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THE GAUSSIAN BEAM METHODS FOR SCHRÖDINGER-POISSON EQUATIONS *

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Abstract

As an important model in quantum semiconductor devices, the Schrödinger-Poisson equations have generated widespread interests in both analysis and numerical simulations in recent years. In this paper, we present Gaussian beam methods for the numerical simulation of the one-dimensional Schrodinger-Poisson equations. The Gaussian beam methods for high frequency waves outperform the geometrical optics method in that the former are accurate even around caustics. The purposes of the paper are first to develop the Gaussian beam methods, based on our previous methods for the linear Schrödinger equation, for the Schrödinger-Poisson equations, and then check their validity for this weakly-nonlinear system.

Mathematics subject classification: 81Q20, 65M99
Key words: Schrödinger-Poisson equations, Gaussian beam methods, Vlasov-Poisson equations.

1. Introduction

The main purpose of this paper is to extend our Gaussian beam method [22], developed for the linear Schrödinger equation, to the one-dimensional nonlinear Schrödinger-Poisson equations

$$i\varepsilon\partial_t\Psi^\varepsilon = -\frac{\varepsilon^2}{2}\partial_{xx}\Psi^\varepsilon + V^\varepsilon\Psi^\varepsilon, \quad x\in\mathbb{R},\ t\geq 0, \tag{1.1}$$

$$\partial_{xx}V^\varepsilon = b(x) - c\left|\Psi^\varepsilon(t,x)\right|^2, \quad E^\varepsilon = \partial_x V^\varepsilon, \tag{1.2}$$

subject to the WKB initial condition

$$\Psi^\varepsilon(0,x) = A_0(x)e^{iS_0(x)/\varepsilon}. \tag{1.3}$$

Here $\Psi^\varepsilon = \Psi^\varepsilon(t,x)$ is the highly oscillatory wave function of wave length $\mathcal{O}(\varepsilon)$ (in the so-called semiclassical regime where the re-scaled Plank constant ε is small). The electric potential $V^\varepsilon =$

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$V^\varepsilon(t,x)$ interacts with the wave function Ψ^ε in a self-consistent way through the Schrödinger equation (1.1) and the Poisson equation (1.2). In the poisson equation (1.2), $b(x) \geq 0$ denotes the fixed positive charged background. The constant c could be ± 1, corresponding to focusing ('+') or defocusing ('-') potential respectively.

The Schrödinger-Poisson equations are a mean-field model for the linear N-particle Schrödinger equation with Coulomb potential [6,7,13], which is based on the Pauli's exclusion principle and the molecular chaos assumption. It is widely used in quantum semiconductor devices modeling [36] and the quantum transport theory [1,2].

The direct simulation of the Schrödinger-Poisson equations is expensive since the wave length $O(\varepsilon)$ is extremely small in the semiclassical regime. The standard time-splitting spectral method [3,4,42] and its adaptive version [5] need the mesh size to be of $\mathcal{O}(\varepsilon)$ and the time step to be of $\mathcal{O}(1)$ to capture the correct physical observables. The finite difference methods [34,35] are even worse since the mesh size and the time step are restricted to be $\mathcal{O}(\varepsilon)$.

One efficient alternative approach is to study the semiclassical limit of the Schrödinger-Poisson equations. When taking the rescaled Planck constant $\varepsilon \to 0$, one can derive the Vlasov-Poisson equations [28,33,49] in the phase space

$$\partial_t f + \xi \partial_x f - \partial_x V \partial_\xi f = 0 \qquad x, \xi \in \mathbb{R},\ t \geq 0, \tag{1.4}$$

$$\partial_{xx} V = b(x) - c \int_{-\infty}^{\infty} f(t,x,\xi) \mathrm{d}\xi, \quad E = \partial_x V, \tag{1.5}$$

or the Euler-Poisson equations in the physical space [30]

$$\partial_t \rho + \partial_x (\rho u) = 0, \qquad x \in \mathbb{R},\ t \geq 0, \tag{1.6}$$

$$\partial_t (\rho u) + \partial_x (\rho u^2) = -\rho \partial_x V, \tag{1.7}$$

$$\partial_{xx} V = b(x) - c\rho. \tag{1.8}$$

There are many papers discussing mathematical analysis and numerical methods for those equations [8, 11, 12, 24, 37], such as the existence and uniqueness of suitable weak solution to Vlasov-Poisson equations [9,19,29,32,50] and numerical methods for capturing the multi-valued solutions to the Euler-Poisson equations [14, 27, 31].

