the classical semiclassical approximation is that the solution may not exist globally. The asymptotic solution ceases to be valid at caustics where the rays intersect and the amplitudes blow up. A remedy for this problem is the Gaussian beam method, see [24, 25] for examples. Gaussian beam method also resorts to the ray tracing system. The difference between the classical geometrical optics and the Gaussian beam method is that while the phase function is real-valued in the former, it is generally complex-valued in the latter. Besides, the imaginary part of the Hessian of phase function is made positively definite in each direction perpendicular to the ray propagating. This ensures that the profile of wave function is bell-shaped, and very importantly, has a width of \( O(\sqrt{\epsilon}) \).

For the one-dimensional Schrödinger equation the Gaussian beam has a form of

\[
\psi = \exp \left\{ \frac{i}{\epsilon} \left( \sum_{j=0}^{+\infty} S_j^i (x - x_c)^j \right) \right\} \times \sum_{k=0}^{+\infty} \left\{ \left( \frac{\epsilon}{\pi} \right)^k \sum_{j=0}^{+\infty} A_{kj} (x - x_c)^j \right\},
\]

where the beam center \( x_c \), the phase parameters \( \{S_j\} \) and the amplitude parameters \( \{A_{kj}\} \) are functions of \( t \). In terms of the WKB ansatz (2.1), we have

\[
S = \sum_{j=0}^{+\infty} S_j^i (x - x_c)^j, \quad A_k = \sum_{j=0}^{+\infty} A_{kj} (x - x_c)^j,
\]

where

\[
S_j = \partial_j^i S(x_c), \quad A_{kj} = \partial_j^i A_k(x_c).
\]

Under the conditions that \( S_0 \) and \( S_1 \) are real, and the imaginary part of \( S_2 \) is positive in the evolution time interval \([0, T_f]\), a valid region for beam profile is defined by

\[
\Omega(u) = \left\{ (x, t) | |x - x_c| < W \sqrt{\epsilon/3S_2}, t \in [0, T_f] \right\},
\]

where \( W \) is an empirical constant which controls the global error of beam solution by extending its value to zero in the outside of \( \Omega(u) \). For example, by taking \( W = 8 \), we have

\[
\left| \exp \left\{ \frac{i}{\epsilon} \frac{S_2}{2} (x - x_c)^2 \right\} \right| \approx 1.27 \times 10^{-14}, \quad \forall x, \quad |x - x_c| \geq W \sqrt{\epsilon/3S_2},
\]

which is close to the machine precision with double digits. In the valid region \( \Omega(u) \), the higher-order phase terms are small quantities compared with the second-order phase term if \( \epsilon \) is small enough. By truncating the series terms of (2.5) in the following way

\[
u_N = \exp \left\{ \frac{i}{\epsilon} \left( \sum_{j=0}^{N+1} S_j^i (x - x_c)^j \right) \right\} \times \sum_{k=0}^{N-1} \left\{ \left( \frac{\epsilon}{\pi} \right)^k \sum_{j=0}^{N-2k} A_{kj} (x - x_c)^j \right\},
\]

we get the \( N \)-th order Gaussian beam formulation, which has an asymptotic accuracy of \( O(\epsilon^{N/2}) \) in \( \Omega(u) \).

Taylor expansion of the potential \( V \) at the beam center \( x_c \) gives

\[
V(x) = \sum_{j=0}^{+\infty} V_j (x - x_c)^j, \quad V_j = \partial_j^i V(x_c).
\]
Substituting this expression together with (2.6) into (2.2)-(2.3) and equating the different powers of \( x - x_c \), after a tedious but trivial computation we derive the ODEs satisfied by the phase parameters \( \{ S_j \}_{j=0}^5 \):

\[
\frac{dx_c}{dt} = S_1, \\
\frac{dS_0}{dt} = \frac{1}{2} S_1^2 - V_0, \\
\frac{dS_1}{dt} = -V_1, \\
\frac{dS_2}{dt} = -S_1^2 - V_2, \\
\frac{dS_3}{dt} = -3S_2S_3 - V_3, \\
\frac{dS_4}{dt} = -4S_2S_4 - 3S_3^2 - V_4, \\
\frac{dS_5}{dt} = -5S_2S_5 - 10S_3S_4 - V_5,
\]

the ODEs satisfied by the amplitude functions \( \{ A_{0j} \}_{j=0}^5 \):

\[
\frac{dA_{00}}{dt} = -\frac{1}{2} S_2 A_{00}, \\
\frac{dA_{01}}{dt} = -\frac{3}{2} S_2 A_{01} - \frac{1}{2} S_4 A_{00}, \\
\frac{dA_{02}}{dt} = \frac{5}{2} S_2 A_{02} - 2S_3 A_{01} - \frac{1}{2} S_4 A_{00}, \\
\frac{dA_{03}}{dt} = -\frac{7}{2} S_2 A_{03} - \frac{9}{2} S_3 A_{02} - \frac{5}{2} S_4 A_{01} - \frac{1}{2} S_5 A_{00},
\]

and the ODEs satisfied by the amplitude functions \( \{ A_{1j} \}_{j=0}^1 \):

\[
\frac{dA_{10}}{dt} = -\frac{1}{2} S_2 A_{10} - \frac{1}{2} A_{02}, \\
\frac{dA_{11}}{dt} = -\frac{3}{2} S_2 A_{11} - \frac{1}{2} S_3 A_{10} - \frac{1}{2} A_{03}.
\]

