An Eulerian Gaussian Beam Method for Semi-classical Limit of the Linear Schrodinger Equation

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High frequency waves

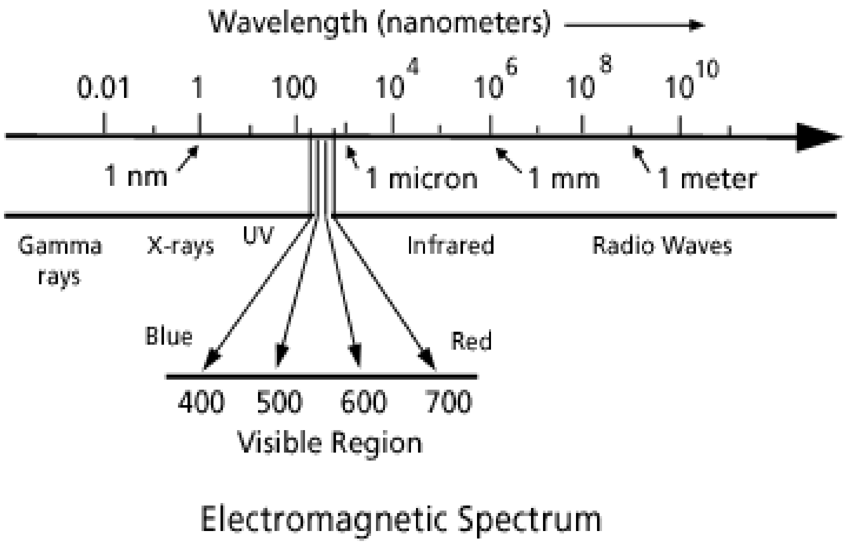


Fig. 1. The electromagnetic spectrum, which encompasses the visible region of light, extends from gamma rays with wave lengths of one hundredth of a nanometer to radio waves with wave lengths of one meter or greater.

- High frequency waves: wave length/domain of computation <<1

Difficulty of high frequecy wave computation

- Consider the example of visible lights in this lecture room:

wave length: $\sim 10^{-6}$ m

computation domain $\sim$ m

1d computation: $10^6 \sim 10^7$

2d computation: $10^{12} \sim 10^{14}$

3d computation: $10^{18} \sim 10^{21}$

do not forget time! Time steps: $10^6 \sim 10^7$

An Example: Linear Schrodinger Equation

$$i\epsilon\psi_t + \frac{\epsilon^2}{2}\Delta\psi - V\psi = 0 \qquad \mathbf{x} \in R^d, \quad t > 0$$

$$\psi(\mathbf{x}, 0) = A_0(\mathbf{x})e^{i\frac{S_0(\mathbf{x})}{\epsilon}}$$

In this equation, $\psi(\mathbf{x}, t)$ is the complex-valued *wave function*, ϵ is or is playing the role of *Planck's constant*. It is assumed to be small here. The solution ψ and the related physical observables become *oscillatory* in space and time in the order of $O(\epsilon)$, causing all the mathematical and numerical challenges.

Semiclassical limit of the linear schrodinger equation

If one can find the asymptotic (semiclassical) limit as $\varepsilon \to 0$ then one can just solve the *limiting* equation numerically.

The WKB Method

We assume that solution has the form (*Madelung Transform*)

$$\psi(\mathrm{x},t) = A(\mathrm{x},t)e^{i\frac{S(\mathrm{x},t)}{\epsilon}}$$

and apply this ansatz into the Schrodinger equation with initial data. Separating the real part from the imaginary part, and keeping only the leading order term, one can get