A well-known drawback to the semiclassical approach is that it can not give accurate solutions around caustics. The Gaussian beam methods, developed for the high frequency linear waves [22, 23, 25, 26, 39, 40, 44, 46, 47] and also in the setting of quantum mechanics [15–17], on the other hand, are efficient asymptotic methods that give accurate solutions even around caustics ([45]). The key idea of the Gaussian beam methods is to complexify the phase function $S(t,x)$ off the beam center. Moreover, the imaginary part of $S(t,x)$ should be chosen delicately so that the solution decays exponentially. In this paper, we extend the Gaussian beam methods, proposed previously by the authors [22] for the linear Schrödinger equation, to the weakly nonlinear Schrödinger-Poisson equation (1.1)-(1.2). The original Gaussian beam methods were developed for linear high frequency waves, based on the linear superposition principle. It is of great mathematical and numerical interests to see if the methods can be extended to (at least weakly-) nonlinear problems. In this paper, we propose a class of Gaussian beam methods, in both Lagrangian and Eulerian frameworks, for the Schrödinger-Poisson equations, and check their validity for this weakly nonlinear system.

Our numerical studies show that the Gaussian beam methods can indeed be extended to this one-dimensional, weakly nonlinear system. Indeed, convergent results can be observed, even around caustics, for both the focusing and defocusing cases, when $\varepsilon \to 0$.

A main feature of our Eulerian Gaussian beam method is that only a few (complex-valued) Liouville equations like (1.4) are solved. Thus the computational methods are similar to that of geometrical optics [10, 20, 21]. As a result, the local level-set techniques [38, 41, 43] can also be applied to further reduce the computational cost.

The paper is organized as follows. In Section 2 we systematically present the Gaussian Beam methods, in both Lagrangian and Eulerian frameworks, for solving (1.1)-(1.2). We conduct numerical experiments in Section 3 to verify the validity and convergence of the numerical methods, and give some conclusive remarks in Section 4.

2. The Gaussian Beam Method

In this section, we introduce the Gaussian beam method in details for solving the Schrödinger-Poisson system (1.1)-(1.2). The main procedure is to solve the Poisson equation (1.2) and the Schrödinger equation (1.1) iteratively. Suppose the solution $\Psi^\varepsilon(t^n, x)$ at time t^n are given, then the solution $\Psi^\varepsilon(t^{n+1}, x)$ at time $t^{n+1} = t^n + \Delta t$ is computed as follows:

- Step 1. We solve the Poisson equation (1.2) first to get the potential $V^{\varepsilon,n}(x)$ by some Poisson solvers.
- Step 2. With $V^{,\varepsilon,n}(x)$ given in step 1, $\Psi^\varepsilon(t^{n+1}, x)$ is computed by solving the Schrödinger equation (1.1) using the Gaussian beam method on a fixed time interval Δt.

The Poisson solvers and the Gaussian beam method are given in the following Section 2.1 and 2.2 respectively.

2.1. Poisson solvers

We use the finite difference method to solve the Poisson equation (1.2) equipped with general boundary conditions (Dirichlet, Neumann etc). Suppose the domain of x is $[x_l, x_r]$ and the mesh point is $x_j = x_l + j\Delta x,\ j = 1, \cdots, N$ where Δx is the mesh size and $x_r = x_l + (N+1)\Delta x$, then the potential $V^{\varepsilon,n}(x)$ and the electric field $E^{n,\varepsilon}(x)$ are solved by the linear system:

$$\frac{V_{j+1}^{\varepsilon,n} - 2V_j^{\varepsilon,n} + V_{j-1}^{\varepsilon,n}}{\Delta x^2} = b_j - c\left|\Psi_j^{n,\varepsilon}\right|^2, \quad E_j^{n,\varepsilon} = \frac{V_{j+1}^{\varepsilon,n} - V_{j-1}^{\varepsilon,n}}{2\Delta x},$$

where $V_j^{\varepsilon,n}$, $E_j^{n,\varepsilon}$, b_j, $\Psi_j^{n,\varepsilon}$ are the approximation of $V^\varepsilon(t^n, x_j)$, $E^\varepsilon(t^n, x_j)$, $b(x_j)$, $\Psi^\varepsilon(t^n, x_j)$ respectively.