From the equations (2.9)-(2.10), one sees that \( S_0 \) and \( S_1 \) are always real if they are real at the initial time. Equation (2.11) is a simple Ricatti equation. If the imaginary part of \( S_2 \) is positive at the initial time, it remains positive at any evolution time. These properties ensure that the profile of beam solution is near the beam center. Away from the beam center, the higher-order terms involved in the phase function would come into play, and the Gaussian-like profile can be completely destroyed. A simple remedy is to further approximate the exponentials of higher-order terms with power series of suitable order. For example, for the fourth-order beam solution, we employ the following approximations

\[
\exp \left\{ \frac{i}{\epsilon} \frac{S_3}{6} \bar{x}^3 \right\} \approx \sum_{j=0}^3 \frac{1}{j!} \left\{ \frac{i}{\epsilon} \frac{S_3}{6} \bar{x}^3 \right\}^j, \quad \exp \left\{ \frac{i}{\epsilon} \sum_{j=4}^5 \frac{5}{j!} S_j \bar{x}^j \right\} \approx 1 + \frac{i}{\epsilon} \sum_{j=4}^5 \frac{5}{j!} S_j \bar{x}^j,
\]
where \( \tilde{x} = x - x_c \). The new formulation of the fourth-order beam is

\[
 u_4 = \exp \left\{ i \sum_{j=0}^{2} \frac{S_j}{j!} \tilde{x}^j \right\} \sum_{j=0}^{3} \frac{1}{j!} \left\{ \frac{i}{\epsilon} S_3 \tilde{x}^3 \right\}^j \left( 1 + i \sum_{j=4}^{5} \frac{S_j}{j!} \tilde{x}^j \right) \times \left( \sum_{j=0}^{3} \frac{A_{0j}}{j!} \tilde{x}^j + \left( \frac{1}{i} \sum_{j=0}^{5} \frac{A_{1j}}{j!} \tilde{x}^j \right) \right),
\]

which has the same asymptotic accuracy \( \mathcal{O}(\epsilon^2) \) as the original fourth-order beam expression (2.7). Analogously, the first three order beams are reformulated as

\[
 u_3 = \exp \left\{ i \sum_{j=0}^{2} \frac{S_j}{j!} \tilde{x}^j \right\} \sum_{j=0}^{2} \frac{1}{j!} \left\{ \frac{i}{\epsilon} S_3 \tilde{x}^3 \right\}^j \left( 1 + i \sum_{j=4}^{5} \frac{S_j}{j!} \tilde{x}^j \right) \times \left( \sum_{j=0}^{3} \frac{A_{0j}}{j!} \tilde{x}^j + \left( \frac{1}{i} \sum_{j=0}^{5} \frac{A_{1j}}{j!} \tilde{x}^j \right) \right),
\]

\[
 u_2 = \exp \left\{ i \sum_{j=0}^{2} \frac{S_j}{j!} \tilde{x}^j \right\} \left( 1 + i \frac{S_3}{\epsilon} \tilde{x}^3 \right) (A_{00} + A_{01} \tilde{x}),
\]

\[
 u_1 = \exp \left\{ i \sum_{j=0}^{2} \frac{S_j}{j!} \tilde{x}^j \right\} A_{00},
\]

which have the asymptotic accuracy of \( \mathcal{O}(\epsilon^{3/2}), \mathcal{O}(\epsilon), \) and \( \mathcal{O}(\epsilon^{1/2}) \) in the valid region respectively.

### 3. Interface conditions.

The profile of Gaussian beams is bell-shaped in the spatial direction. For a traveling beam, i.e., \( S_1 \neq 0 \), it is also bell-shaped in the time direction. When a beam arrives at a singular point of the potential \( V(x) \), it splits into a reflected wave and a transmitted wave. Asymptotically both of them have the same phase at the singular point.

#### 3.1. Parameters transformation.

First we study the relation between the Spatial Profile Parameters (SPPs) of a Gaussian beam and its Temporal Profile Parameters (TPPs). We only consider this issue for Gaussian beams up to fourth order. Suppose the beam arrives at \( x_s \) after a traveling time \( t_s \). With the SPPs, the fourth-order beam at \( x = x_s \) is formulated as

\[
 u_4 = \exp \left\{ i \sum_{j=0}^{5} \frac{S_j}{j!} (x_s - x_c)^j \right\} \times \left( \sum_{j=0}^{3} \frac{A_{0j}}{j!} (x_s - x_c)^j + \frac{1}{i} \sum_{j=0}^{5} \frac{A_{1j}}{j!} (x_s - x_c)^j \right),
\]

and with the TPPs, it is formulated as

\[
 u_4 = \exp \left\{ i \sum_{j=0}^{5} \frac{S_j}{j!} (t_s - t)^j \right\} \times \left( \sum_{j=0}^{3} \frac{a_{0j}}{j!} (t_s - t)^j + \frac{1}{i} \sum_{j=0}^{5} \frac{a_{1j}}{j!} (t_s - t)^j \right). \tag{3.1}
\]