$$S_t + \frac{1}{2}|\nabla S|^2 + V = 0 \qquad \text{eiconal equation}$$

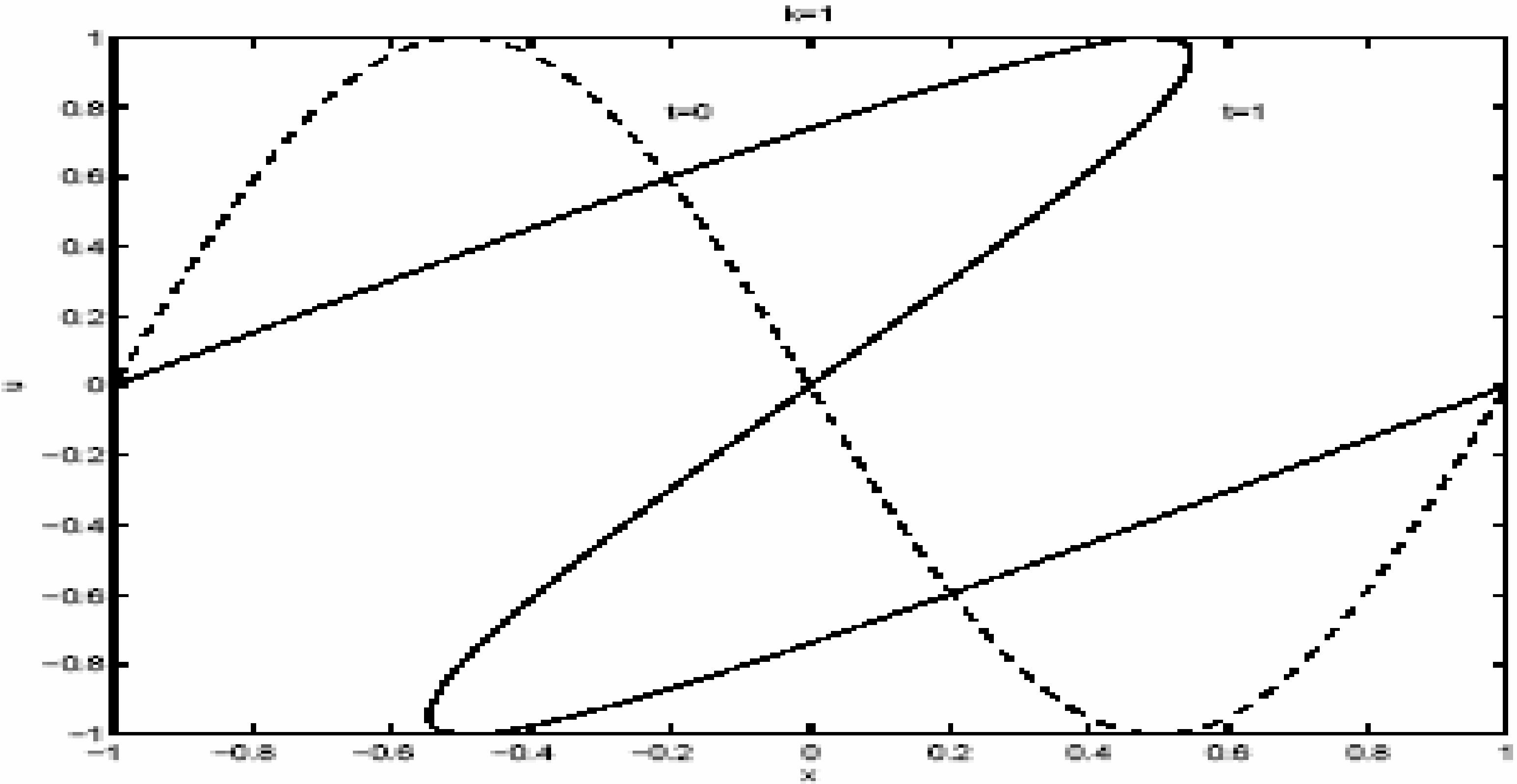
$$(|A|^2)_t + \nabla \cdot (|A|^2 \nabla S) = 0 \quad \text{transport equation}$$