If the periodic boundary condition is considered for (1.2), the pseudo spectral method will be applied for faster performance. By using the fourier transform $\mathcal{F}$, we can get

$$\mathcal{F}(V^{\varepsilon,n})_k = (\frac{x_r - x_l}{2\pi k})^2 \left(\mathcal{F}(b - c\left|\Psi^{n,\varepsilon}\right|^2)_k\right),$$

and we set $\mathcal{F}(V^{\varepsilon,n})_0 = 0$ for each n. Inverse fourier transform follows after updating $\mathcal{F}(b - c\left|\Psi^{n,\varepsilon}\right|^2)_k$ and $\mathcal{F}(V^{\varepsilon,n})_k$. Remark that the periodic boundary condition forces the following compatibility constraint:

$$\int_{x_l}^{x_r} b(x) - c\left|\Psi^\varepsilon(t,x)\right|^2 dx = 0,$$

which explains why we could set $\mathcal{F}(V^{\varepsilon,n})_0 = 0$ for each n.

2.2. Gaussian beam method

In this subsection we describe how to solve (1.1) on a fixed time interval Δt by the Gaussian beam methods [22] and discuss the issue of constructing the potential $V^{\varepsilon,n+1}(x)$ from the summation of the Gaussian beams. Since the potential $V^{\varepsilon,n}(x)$ is given for computing $\Psi^{\varepsilon}(t^{n+1},x)$, we denote it as V for simplicity.

2.2.1. Lagrangian formulation

The Lagrangian Gaussian beam ansatz is

$$\varphi^{\varepsilon}_{la}(t,x,y_0) = A(t,y)e^{iT(t,x,y)/\varepsilon},$$

where $y = y(t,y_0)$ and $T(t,x,y)$ is given by

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

here $S,p \in \mathbb{R}$, $A,M \in \mathbb{C}$. The time evolution equations of these quantities can be written as a set of ODEs ([22])

$$\frac{\mathrm{d}y}{\mathrm{d}t} = p, \tag{2.1a}$$
$$\frac{\mathrm{d}p}{\mathrm{d}t} = -\partial_y V, \tag{2.1b}$$
$$\frac{\mathrm{d}M}{\mathrm{d}t} = -M^2 - \partial_{yy}V, \tag{2.1c}$$
$$\frac{\mathrm{d}S}{\mathrm{d}t} = \frac{1}{2}|p|^2 - V, \tag{2.1d}$$
$$\frac{\mathrm{d}A}{\mathrm{d}t} = -\frac{1}{2}\big(\mathrm{Tr}(M)\big)A. \tag{2.1e}$$

The Lagrangian Gaussian beam summation solution to the Schrödinger equation (1.1) at time t^{n+1} is constructed as

$$\Phi^{\varepsilon}_{la}(t^{n+1},x) = \int_{\mathbb{R}} \left(\frac{1}{2\pi\varepsilon}\right)^{\frac{1}{2}} r_\theta(x - y(t^{n+1},y_n))\varphi^{\varepsilon}_{la}(t^{n+1},x,y_n)\mathrm{d}y_n. \tag{2.2}$$

where $y_n = y(t^n)$ and $r_\theta \in C_0^\infty(\mathbb{R})$, $r_\theta \geq 0$ is a truncation function with $r_\theta \equiv 1$ in a ball of radius $\theta > 0$ about the origin. The initial conditions at $t = 0$ come from the approximation of the initial condition (1.3) ([18]):

$$y(t^n,y_0) = y_0, \tag{2.3a}$$
$$p(t^n,y_0) = \partial_x S_0(y_0), \tag{2.3b}$$
$$M(t^n,y_0) = \partial_{xx}S_0(y_0) + iI, \tag{2.3c}$$
$$S(t^n,y_0) = S_0(y_0), \tag{2.3d}$$
$$A(t^n,y_0) = A_0(y_0). \tag{2.3e}$$

The discrete form of (2.2) is given as

$$\Phi^{\varepsilon}_{la}(t^{n+1},x) = \sum_{j=1}^{N_{y_n}} \left(\frac{1}{2\pi\varepsilon}\right)^{\frac{1}{2}} r_\theta(x - y(t^{n+1},y_n^j))\varphi^{\varepsilon}_{la}(t^{n+1},x,y_n^j)\Delta y_n, \tag{2.4}$$

where y_n^j's are the Lagrangian mesh points, and N_{y_n} is the number of the beams at time t^n.