Note that generally the above two expressions are equal only asymptotically within an \( \mathcal{O}(\epsilon^2) \) error in the valid region. Performing Taylor expansion and using the ODEs
(2.8)-(2.20), we obtain
\[ s_0 = S_0, \quad (3.2) \]
\[ s_1 = \frac{1}{2} S_1^2 + V_0, \quad (3.3) \]
\[ s_2 = S_2^2 S_2 + V_1 S_1, \quad (3.4) \]
\[ s_3 = S_3^3 S_3 + 3 S_1^2 S_1^2 + V_2 S_1^2 + 3 V_1 S_1 S_2 + V_1^2, \quad (3.5) \]
\[ s_4 = S_4^4 S_4 + 12 S_3 S_1^3 S_2 + V_3 S_1^3 + 12 S_1^2 S_1^2 S_2 + 8 V_2 S_1^2 S_2 + 6 V_1 S_1 S_2 + 5 V_2 S_1 + 3 V_1^2 S_2, \quad (3.6) \]
\[ s_5 = S_5^5 S_5 + 20 S_4 S_1^4 S_2 + 15 S_1^3 S_1^3 S_2 + V_4 S_1^3 S_2 + V_2 S_1^2 S_1 S_2 + 15 V_1 S_1 S_2 + 9 V_1 V_3 S_1^2 S_2 + 8 V_2 S_1^2 + 6 V_1 S_1 S_2 + 4 V_1 V_2 S_1 S_2 + 15 V_1^2 S_1 S_3 + 15 V_1^2 S_2 + 8 V_1^2 V_2, \quad (3.7) \]

and
\[ a_{00} = A_{00}, \quad (3.8) \]
\[ a_{01} = \frac{1}{2} S_2 A_{00} + S_1 A_{01}, \quad (3.9) \]
\[ a_{02} = S_2^2 A_{02} + 3 S_2 S_1 A_{01} + S_3 S_1 A_{00} + \frac{3}{4} S_2^2 A_{00} + \frac{1}{2} V_2 A_{00} + V_1 A_{01}, \quad (3.10) \]
\[ a_{03} = S_3^3 A_{03} + \frac{15}{8} S_1^3 A_{00} + \frac{3}{2} V_1 S_1 A_{00} + \frac{7}{4} V_2 S_2 A_{00} + V_2 S_1 A_{00} + \frac{9}{2} V_1 S_2 A_{01} + 3 V_1 S_3 A_{02} + 7 V_2 S_1 A_{01} + \frac{3}{2} S_1^2 S_4 A_{00} + 45 S_1^2 S_2 A_{01} + 6 S_1^3 S_1 A_{01} + 15 \frac{S_2^2 S_2 A_{02}}{2} + \frac{15}{2} S_1 S_2 S_3 A_{00}, \quad (3.11) \]

and
\[ a_{10} = A_{10}, \quad (3.12) \]
\[ a_{11} = \frac{1}{2} S_2 A_{10} + \frac{1}{2} A_{02} + S_1 A_{11}. \quad (3.13) \]

Considering \( s_0 \) and \( s_1 \) are real, the imaginary part of \( s_2 \) has the same sign as that of \( S_2 \). Confining to the valid region, the profile of \( u_4 \) given in (3.1) is thus bell-shaped asymptotically.

**3.2. Impedances.** We would like to compute the impedances of the monochromatic waves with energy \( E \). Let
\[ u(x, t) = U(x) e^{-iEt/c}. \quad (3.14) \]

Substituting (3.14) into the Schrödinger equation (1.1) gives
\[ EU + \frac{\epsilon^2}{2} U_{xx} = V(x) U. \quad (3.15) \]

Suppose the harmonic monochromatic wave solution \( U \) has the following asymptotic expansion
\[ U = e^{iS/c} \sum_{k=0}^{\infty} \left( \frac{\epsilon}{i} \right)^k B_k, \quad (3.16) \]
where $S$ and $B_k$ are functions of $x$. Substituting (3.16) into the harmonic wave equation (3.15) and equating the different powers of $\epsilon$, we derive

\[
S_x^2 = 2(E - V),
\]
\[
S_{xx}B_0 + 2S_xB_{0,x} = 0,
\]
\[
S_{xx}B_k + 2S_xB_{k,x} + B_{k-1,xx} = 0, \quad \forall k \geq 1.
\]

At a fixed spatial point, say $x = 0$, the initial conditions can be set as

\[
S(0) = 0, \quad B_0(0) = 1, \quad B_k(0) = 0, \quad k \geq 1.
\]

The impedance associated with the harmonic wave solution $U$ is

\[
\frac{U'(0)}{U(0)} = \frac{iS_x(0)}{\epsilon} + \sum_{k=0}^{\infty} \left( \frac{\epsilon}{i} \right)^k B_{k,x}(0).
\]

Introducing the local wave number $k$ as

\[
k = \sqrt{2(E - V(0))},
\]

we have

\[
S_x(0) = \pm k, \quad (3.17)
\]
\[
S_{xx}(0) = \mp \frac{V'(0)}{k}, \quad (3.18)
\]
\[
A_{0,x}(0) = \frac{V'(0)}{2k^2}. \quad (3.19)
\]

Thus within the accuracy to $O(\epsilon)$, the impedance is

\[
\frac{U'(0)}{U(0)} = \pm \frac{ik}{\epsilon} + \frac{V'(0)}{2k^2} + O(\epsilon).
\]

The plus sign corresponds to the right-going wave, while the minus sign to the left-going wave. That is to say, if denoting by $U^+$ the right-going wave and by $U^-$ the left-going wave, we have $U^\pm(0) = 1$ and

\[
\frac{\partial_x U^+(0)}{U^+(0)} = \frac{ik}{\epsilon} + \frac{V'(0)}{2k^2} + O(\epsilon), \quad \frac{\partial_x U^-(0)}{U^+(0)} = -\frac{ik}{\epsilon} + \frac{V'(0)}{2k^2} + O(\epsilon). \quad (3.20)
\]