Multivalued solutions

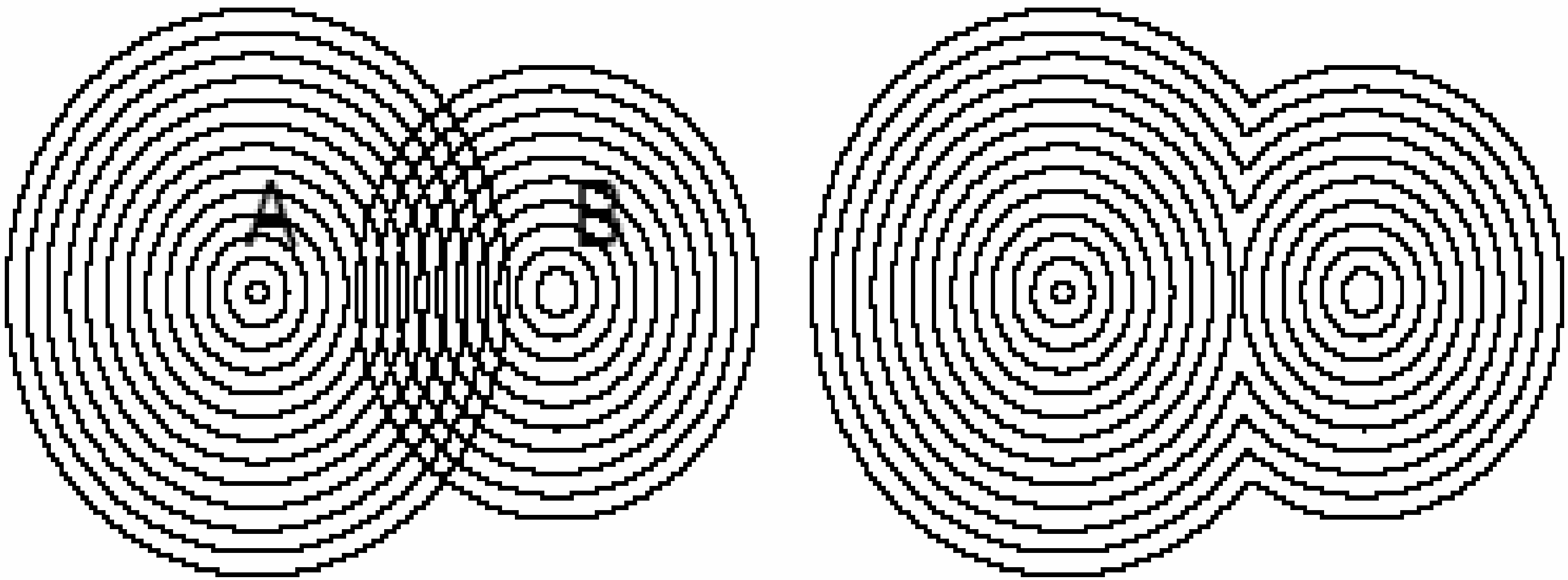
This limit is not valid at and beyond caustics; Multivalued solution (rather than the viscosity solution) is the correct one beyond caustics:

- *Homander, Maslov, Keller, Whitham, Flashka-Forest-MacLaughlin, Lax-Levemore, Majda-Majda-Zheng, Brenier, Gosse, Sparber-Markowich-Mauser, Jin-Li, Engquist-Runborg, Jin-Osher-Cheng-Liu-Tsai,* etc.

Shock vs. multivalued solution for velocity



Multivalued phase



(a) Correct solution (b) Eikonal equation

Semiclassical limit in the phase space

Wigner Transform

$$W^{\epsilon}(\mathrm{x}, \mathrm{k}) = \left(\frac{1}{2\pi}\right)^{d} \int_{R^d} e^{i\mathbf{k}\cdot\mathbf{y}} \psi(\mathrm{x} - \frac{\mathrm{y}}{2}) \overline{\psi}(\mathrm{x} + \frac{\mathrm{y}}{2}) d\mathrm{y}$$

where \overline{ψ} is the complex conjugate of ψ.

A convenient tool to study the semiclassical limit

(**Lions-Paul; Gerard, Markowich, Mauser, Poupaud**)

The semiclassical limit in phase space

As $\epsilon \to 0$, the limit Wigner equation is the **Liouville equation** in phase space

$$W_t + \mathbf{k} \cdot \nabla_{\mathbf{x}} W - \nabla V \cdot \nabla_{\mathbf{k}} W = 0$$

with the initial condition

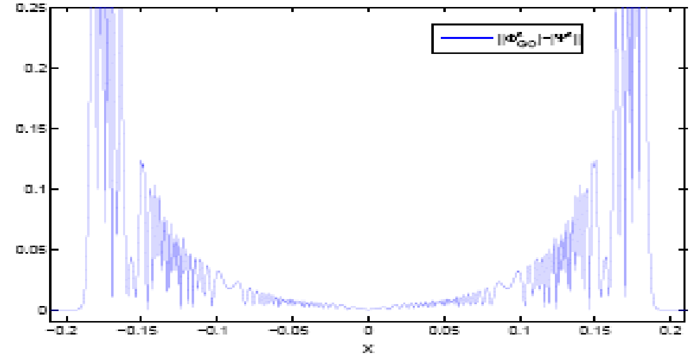
$$W(0, \mathbf{x}, \mathbf{k}) = |A_0(\mathbf{x})|^2 \delta(\mathbf{k} - \nabla S_0(\mathbf{x}))$$