For the evolution from t^{n+1} to t^{n+2}, we need to construct $V^{\varepsilon,n+1}$, $\partial_y V^{\varepsilon,n+1}$ and $\partial_y^2 V^{\varepsilon,n+1}$ from the beam summation solution (2.2) which is done by the following procedure:

- Step 1, we compute (2.2) on a fixed gird of x, then solve $V^{\varepsilon,n+1}(x)$ and $E^{n+1,\varepsilon}(x) = \partial_x V^{\varepsilon,n+1}$ from (1.2) by some Poisson solver given in Section 2.1. Interpolate $V^{\varepsilon,n+1}(x)$ and $\partial_x V^{\varepsilon,n+1}$ to get their values on the Lagrangian mesh points y_n^j. Note that $V^{\varepsilon,n+1}(x)$ and $\partial_x V^{\varepsilon,n+1}$ are the integration functions of the density $|\Psi^\varepsilon|^2$ which implies that they are oscillatory but with *very small* oscillatory magnitudes (see, e.g., Fig. 6 of [19]). This feature implies that if one implements the interpolation on a coarse mesh gird, although the numerical result could not capture the small scale oscillations, it provides good approximation for the envelope of the solution, which in fact is very close to the true solution due to the oscillation amplitude is *very small*.
- Step 2, we compute $\partial_{yy} V^{\varepsilon,n+1}$ directly for each y_n^j using the Poisson equation (1.2), i.e.
$$\partial_{yy} V^{\varepsilon,n+1} = b(y) - c\,|\Phi_{la}^\varepsilon|^2 .$$
The reason we have to compute $\partial_{yy} V^{\varepsilon,n+1}$ directly instead of using interpolation is that, the oscillatory magnitude of $\partial_{yy} V^{\varepsilon,n+1}$ is *comparable* to that of the density $|\Psi^\varepsilon|^2$.

Note that we have two sets of meshes here: one is the Eulerian mesh for x, and the other is the Lagrangian mesh for y. The values exchanged between these two meshes are through high order interpolation. This inevitably complicates the algorithms and the notations which could be avoided by the Eulerian formulation below.

2.2.2. Eulerian formulation

For the Eulerian formulation of the Gaussian beam approximation, we have

$$\varphi_{eu}^\varepsilon(t,x,y,\xi) = A(t,y,\xi)e^{iT(t,x,y,\xi)/\varepsilon},$$

with

$$T(t,x,y,\xi) = S(t,y,\xi) + \xi(x-y) + \frac{1}{2}M(t,y,\xi)(x-y)^2.$$

Define the linear Liouville operator as

$$\mathcal{L} = \partial_t + \xi\partial_y - \partial_y V \partial_\xi,$$

then the Eulerian Gaussian beam method is constructed by solving the following Liouville equations:

$$\mathcal{L}\phi = 0, \tag{2.5a}$$
$$\mathcal{L}S = \frac{1}{2}|\xi|^2 - V, \tag{2.5b}$$
$$\mathcal{L}f = 0. \tag{2.5c}$$

where $\phi \in \mathbb{C}$, and $S, f \in \mathbb{R}$. M and amplitude A are computed by

$$M(t,y,\xi) = -\partial_y\phi(\partial_\xi\phi)^{-1},$$
$$A(t,y,\xi) = (\det(\partial_\xi\phi)^{-1}f)^{1/2}.$$

The Eulerian Gaussian beam summation solution to the Schrödinger equation (1.1) is constructed via

$$\Phi^{\varepsilon}_{eu}(t^{n+1},x)=\int_{\mathbb{R}}\int_{\mathbb{R}}\left(\frac{1}{2\pi\varepsilon}\right)^{\frac{1}{2}} r_\theta(x-y)\varphi^{\varepsilon}_{eu}(t^n,x,y,\xi)\delta(\mathrm{Re}[\phi])\mathrm{d}\xi\mathrm{d}y, \tag{2.6}$$

in which δ is the Dirac delta function.