### 3.3. Reflection and transmission operators.

First let us go to the frequency domain and compute the reflection and transmission coefficients for a monochromatic wave with energy $E$. Suppose $x = 0$ is the singular point. Set

\[
V_0^l = \lim_{x \to 0^-} V(x), \quad V_1^l = \lim_{x \to 0^-} V'(x), \quad k^l = \sqrt{2(E - V_0^l)}, \quad (3.21)
\]

and

\[
V_0^r = \lim_{x \to 0^+} V(x), \quad V_1^r = \lim_{x \to 0^+} V'(x), \quad k^r = \sqrt{2(E - V_0^r)}. \quad (3.22)
\]
Suppose the wave travels from the left to the right. On the left of \( x = 0 \), the wave field \( U \) is a linear combination of incident wave \( U_1^+ \) and its reflected wave \( U_1^- \), and on the right, it is a transmitted wave proportional to \( U_r^+ \). That is to say, we have

\[
U(x) = \begin{cases} 
U_(x), & x < 0, \\
U_r(x), & x > 0,
\end{cases}
\]

with

\[
U_1 = U_1^+ + RU_1^-, \quad U_r = TU_r^+,
\]

where \( R = R(E) \) and \( T = T(E) \) denote the reflection and transmission coefficients, respectively. In terms of the \( C^1 \)-continuity condition, applying (3.20) we have

\[
1 + R = T, \quad \left( \frac{ik^l}{c} + \frac{V_l^l}{2(k^l)^2} \right) + R \left( -\frac{ik^l}{c} + \frac{V_l^l}{2(k^l)^2} \right) = T \left( \frac{ik^r}{c} + \frac{V_l^r}{2(k^r)^2} \right) + O(\epsilon). \tag{3.23}
\]

Expanding \( R \) and \( T \) up to the linear terms with respect to \( \epsilon \), i.e.,

\[
R = R_0 + \left( \frac{\epsilon}{2} \right) R_1 + O(\epsilon^2), \quad T = T_0 + \left( \frac{\epsilon}{2} \right) T_1 + O(\epsilon^2),
\]

and substituting these expressions into (3.23)-(3.24), we derive

\[
R_0 = \frac{k^l - k^r}{k^l + k^r}, \quad T_0 = \frac{2k^l}{k^l + k^r}, \quad R_1 = \frac{V_l^l(k^l)^2 - V_l^r(k^r)^2}{k^l(k^r)^2(k^l + k^r)^2}, \quad T_1 = \frac{V_l^r(k^r)^2 - V_l^l(k^l)^2}{k^l(k^r)^2(k^l + k^r)^2}.
\]

Since \( k^l,r \) are functions of \( E \) (see (3.21)-(3.22)), so are \( \{R_0, R_1\} \) and \( \{T_0, T_1\} \). For a Gaussian beam with central Hamiltonian \( s_1 \), the energy band is of the size \( O(\sqrt{\epsilon}) \) centered at \( E_\epsilon = s_1 \). To maintain the same form as (3.1) for the reflected and transmitted waves, we need to expand \( R \) and \( T \) into power forms. Suppose

\[
R = \sum_{j=0}^{\infty} \frac{R_0}{j!} (E - E_\epsilon)^j + \left( \frac{\epsilon}{2} \right) \sum_{j=0}^{1} \frac{R_1}{j!} (E - E_\epsilon)^j + O(\epsilon^2), \tag{3.25}
\]

\[
T = \sum_{j=0}^{\infty} \frac{T_0}{j!} (E - E_\epsilon)^j + \left( \frac{\epsilon}{2} \right) \sum_{j=0}^{1} \frac{T_1}{j!} (E - E_\epsilon)^j + O(\epsilon^2). \tag{3.26}
\]

Setting \( k^l,r = \sqrt{2(s_1 - V_l^l,r)} \), a direct computation shows that

\[
R_{00} = \frac{k^l_1 - k^r_1}{k^l_1 + k^r_1}, \quad T_{00} = \frac{2k^l_1}{k^l_1 + k^r_1},
\]

\[
R_{01} = T_{01} = \frac{2(k^r_1 - k^l_1)}{k^l_1 k^r_1(k^l_2 + k^r_2)}, \quad R_{02} = T_{02} = \frac{2}{k^l_2 (k^l_1)^3} = \frac{2}{k^r_2 (k^r_1)^3},
\]

\[
R_{03} = T_{03} = \frac{6}{(k^l_1)^3 k^l_2} - \frac{6}{(k^r_1)^3 k^r_2}, \quad R_{10} = T_{10} = \frac{V_l^l (k^l_1)^2 - V_l^r (k^r_1)^2}{k^l_1 (k^r_1)^2 (k^l_2 + k^r_2)^2},
\]

\[
R_{11} = T_{11} = -2V_l^l (k^l_1)^2 (k^r_1)^3 + V_l^l (k^l_2)^4 k^l_1 - 2V_l^r (k^r_1)^5 + 2V_l^r (k^l_1)^4 k^r_1 + V_l^r (k^r_1)^2 (k^l_1)^3.
\]
Returning to the time domain, the reflection operator $\mathcal{R}$ and the transmission operator $T$ are (with the accuracy to $O(\epsilon^2)$, see (3.25)-(3.26))

$$\mathcal{R} = \sum_{j=0}^{3} \frac{R_{0j}}{j!}(ie\partial_t - s_1)^j + \left(\frac{\epsilon}{7}\right) \sum_{j=0}^{1} \frac{R_{1j}}{j!}(ie\partial_t - s_1)^j,$$