Problem at caustics

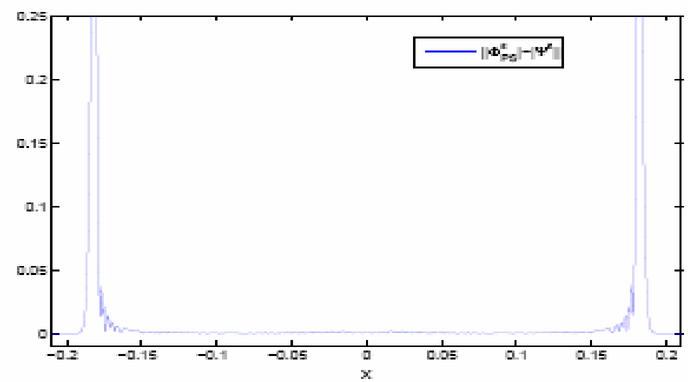
- The GO limit is invalid at caustics since the density blows up there – inaccurate for seismic imaging (*Hill*, Geophys, 1990, 2001)

Errors at caustics

- Semiclassical limit
  (Liouville equation)



- Semiclassical limit
  with phase-shift
  (Keller-Maslov index)
  (*Jin-Yang*, JSC 08)



Gaussian beam method

- More accurate at caustics

$$\varphi^{\varepsilon}_{la}(t, x, y_0) = A(t, \boldsymbol{y}) e^{iT(t,\boldsymbol{x},\boldsymbol{y})/\varepsilon}, \tag{2.1}$$

where $\boldsymbol{y} = \boldsymbol{y}(t, \boldsymbol{y}_0)$ and $T(t, \boldsymbol{x}, \boldsymbol{y})$ is given by the Taylor expansion

$$T(t, \boldsymbol{x}, \boldsymbol{y}) = S(t, \boldsymbol{y}) + \boldsymbol{p}(t, \boldsymbol{y}) \cdot (\boldsymbol{x} - \boldsymbol{y}) + \frac{1}{2}(\boldsymbol{x} - \boldsymbol{y})^{\top} M(t, \boldsymbol{y})(\boldsymbol{x} - \boldsymbol{y}) + O(|\boldsymbol{x} - \boldsymbol{y}|^3), \tag{2.2}$$

in which $(\boldsymbol{x} - \boldsymbol{y})^{\top}$ is the transpose of $(\boldsymbol{x} - \boldsymbol{y})$. Here $S \in \mathbb{R}$, $\boldsymbol{p} \in \mathbb{R}^n$, $A \in \mathbb{C}$, $M \in \mathbb{C}^{n \times n}$. The imaginary part of M will be chosen so that (2.1) has a Gaussian beam profile. We call (2.1) as the beam-shaped ansatz.

Lagrangian formulation

- Applying this ansatz to the Schrodinger equation, ignoring $O(\varepsilon^2)$ and $O(|x-y|^3)$ terms, one can derive the following set of ODEs (in the Lagrangian coordinate
  dy/dt=p) for M(t,y), S(t,y), and A(t,y):

Lagrangian formulation

$$
\begin{aligned}
\frac{\mathrm{d}\boldsymbol{y}}{\mathrm{d}t} &= \boldsymbol{p}, \\
\frac{\mathrm{d}\boldsymbol{p}}{\mathrm{d}t} &= -\nabla_{\boldsymbol{x}} V, \\
\frac{\mathrm{d}M}{\mathrm{d}t} &= -M^2 - \nabla_{\boldsymbol{x}}^2 V, \\
\frac{\mathrm{d}S}{\mathrm{d}t} &= \frac{1}{2}\,|\boldsymbol{p}|^2 - V, \\
\frac{\mathrm{d}A}{\mathrm{d}t} &= -\frac{1}{2}\big(\mathrm{Tr}(M)\big)A.
\end{aligned}
$$

$$
\begin{aligned}
\boldsymbol{y}(0, \boldsymbol{y}_0) &= \boldsymbol{y}_0, \\
\boldsymbol{p}(0, \boldsymbol{y}_0) &= \nabla_{\boldsymbol{x}} S_0(\boldsymbol{y}_0), \\
M(0, \boldsymbol{y}_0) &= \nabla_{\boldsymbol{x}}^2 S_0(\boldsymbol{y}_0) + iI, \\
S(0, \boldsymbol{y}_0) &= S_0(\boldsymbol{y}_0), \\
A(0, \boldsymbol{y}_0) &= A_0(\boldsymbol{y}_0).
\end{aligned}
$$