According to [22], the initial data for (2.5) are given by

$$\phi(0,y,\xi)=-iy+(\xi-\partial_y S_0(y)), \tag{2.7a}$$

$$S(0,y,\xi)=S_0(y), \tag{2.7b}$$

$$f(0,y,\xi)=A_0^2(y). \tag{2.7c}$$

The construction of $V^{\varepsilon,n+1}$, $\partial_y V^{\varepsilon,n+1}$ and $\partial_{yy}V^{\varepsilon,n+1}$ from (2.6) is simple in the Eulerian framework since every quantity is computed in a fixed grid. All we need to do is to take the same mesh for x as that for y and solve (1.2) by some Poisson solver given in Section 2.1. For the numerical computation of (2.6), the discretized delta function integration method [48] is recommended since it avoids the difficulty of computing singular integrals [22].

3. The Numerical Examples

In this section, we will present both focusing and defocusing numerical results of the Schrödinger-Poisson equations (1.1)-(1.2) by using the Gaussian beam method proposed in section 2. In our computations, the initial condition is always chosen in the WKB form (1.3). We compute the reference solution Ψ^{ε} using the Strang splitting spectral method [3–5] with mesh size Δx and time step Δt small enough. We always take a large computational domain such that the periodic boundary condition does not introduce a significant error to the whole problem. To diminish the cut-off error, the truncation parameter θ appears in (2.6) is picked fairly large as we discussed in [22]. We will denote solutions obtained by (2.6) as Φ^{ε}_{GB}.

Example 1. Consider the 1D Schrödinger-Poisson equation on computational domain $[-0.5,0.5]$ with a focusing potential

$$V_{xx}=\frac{\sqrt{2\pi}}{10}-|\psi(x)|^2.$$

The initial conditions are given by

$$A_0(x)=e^{-25x^2},\quad S_0(x)=\frac{1}{\pi}\cos(x).$$

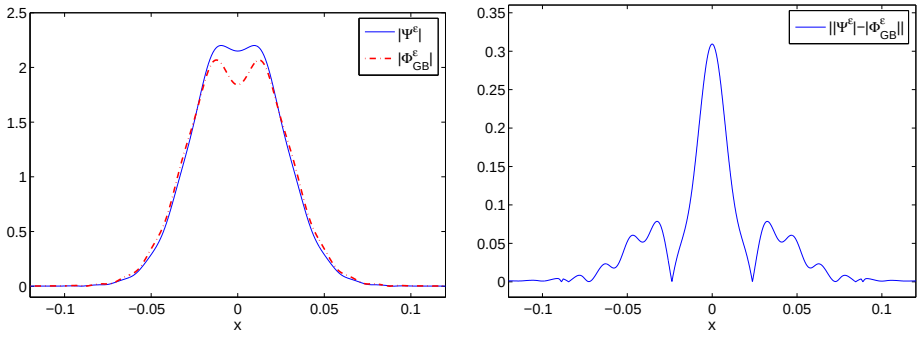
At time $t=0.4$, we output the l^1, l^2 and l^∞ error of the wave amplitude in Table 3.1. We can see the convergence rate in ε is of order 0.9006 in the l^1 norm. Here the number of Gaussian beams N_y is optimized with ε, see discussion in [22]. In Figure 3.1, we plot the wave amplitude and absolute error for different ε.

Example 2. Consider the 1D defocusing Schrödinger-Poisson equation

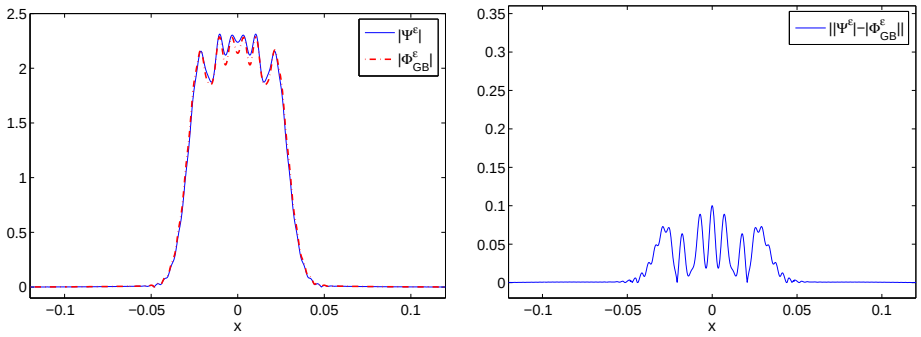
$$V_{xx}=-\frac{\sqrt{2\pi}}{10}+|\psi(x)|^2.$$