(3.27)

$$T = \sum_{j=0}^{3} \frac{T_{0j}}{j!}(ie\partial_t - s_1)^j + \left(\frac{\epsilon}{7}\right) \sum_{j=0}^{1} \frac{T_{1j}}{j!}(ie\partial_t - s_1)^j.$$  

(3.28)

Note that the reflected and transmitted waves have the same phase of the incident wave in the TPP representation. The TPP amplitude parameters $\{a_{ij}^{(R)}\}$ of the reflected wave are then obtained by acting the reflection operator $\mathcal{R}$ in (3.27) onto the expression (3.1). The results are

$$a_{00}^{(R)} = R_{00}a_{00},$$

(3.29)

$$a_{01}^{(R)} = R_{00}a_{01} + R_{01}s_2a_{00},$$

(3.30)

$$a_{02}^{(R)} = R_{00}a_{02} + R_{01}a_{2} + R_{02}s_2a_{00} + 2R_{01}s_2a_{01},$$

(3.31)

$$a_{03}^{(R)} = R_{00}a_{03} + 3R_{01}s_2a_{02} + 3R_{02}s_3a_{01} + R_{01}s_3a_{00} + 3R_{02}s_3a_{02}a_{00} + 3R_{03}s_3a_{00} + 3R_{02}s_3a_{00}a_{02},$$

(3.32)

$$a_{10}^{(R)} = R_{00}a_{10} + R_{01}a_{01} + \frac{1}{2}R_{02}s_3a_{02} + R_{10}a_{00},$$

(3.33)

$$a_{11}^{(R)} = R_{00}a_{11} + R_{01}(a_{02} + a_{10}s_2) + \frac{3}{2}R_{02}a_{01}s_2 + \frac{1}{2}R_{02}a_{00}s_3 + \frac{1}{2}R_{03}a_{00}s_2 + R_{10}a_{01} + R_{11}a_{00}s_2.$$  

(3.34)

The TPP amplitude parameters $\{a_{ij}^{(T)}\}$ of the transmitted wave at the singular point are analogously derived by replacing the symbol $R$ with $T$ in the above formulations.

We should remark that the above asymptotic analysis is only valid when $k^{\ast}_{1r} = O(1)$. If this condition is violated, the corresponding analysis is still open, to the authors’ knowledge.

### 3.4. Determining the reflected wave and transmitted wave

The last subsection presented the TPPs for both the reflected and transmitted waves of a traveling Gaussian beam at a singular point. Now we discuss the possibility of transforming TPPs back to SPPs. Notice that after $S_1$ is determined through the Hamiltonian expression (3.3), other SPPs are then determined uniquely through the equations (3.2), (3.4)-(3.13). For the reflected wave, the inverse transformation from TPPs to SPPs at the singular point is always possible, which implies that the reflected wave is still a Gaussian beam. The speed of reflected beam is uniquely determined as $S_1^{(R)} = -S_1$, where $S_1$ is the speed of the traveling beam. For the transmitted wave, things are more complicated. If $s_1 > V^r_\epsilon$, which means the beam energy is large enough to climb over the energy barrier, the transmitted wave is also a Gaussian beam with the speed $S_1^{(T)} = \sqrt{2(s_1 - V^r_\epsilon)}$. If $s_1 < V^r_\epsilon$, the equation (3.3) has no real root, which implies that the transmitted wave is not traveling but evanescent. A boundary layer of size $O(\epsilon)$ (NOT $O(\epsilon^{1/2})$) appears, and the ODE system (2.9)-(2.20) could no longer describe the dynamics of the transmitted wave. We have to find a different way to compute the transmitted wave away from the singular point.
Using the right-going wave expression (see (3.17)-(3.19)) for the monochromatic wave of energy $E$, we have

$$u_r(x, E) = \exp \left( \frac{i}{\epsilon} \left( S_r(0) + S_{xx}(0)x^2/2 \right) \right) \left( 1 + B_{0,r}(0)x \right) + O(\epsilon^2)$$

$$= \left( 1 + \frac{V'_r x}{2(k^r)^2} \right) \exp \left\{ \frac{i}{\epsilon} \left( k_r^r x - \frac{V'_r x^2}{2k^r} \right) \right\} + O(\epsilon^2)$$

$$= \left( 1 + \frac{V'_r x}{2(k^r)^2} - \frac{iV''_r x^2}{2k^r} \right) \exp \left\{ \frac{ik_r^r x}{\epsilon} \right\} + O(\epsilon^2).$$

Here we have used the facts that $B_{0,0}(0) = 1$, $B_{1,0}(0) = 0$, $S(0) = 1$, and $x$ is at most of $O(\epsilon)$ in the valid region of evanescent transmitted wave. Since $u_r$ is defined in the frequency domain, to derive a computation formulation in the time domain, we need to expand $u_r$ into power form around the central Hamiltonian $E^* = s_1$ for any fixed $x$. To maintain the second order accuracy, we need to keep up to the cubic terms, i.e.,

$$u_r(x, E) = \sum_{j=0}^{3} \frac{\tilde{T}_j(x, \epsilon)}{j!} (E - E^*)^j + O(\epsilon^2).$$

Here $\{\tilde{T}_j\}$ could be computed either analytically or numerically. Then we use the transformation relations (3.29)-(3.34) (replacing $R_0$ with $\tilde{T}_j$ and $R_1$ with $0$) to compute the TPPs at the point $x$. The wave field is finally computed with the asymptotic expression (3.1).

Finally we should remark that the interface conditions have also been studied recently by Tanushev, Engquist and Tsai [28] for the hyperbolic wave equation.