Properties (following *Ralston* '82)

Theorem 2.1 *Let $P(t, \boldsymbol{y}(t, \boldsymbol{y}_0))$ and $R(t, \boldsymbol{y}(t, \boldsymbol{y}_0))$ be the (global) solutions of the equations*

$$\frac{\mathrm{d}P}{\mathrm{d}t} = R, \quad \frac{\mathrm{d}R}{\mathrm{d}t} = -(\nabla^2_{\boldsymbol{x}} V)P, \tag{2.17}$$

with initial conditions

$$P(0, \boldsymbol{y}_0) = I, \ R(0, \boldsymbol{y}_0) = M(0, \boldsymbol{y}_0), \tag{2.18}$$

where matrix I is the identity matrix and $Im(M(0, \boldsymbol{y}_0))$ is positive definite. Assume $M(0, \boldsymbol{y}_0)$ is symmetric, then for each initial position $\boldsymbol{y}_0$, we have the following results:

1. *$P(t, \boldsymbol{y}(t, \boldsymbol{y}_0))$ is invertible for all $t > 0$.*
2. *The solution to equation (2.14) is given by*

$$M(t, \boldsymbol{y}(t, \boldsymbol{y}_0)) = R(t, \boldsymbol{y}(t, \boldsymbol{y}_0))P^{-1}(t, \boldsymbol{y}(t, \boldsymbol{y}_0)) \tag{2.19}$$

3. *$M(t, \boldsymbol{y}(t, \boldsymbol{y}_0))$ is symmetric and $Im(M(t, \boldsymbol{y}(t, \boldsymbol{y}_0)))$ is positive definite for all $t > 0$.*

Density does not blow up

- Moreover, $A^2 \det(P^{-1})$ is conserved in time, thus $|A|$ is always finite if it is initially (note $P_0=I$)

- Lagrangian Gaussian beams for waves:

  Cerveny-Popov-Psencik ('82), *Hill* ('90, '01), *Tanushev-Qian-Ralston-Leung-Burridge* ('07-), *Matamed-Runborg* ('08)
- Gaussian beams in quantum chemistry: *Heller,* etc.
- Laser physics, etc.

The Lagrangian beam summation

$$\Phi_{la}^{\varepsilon}(t,x) = \int_{\mathbb{R}^n} \left(\frac{1}{2\pi\varepsilon}\right)^{\frac{n}{2}} r_\theta(x - y(t,y_0))\varphi_{la}^{\varepsilon}(t,x,y_0)\mathrm{d}y_0. \qquad ($$

The discrete form of (2.28) in a bounded domain is given by

$$\Phi_{la}^{\varepsilon}(t,x) = \sum_{j=1}^{N_{y_0}} \left(\frac{1}{2\pi\varepsilon}\right)^{\frac{n}{2}} r_\theta(x - y(t,y_0^j))\varphi_{la}^{\varepsilon}(t,x,y_0^j)\Delta y_0, \qquad ($$

The Eulerian formulation

- Recall the semiclassical limit of the linear Schrodinger equation is (via Wigner transform) is the Liouville equation:

$$\boldsymbol{L}\, f = \partial_t f + \xi \cdot \nabla_y f - \nabla_y V \cdot \nabla_\xi f = 0$$

$$f(0, x, \xi) = |A_0|^2\, \delta(\xi - \nabla_y S_0)$$

Level set method

- This initial value problem can be solved by (ϕ is the level set function whose zero gives multivalued $u=\nabla_x S$)

$$\mathbf{\mathit{L}}\, \phi = 0, \quad \phi \in R^n$$
$$\phi(0, x, \xi)=\xi - \nabla_x S_0$$

(ϕ is the level set function whose zero gives multivalued $u=\nabla_x S$)

$$\mathbf{\mathit{L}}\, \psi = 0, \quad \psi \in R$$
$$\psi(0, x, \xi)=|A|^2$$

$$f = \psi\, \delta\, (\phi)$$

(*Jin-Osher*, *Cheng-Liu-Osher, Jin-Liu-Osher-Tsai, 03-06*)