Table 3.1: the l^1, l^2 and l^∞ errors of the wave amplitude for $\varepsilon = \frac{1}{256}, \frac{1}{1024}, \frac{1}{4096}$ for Example 1.

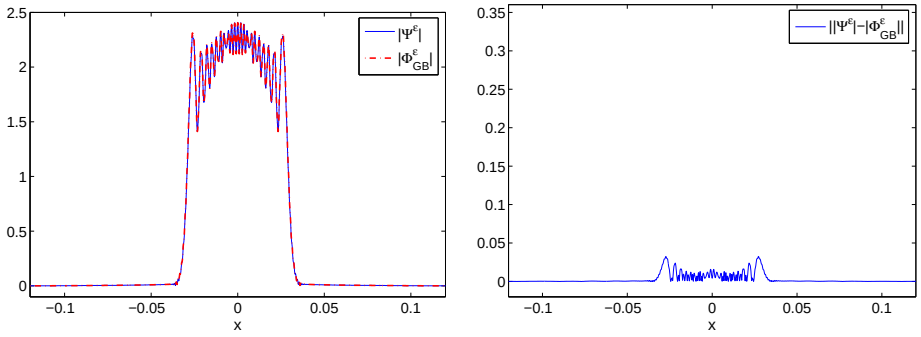
(ε, N_y)	$(\frac{1}{256}, 128)$	$(\frac{1}{1024}, 256)$	$(\frac{1}{4096}, 512)$
l^1 error	1.12×10^{-2}	3.93×10^{-3}	9.22×10^{-4}
l^2 error	4.09×10^{-2}	1.47×10^{-2}	3.80×10^{-3}
l^∞ error	3.09×10^{-1}	1.09×10^{-1}	3.09×10^{-2}



(a) $\varepsilon = \dfrac{1}{256}$



(b) $\varepsilon = \dfrac{1}{1024}$



(c) $\varepsilon = \dfrac{1}{4096}$

Fig. 3.1. Example 1, the Schrödinger-Poisson solution $|\Psi^\varepsilon|$ versus the Gaussian beams solution $|\Phi^\varepsilon_{eu}|$ for different values of ε. The left figures are the comparisons of the wave amplitude at $t = 0.4$; the right figures plot the errors $||\Phi^\varepsilon_{GB}| - |\Psi^\varepsilon||$.

Table 3.2: the l^1, l^2 and l^∞ errors of the wave amplitude for $\varepsilon = \frac{1}{256}, \frac{1}{1024}, \frac{1}{4096}$ for Example 2.

(ε, N_y)	$(\frac{1}{256}, 128)$	$(\frac{1}{1024}, 256)$	$(\frac{1}{4096}, 512)$
l^1 error	8.16×10^{-3}	2.60×10^{-3}	8.35×10^{-4}
l^2 error	3.20×10^{-2}	9.24×10^{-3}	2.94×10^{-3}
l^∞ error	1.74×10^{-1}	5.30×10^{-2}	1.95×10^{-2}

with same boundary condition and initial data as in Example 1. At time $t = 0.4$, the l^1, l^2 and l^∞ error of the wave amplitude are also given in Table 3.2. We can see the convergence rate in ε is of order 0.8221 in the l^1 norm. The wave amplitude and absolute error for different ε are plotted in Figure 3.2.

Example 3. Consider the same defocusing potential as in Example 2. The initial conditions are changed to be

$$A_0(x) = e^{-25x^2}, \quad S_0(x) = 0.$$

In this example, we examine the convergence when there is no caustics. This, along with the above two caustic examples, will show that the Gaussian beam method we propose here gives satisfactory results from the numerical point of view. We evolve the solution to time $t = 0.5$, and the l^1, l^2 and l^∞ errors of the wave amplitude are given in Table 3.3. The convergence rate in ε is of order 0.9389 in the l^1 norm. In Figure 3.3, the wave amplitude and absolute error are plotted for different ε. We remark that since the solution is not as oscillatory as in the last two examples, only a very small number of beams are needed to get the accurate solution.