4. Numerical tests. In this section, we present some numerical tests to validate the Gaussian beam formulations given in Section 2, and the interface conditions proposed in Section 3. The initial data is set as

$$u_0(x) = \exp \left\{ \frac{i}{\epsilon} \left( 2(x - x_0) + \frac{i}{2}(x - x_0)^2 \right) \right\},$$

with $x_0 = -0.5$. We consider two different potentials

$$V_{\text{one}} = \begin{cases} 0, & x < 0 \\ \Delta V, & x > 0 \end{cases}, \quad V_{\text{two}} = \begin{cases} x/5, & x < 0 \\ \Delta V - x/5, & x > 0 \end{cases},$$

where $\Delta V$ denotes the potential jump at $x = 0$.

For the sake of comparison, a reference solution for each potential is computed by the characteristic expansion method. The details of the method are as follows. We confine the computation domain into $[-1, 1]$, and impose Neumann boundary conditions at the two boundary points $\pm 1$. This treatment is reasonable since in our computation the wave field does not reach the boundaries and the boundary conditions do not have any significant effect. The Schrödinger operator $-\frac{\epsilon^2}{2} \partial_x^2 + V(x)$ is discretized by eighth-order finite element method with mesh size $\frac{1}{1024}$. Then we compute the eigenvalues and their associated orthonormal eigenfunctions. Since the spectra of $u_0(x)$ is centered around $2 + V(x_0)$, and has a width of $O(\sqrt{\epsilon})$, only a few modes have non-negligible contributions to the wave solution. In the numerical tests of this section, we compute 300 eigenvalues closest to $2 + V(x_0)$ with the Matlab
function “eigs”. The wave solution at any given time point $t$ is then obtained by evolving 300 simple ODEs and composing the corresponding modes together.

We perform four numerical tests:

- **PA**: $V = V_{\text{one}}, \Delta V = 1$
- **PB**: $V = V_{\text{one}}, \Delta V = 3$
- **PC**: $V = V_{\text{two}}, \Delta V = 0$
- **PD**: $V = V_{\text{two}}, \Delta V = 3$

For PA, PB and PD, the potential is not continuous at $x = 0$. The potential of PC is continuous at $x = 0$, but its first derivative has a jump of $-0.4$. Let $t_*$ denote the traveling time for the beam arriving at the singular point $x = 0$. For PA and PB, $t_* = 0.25$, while for PC and PD, $t_* \approx 0.25321$. When $\epsilon = \frac{1}{1024}$, the moduli of reference solutions at $t = t_*$ and $t = 2t_*$ are plotted in Fig. 4.1 and Fig. 4.2, respectively. The wave reflection is obvious except PC. The reflection effect for PC is not as significant as other cases, but it does exist, see the zoomed plot in Fig. 4.3 at $t = 2t_*$. At $t = t_*$, due to the interference of reflected wave and propagating beam, the wave field becomes very oscillatory on the left hand side of the singular point. We could also observe that for PB and PD, the propagating beam cannot penetrate the potential barrier. At $t = t_*$, a sharp boundary layer appears on the right hand side of the singular point $x = 0$.

![Fig. 4.1. Modulus of reference solution at $t = t_*$. $t_*$ denotes the traveling time for Gaussian beams arriving at the singular point $x = 0$. $\epsilon = 1/1024$. Top left: PA. Top right: PB. Bottom left: PC. Bottom right: PD.](image)

At any time, the Gaussian beam solution to the Schrödinger equation (1.1) is a summation of the propagating beam, the reflected wave and the transmitted wave. In Fig. 4.4 and Fig. 4.5, we plot the error between the different order Gaussian beam solutions and the reference solution for $\epsilon = \frac{1}{1024}$ at $t = t_*$ and $t = 2t_*$, respectively. It
Fig. 4.2. Modulus of reference solution at \( t = 2t^* \). \( t^* \) denotes the traveling time for Gaussian beams arriving at the singular point \( x = 0 \), \( \epsilon = 1/1024 \). Top left: PA. Top right: PB. Bottom left: PC. Bottom right: PD.

Fig. 4.3. Modulus of reference solution at \( t = 2t^* \). \( t^* \) denotes the traveling time for Gaussian beams arriving at the singular point \( x = 0 \), \( \epsilon = 1/1024 \). PC.
could be observed that high-order beam solutions are much more accurate than low-order ones. In particular for PC, the first and second order beams solutions cannot resolve the weak reflected wave at all, see Fig. 4.6, since in these cases, the reflection operator is simply approximated with zero in the first and second order interface conditions. Comparatively, the fourth order beam solution matches the reference solution very well, and no difference can be detected. In Table 4.1-4.4, we list the relative $L^2$ errors at $t = t^*$ for all those test problems. As expected, the convergence rate for the first to fourth beam solutions is close to $1/2$, $1$, $3/2$ and $2$ respectively.

![Graph showing modulus of errors for different orders of beams](image)

**Fig. 4.4.** Errors between Gaussian beam solutions and the reference solution at $t = t^*$. Modulus is plotted. $\epsilon = 1/2^{0.5}$. Top left: PA. Top right: PB. Bottom left: PC. Bottom right: PD.