Eulerian method for the Hessian of S

- Leung, Qian, Burridge '07, '08

$\boldsymbol{L}\, R = -\,(\nabla^2_y V)\, P; \qquad R \in C^{n\times n}$

$\boldsymbol{L}\, P = R \qquad\qquad P \in C^{n\times n}$

$M = R\, P^{-1}$

This requires to solve $2n^2$ complex-valued, inhomogeneous Liouville equations

A key observation

Recall the level set equation

$$\boldsymbol{L}\,\phi = 0 \qquad (*)$$

by taking the y and ξ-derivatives:

$$\boldsymbol{L}\,(\nabla_y \phi) = \nabla^2_y V \nabla_\xi \phi, \qquad \boldsymbol{L}\,(\nabla_\xi \phi) = -\nabla_y \phi$$

and comparing these equations with:

$$\boldsymbol{L}\,R = -(\nabla^2_y V)\,P; \quad \boldsymbol{L}\,P = R$$

we find that $R = -\nabla_y \phi, \;\; P = \nabla_\xi \phi$

provides they are given the same initial data and ϕ is made complex

Thus $M = -\nabla_y \phi\,(\nabla_\xi \phi)^{-1}$

so the 2n^2 complex-valued R-P equations are redundant, all we need is to use complex ϕ that solves (*), and then compute its partial derivatives to get M !

Our level set method

- Solve $\boldsymbol{L}\,\phi = 0 \quad \phi \in C^n$

  with $\phi(0,y,\xi)=-i\,y+(\xi-\nabla_y S_0)$

  (note $Re(\phi)=0$ at $\xi=u=\nabla_y S$)
- The above Liouville fluxes give $\nabla_y \phi$ and $\nabla_\xi \phi$ thus M
- From u one can obtain S (*Gosse, Jin-Yang*)
- Solves $\boldsymbol{L}\,\psi=0, \ \psi\in R$

  with $\psi(0, y, \xi)=|A_0|^2$

  then $A(t, x)= (\det(\nabla_\xi \phi)^{-1})\,\psi)^{1/2}$ (principle value)

The complexity is comparable to the level set method for semiclassical limit; only now that $\phi \in C^n$ rather than R^n

The method is well-defined!

- The density A does not blow up!

Theorem 3.2 *Let* $\phi = \phi(t, \boldsymbol{y}, \boldsymbol{\xi}) \in \mathbb{C}$ *be the solution of (3.5) with initial data (3.14). Then we have the following: properties*

1. $\nabla_{\boldsymbol{\xi}}\phi$ *is non-degenerate for all* $t > 0$.

2. $Im\left(-\nabla_{\boldsymbol{y}}\phi(\nabla_{\boldsymbol{\xi}}\phi)^{-1}\right)$ *is positive definite for all* $t > 0$, $\boldsymbol{y}, \boldsymbol{\xi} \in \mathbb{R}^n$.

The Eulerian Gaussian beam summation

Define

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

where

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

then the wave function is constructed via the following Eulerian Gaussian beam summation formula:

$$\Phi_{eu}^{\varepsilon}(t,\boldsymbol{x}) = \int_{\mathbb{R}^n}\int_{\mathbb{R}^n}\left(\frac{1}{2\pi\varepsilon}\right)^{\frac{n}{2}} r_\theta(\boldsymbol{x}-\boldsymbol{y})\varphi_{eu}^{\varepsilon}(t,\boldsymbol{x},\boldsymbol{y},\boldsymbol{\xi})\Pi_{j=1}^{n}\delta(\mathrm{Re}[\phi_j])\mathrm{d}\boldsymbol{\xi}\mathrm{d}\boldsymbol{y}, \tag{3.20}$$

in which $r_\theta \in C_0^\infty(\mathbb{R}^n)$, $r_\theta \geq 0$ is a truncation function with $r_\theta \equiv 1$ in a ball of radius $\theta > 0$ about the origin and δ is the Dirac delta function. The