Table 3.3: the l^1, l^2 and l^∞ errors of the wave amplitude for $\varepsilon = \frac{1}{256}, \frac{1}{1024}, \frac{1}{4096}$ for Example 3.

(ε, N_y)	$(\frac{1}{256}, 16)$	$(\frac{1}{1024}, 32)$	$(\frac{1}{4096}, 64)$
l^1 error	3.31×10^{-2}	9.40×10^{-3}	2.45×10^{-3}
l^2 error	4.26×10^{-2}	1.25×10^{-2}	3.30×10^{-3}
l^∞ error	1.05×10^{-1}	3.28×10^{-2}	8.92×10^{-3}

4. Conclusion

In this paper, we extended the Gaussian beam methods, in both Lagrangian and Eulerian framework, to the one dimensional Schrödinger-Poisson equations. Using the method introduced in [22], the Schödinger equation (1.1) can be directly simulated in each time step. For the poisson equation (1.2), the potential function and its derivatives only need to be constructed at mesh points. Such a setup makes the Gaussian beam method valid and efficient for solving the one-dimensional Schrödinger-Poisson equations. Several examples have been given to confirm the convergence and accuracy.

It will be of interest to study the method in higher space dimension, which will be the subject of our future study.

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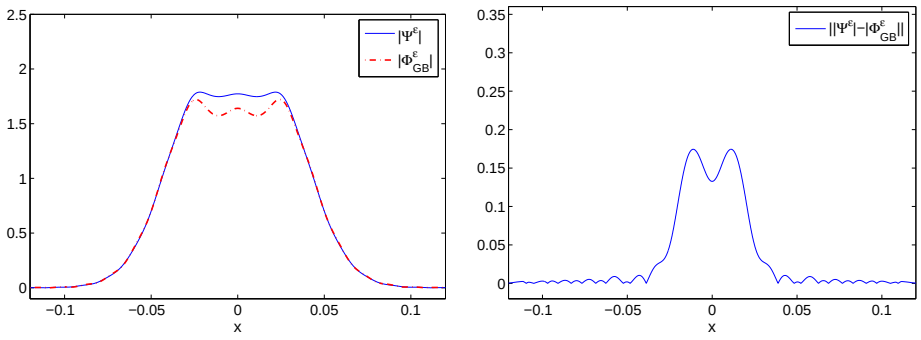
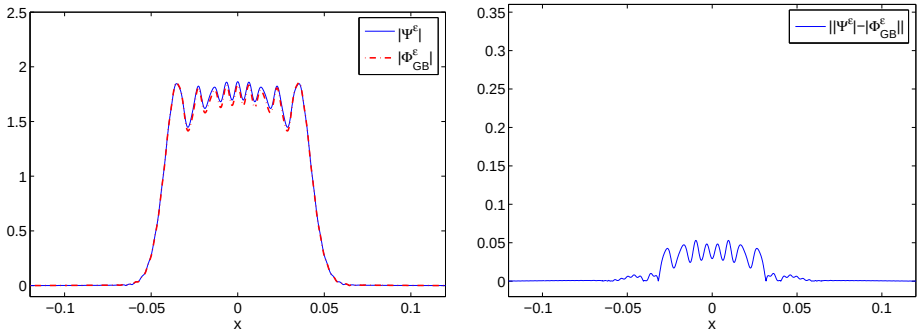
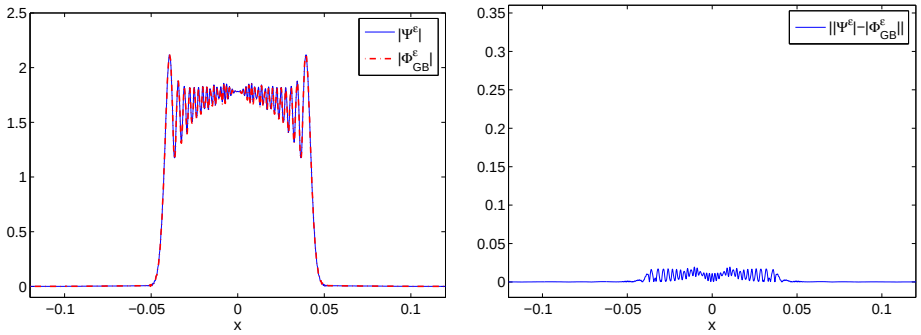


(a) $\varepsilon = \dfrac{1}{256}$



(b) $\varepsilon = \dfrac{1}{1024}$



(c) $\varepsilon = \dfrac{1}{4096}$

Fig. 3.2. Fig. 3.2. Same as Fig. 3.1, excep for Example 2.