<table>
<thead>
<tr>
<th>Order</th>
<th>$\epsilon = 1/2^{0.5}$</th>
<th>$\epsilon = 1/2^{1.5}$</th>
<th>$\epsilon = 1/2^{2.5}$</th>
<th>$\epsilon = 1/2^{10}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>First order</td>
<td>1.0633e-002</td>
<td>8.9639e-003</td>
<td>7.5554e-003</td>
<td>6.3669e-003</td>
</tr>
<tr>
<td>Convergence rate</td>
<td>—</td>
<td>—</td>
<td>—</td>
<td>—</td>
</tr>
<tr>
<td>Second order</td>
<td>1.1284e-003</td>
<td>7.9810e-004</td>
<td>5.6462e-004</td>
<td>3.9950e-004</td>
</tr>
<tr>
<td>Convergence rate</td>
<td>—</td>
<td>—</td>
<td>—</td>
<td>—</td>
</tr>
<tr>
<td>Third order</td>
<td>1.8589e-004</td>
<td>1.1019e-004</td>
<td>6.5373e-005</td>
<td>3.8808e-005</td>
</tr>
<tr>
<td>Convergence rate</td>
<td>—</td>
<td>—</td>
<td>—</td>
<td>—</td>
</tr>
<tr>
<td>Fourth order</td>
<td>4.2701e-005</td>
<td>2.1233e-005</td>
<td>1.0608e-005</td>
<td>5.3128e-006</td>
</tr>
<tr>
<td>Convergence rate</td>
<td>—</td>
<td>—</td>
<td>—</td>
<td>—</td>
</tr>
</tbody>
</table>

As a final numerical test, we use the proposed formulations and the Gaussian beam approach to study the solution of the Schrödinger equation with the following
Fig. 4.5. Errors between Gaussian beam solutions and the reference solution at $t = 2t^*$. Modulus is plotted. $\epsilon = \frac{1}{1024}$. Top left: PA. Top right: PB. Bottom left: PC. Bottom right: PD.

Fig. 4.6. Gaussian beam solutions and the reference solution at $t = 2t^*$. PC. Modulus is plotted. $\epsilon = \frac{1}{1024}$. 
### Table 4.2
Relative $L^2$ errors of Gaussian beams. $V = V_{\text{one}}$ with $\Delta V = 3$.  

<table>
<thead>
<tr>
<th>Relative $L^2$ error</th>
<th>$\epsilon = 1/2^{2.5}$</th>
<th>$\epsilon = 1/2^{2}$</th>
<th>$\epsilon = 1/2^{2.5}$</th>
<th>$\epsilon = 1/2^{10}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>First order</td>
<td>3.7532e-002</td>
<td>3.1499e-002</td>
<td>2.6447e-002</td>
<td>2.2212e-002</td>
</tr>
<tr>
<td>Convergence rate</td>
<td>—</td>
<td>5.0565e-001</td>
<td>5.0441e-001</td>
<td>5.0347e-001</td>
</tr>
<tr>
<td>Second order</td>
<td>2.2616e-003</td>
<td>1.5755e-003</td>
<td>1.1005e-003</td>
<td>7.7041e-004</td>
</tr>
<tr>
<td>Convergence rate</td>
<td>—</td>
<td>1.0431e+000</td>
<td>1.0352e+000</td>
<td>1.0289e+000</td>
</tr>
<tr>
<td>Third order</td>
<td>1.6045e-004</td>
<td>9.3818e-005</td>
<td>5.5099e-005</td>
<td>3.2458e-005</td>
</tr>
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<td>Convergence rate</td>
<td>—</td>
<td>1.5483e+000</td>
<td>1.5357e+000</td>
<td>1.5269e+000</td>
</tr>
<tr>
<td>Fourth order</td>
<td>2.7111e-005</td>
<td>1.2824e-005</td>
<td>6.1150e-006</td>
<td>2.9347e-006</td>
</tr>
<tr>
<td>Convergence rate</td>
<td>—</td>
<td>2.1602e+000</td>
<td>2.1368e+000</td>
<td>2.1183e+000</td>
</tr>
</tbody>
</table>

### Table 4.3
Relative $L^2$ errors of Gaussian beams. $V = V_{\text{two}}$ with $\Delta V = 0$.  

<table>
<thead>
<tr>
<th>Relative $L^2$ error</th>
<th>$\epsilon = 1/2^{2.5}$</th>
<th>$\epsilon = 1/2^{2}$</th>
<th>$\epsilon = 1/2^{2.5}$</th>
<th>$\epsilon = 1/2^{10}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>First order</td>
<td>2.0864e-003</td>
<td>1.7607e-003</td>
<td>1.4852e-003</td>
<td>1.2521e-003</td>
</tr>
<tr>
<td>Convergence rate</td>
<td>—</td>
<td>4.8964e-001</td>
<td>4.9114e-001</td>
<td>4.9244e-001</td>
</tr>
<tr>
<td>Second order</td>
<td>9.9862e-005</td>
<td>7.0947e-005</td>
<td>5.0371e-005</td>
<td>3.5741e-005</td>
</tr>
<tr>
<td>Third order</td>
<td>6.7654e-006</td>
<td>4.0344e-006</td>
<td>2.4050e-006</td>
<td>1.4332e-006</td>
</tr>
<tr>
<td>Convergence rate</td>
<td>—</td>
<td>1.4917e+000</td>
<td>1.4926e+000</td>
<td>1.4936e+000</td>
</tr>
<tr>
<td>Fourth order</td>
<td>4.3397e-007</td>
<td>2.1843e-007</td>
<td>1.0986e-007</td>
<td>5.5868e-008</td>
</tr>
<tr>
<td>Convergence rate</td>
<td>—</td>
<td>1.9808e+000</td>
<td>1.9831e+000</td>
<td>1.9511e+000</td>
</tr>
</tbody>
</table>