Evaluation of the singular integral

- This (singular) integral can be written as

$$\Phi^{\varepsilon}_{eu}(t,\boldsymbol{x}) = \int_{\mathbb{R}^n} \left(\frac{1}{2\pi\varepsilon}\right)^{\frac{n}{2}} r_\theta(\boldsymbol{x}-\boldsymbol{y}) \sum_k \frac{\varphi^{\varepsilon}_{eu}(t,\boldsymbol{x},\boldsymbol{y},\boldsymbol{u}_k)}{|\det(\mathrm{Re}[\nabla_{\boldsymbol{\xi}}\phi]_{\boldsymbol{\xi}=\boldsymbol{u}_k})|} \mathrm{d}\boldsymbol{y}, \qquad (3.21)$$

Since $\det\left(\mathrm{Re}[\nabla_{\boldsymbol{\xi}}\phi]\right) = 0$ at caustics, a direct numerical integration of (3.21) loses accuracy around singularities (see Example 3 in Section 5 for the detailed numerical demonstrations). To get a better accuracy, we split (3.21) into two parts

$$I_1 = \sum_k \int_{L_1} \left(\frac{1}{2\pi\varepsilon}\right)^{\frac{n}{2}} r_\theta(\boldsymbol{x}-\boldsymbol{y}) \frac{\varphi^{\varepsilon}_{eu}(t,\boldsymbol{x},\boldsymbol{y},\boldsymbol{u}_k)}{|\det(\mathrm{Re}[\nabla_{\boldsymbol{\xi}}\phi]_{\boldsymbol{\xi}=\boldsymbol{u}_k})|} \mathrm{d}\boldsymbol{y}, \qquad (3.22)$$

$$I_2 = \sum_k \int_{L_2} \left(\frac{1}{2\pi\varepsilon}\right)^{\frac{n}{2}} r_\theta(\boldsymbol{x}-\boldsymbol{y}) \frac{\varphi^{\varepsilon}_{eu}(t,\boldsymbol{x},\boldsymbol{y},\boldsymbol{u}_k)}{|\det(\mathrm{Re}[\nabla_{\boldsymbol{\xi}}\phi]_{\boldsymbol{\xi}=\boldsymbol{u}_k})|} \mathrm{d}\boldsymbol{y}, \qquad (3.23)$$

where

$$L_1 = \left\{\boldsymbol{y} \middle| \left|\det(\mathrm{Re}[\nabla_{\boldsymbol{p}}\phi](t,\boldsymbol{y},\boldsymbol{p}_j))\right| \geq \tau\right\},$$

$$L_2 = \left\{\boldsymbol{y} \middle| \left|\det(\mathrm{Re}[\nabla_{\boldsymbol{p}}\phi](t,\boldsymbol{y},\boldsymbol{p}_j))\right| < \tau\right\},$$

with τ being a small parameter.

In our numerical simulations, I_1 is treated using the trapezoid quadrature rule, while the singular integral I_2 is treated by the semi-Lagrangian method introduced in [19]. For convenience we summarize the semi-Lagrangian method here. Suppose we take a number of discrete beams centered at $\boldsymbol{y}^j,\ j = 1, \cdots, M_y$ with the velocity $\boldsymbol{u}_k^j$ on the contour, the idea is to trace each individual $(\boldsymbol{y}^j, \boldsymbol{u}_k^j)$ back to the initial position $(\boldsymbol{y}_0^j, \boldsymbol{u}_{k,0}^j)$ using (2.12)-(2.13) with $t \to -t$, then determine the weight function $\omega(\boldsymbol{y}_0^j)$ for it. For example in one dimension, if the two adjacent points of y_0^j are y_0^{j1} and y_0^{j2} such that $y_0^{j1} < y_0^j < y_0^{j2}$, then $\omega(y_0^j) = (y_0^{j2} - y_0^{j1})/2$ (see Page 68 in [19] for details). In this process one gets rid of the singular term by noticing that $\mathrm{d}\boldsymbol{y}_0 = \dfrac{1}{|\det(\mathrm{Re}[\nabla_{\boldsymbol{\xi}}\phi]_{\boldsymbol{\xi}=\boldsymbol{u}_k})|}\mathrm{d}\boldsymbol{y}$. The discrete form of (3.23) reads as

$$\widetilde{I}_2 = \sum_{j=1}^{M_y} \sum_k \left(\frac{1}{2\pi\varepsilon}\right)^{\frac{n}{2}} r_\theta(\boldsymbol{x} - \boldsymbol{y}^j)\varphi_{eu}^{\varepsilon}(t, \boldsymbol{x}, \boldsymbol{y}^j, \boldsymbol{u}_k^j)\omega(\boldsymbol{y}_0^j). \tag{3.24}$$