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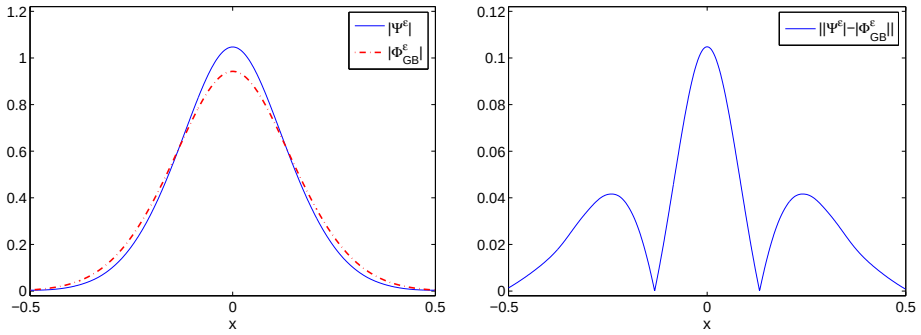
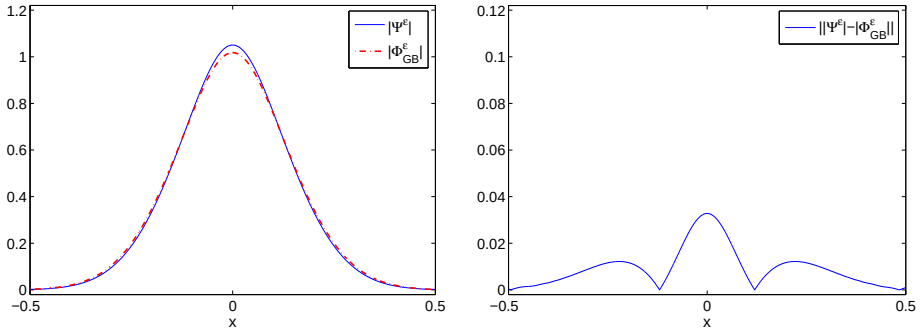
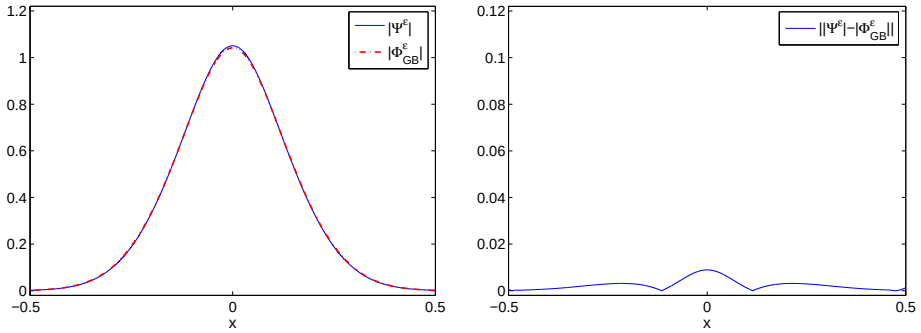


(a) $\varepsilon = \dfrac{1}{256}$



(b) $\varepsilon = \dfrac{1}{1024}$



(c) $\varepsilon = \dfrac{1}{4096}$

Fig. 3.3. Example 3, the Schrödinger-Poisson solution $|\Psi^\varepsilon|$ versus the Gaussian beams solution $|\Phi^\varepsilon_{eu}|$ for $\varepsilon = \frac{1}{256}, \frac{1}{1024}, \frac{1}{4096}$. The left figures are the comparisons of the wave amplitude at $t = 0.5$; the right figures plot the errors $||\Phi^\varepsilon_{GB}| - |\Psi^\varepsilon||$.

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