Initial data:

$$u_0(x) = \exp \left\{ -36(x + 1)^2 + \frac{2ix}{\epsilon} \right\}.$$  

Our initial data decomposition is performed as the following. First we find a function $h_\epsilon(x)$ such that

$$\exp \left\{ -36(x + 1)^2 \right\} = h_\epsilon(x) \ast \exp \left\{ -\frac{x^2}{2\epsilon} \right\}.$$  

Then,

$$u_0(x) = \exp \left\{ \frac{2ix}{\epsilon} \right\} \int_{\mathbb{R}} h_\epsilon(y) \exp \left\{ -\frac{(x - y)^2}{2\epsilon} \right\} dy.$$  

Using the trapezoidal rule to approximate the integral, we have

$$u_0(x) \approx \exp \left\{ \frac{2ix}{\epsilon} \right\} \sum_{j \in \mathbb{Z}} \Delta x h_\epsilon(j \Delta x) \exp \left\{ -\frac{(x - j\Delta x)^2}{2\epsilon} \right\}$$

$$= \sum_{j \in \mathbb{Z}} \Delta x h_\epsilon(j \Delta x) \exp \left\{ \frac{i}{\epsilon} \left( 2j \Delta x + 2(x - j\Delta x) + \frac{i(x - j\Delta x)^2}{2} \right) \right\}.$$  

Notice that the initial wave packet is well-supported in the interval $[-2, 0]$, so is the function $h_\epsilon$. Thus $h_\epsilon$ can be efficiently computed with FFT. In our computations,
Table 4.4

<table>
<thead>
<tr>
<th>Relative $L^2$ error</th>
<th>$\epsilon = 1/2^{5.5}$</th>
<th>$\epsilon = 1/2^7$</th>
<th>$\epsilon = 1/2^{9.5}$</th>
<th>$\epsilon = 1/2^{10}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>First order</td>
<td>3.6109e-002</td>
<td>3.0292e-002</td>
<td>2.5425e-002</td>
<td>2.1347e-002</td>
</tr>
<tr>
<td>Convergence rate</td>
<td>—</td>
<td>5.0684e-001</td>
<td>5.0538e-001</td>
<td>5.0433e-001</td>
</tr>
<tr>
<td>Second order</td>
<td>2.1854e-003</td>
<td>1.5261e-003</td>
<td>1.0682e-003</td>
<td>7.4903e-004</td>
</tr>
<tr>
<td>Convergence rate</td>
<td>—</td>
<td>1.0361e+000</td>
<td>1.0293e+000</td>
<td>1.0242e+000</td>
</tr>
<tr>
<td>Third order</td>
<td>1.3436e-004</td>
<td>7.8698e-005</td>
<td>4.6269e-005</td>
<td>2.7274e-005</td>
</tr>
<tr>
<td>Convergence rate</td>
<td>—</td>
<td>1.5434e+000</td>
<td>1.5326e+000</td>
<td>1.5250e+000</td>
</tr>
<tr>
<td>Fourth order</td>
<td>2.0036e-005</td>
<td>9.5506e-006</td>
<td>4.5798e-006</td>
<td>2.2087e-006</td>
</tr>
<tr>
<td>Convergence rate</td>
<td>—</td>
<td>2.1417e+000</td>
<td>2.1206e+000</td>
<td>2.1042e+000</td>
</tr>
</tbody>
</table>

we set $\Delta x = 2\sqrt{\epsilon}$. Numerical tests show that if $\epsilon \leq \frac{1}{256}$, the maximum error of the above beam sum approximation is less than $6 \times 10^{-14}$. We consider PA and PB. The reference solutions with $\epsilon = 2^{-10}$ are shown in Fig. 4.7. The relative $L^2$ errors are shown in Fig. 4.8. The convergence rates are 0.93, 1.55, 2.01 and 2.12 for the first to fourth order summation methods in the case of PA, and 1.00, 2.00, 3.01 and 3.92 in the case of PB. An interesting thing is that the convergence rates are too much abnormal for PB. Based on the analysis in [23], we know that due to the cancelation effect between the Gaussian beams, the odd order beam summation method in fact has the same accuracy as its one-order-higher even order method. This implies that the first order and second order methods would have the same first order convergence rate with respect to $\epsilon$. However, the numerical tests for PB show that the convergence rate can be even one-order-higher for the second order and fourth order beam methods. This interesting phenomenon needs to be further studied.

5. Conclusion. In this paper we have presented the equations of the first four order Gaussian beams, which are asymptotic solutions to the one-dimensional linear Schrödinger equation with general smooth potential. If the potential is not smooth enough, the Gaussian beam will split into a reflected wave and a transmitted wave after it arrives at any singular point. The reflected wave is always beam-like, but the transmitted wave could be either beam-like or evanescent. In the latter case, a sharp boundary layer of width $O(\epsilon)$ would appear near the singular point. We have studied the interface conditions which specify the way how the reflected beam and the transmitted wave relate to the propagating Gaussian beam. Numerical tests have

![Fig. 4.7. Reference solutions. $\epsilon = 2^{-10}$. Left: PA. Right: PB.](image-url)
been given to validate the accuracy of different order Gaussian beam solutions and the interface conditions, and it has been shown that high-order Gaussian beams have great advantage over low-order ones.

Throughout this paper, we have assumed that all parameters involved in the beam formulations are of $O(1)$. This assumption does not hold if the potential jump is very close to the central Hamiltonian of the propagating beam. In this case, neither the transmitted wave nor the reflected wave behaves like a beam. Some new ansatz is thus needed to seek the correct semi-analytical asymptotic solutions. This issue is now under investigation.

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REFERENCES