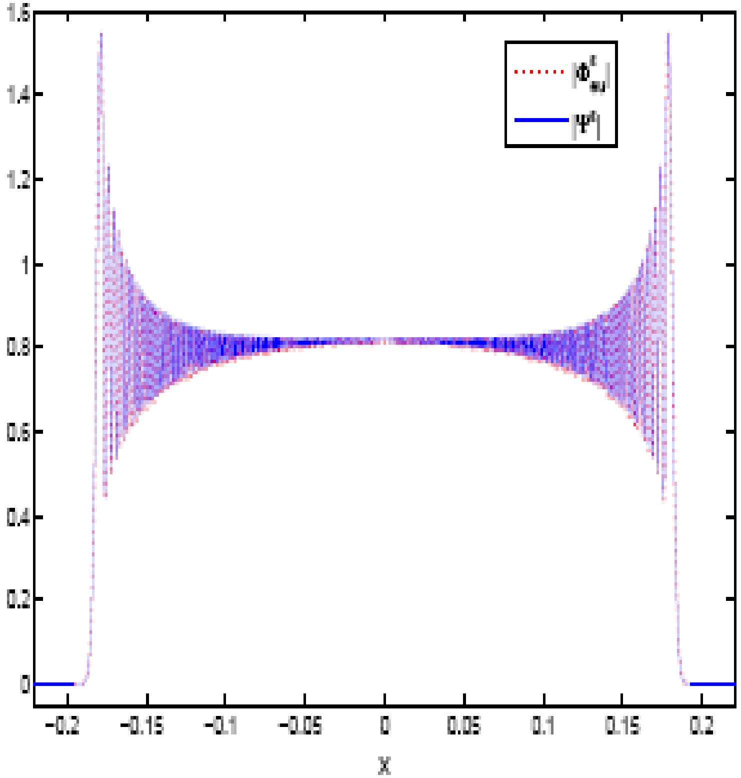
- Note we use the semi-Lagrangian method only locally (around caustics). This maintains the efficiency and accuracy of the Eulerian method

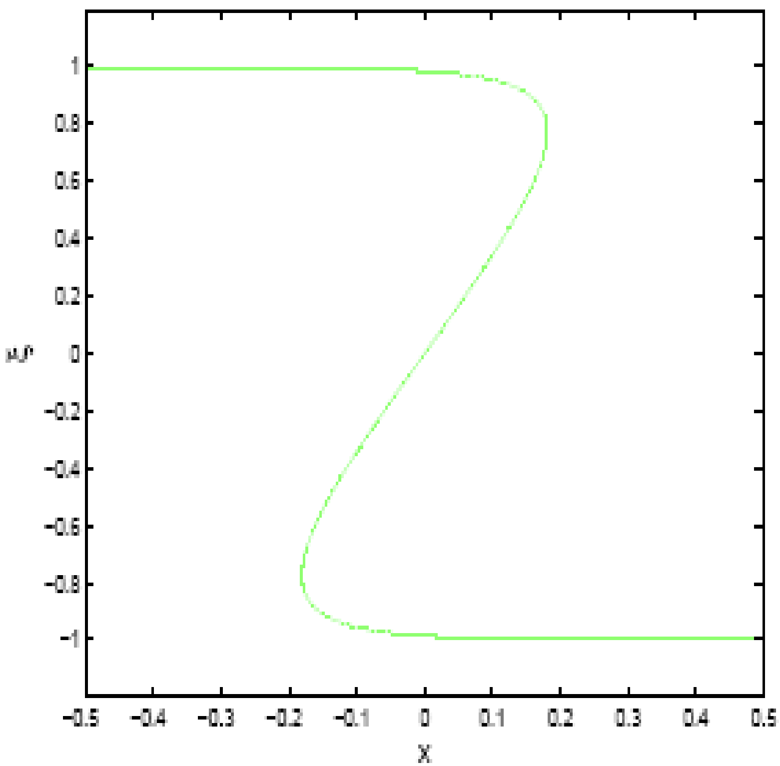
Computational cost

- Use Δ y= $O(\varepsilon^{1/2})$, Δ t= $O(\varepsilon^{1/2})$
  cost: $O(\varepsilon^{-(n+1)/2} \ln \varepsilon^{-1/2})$

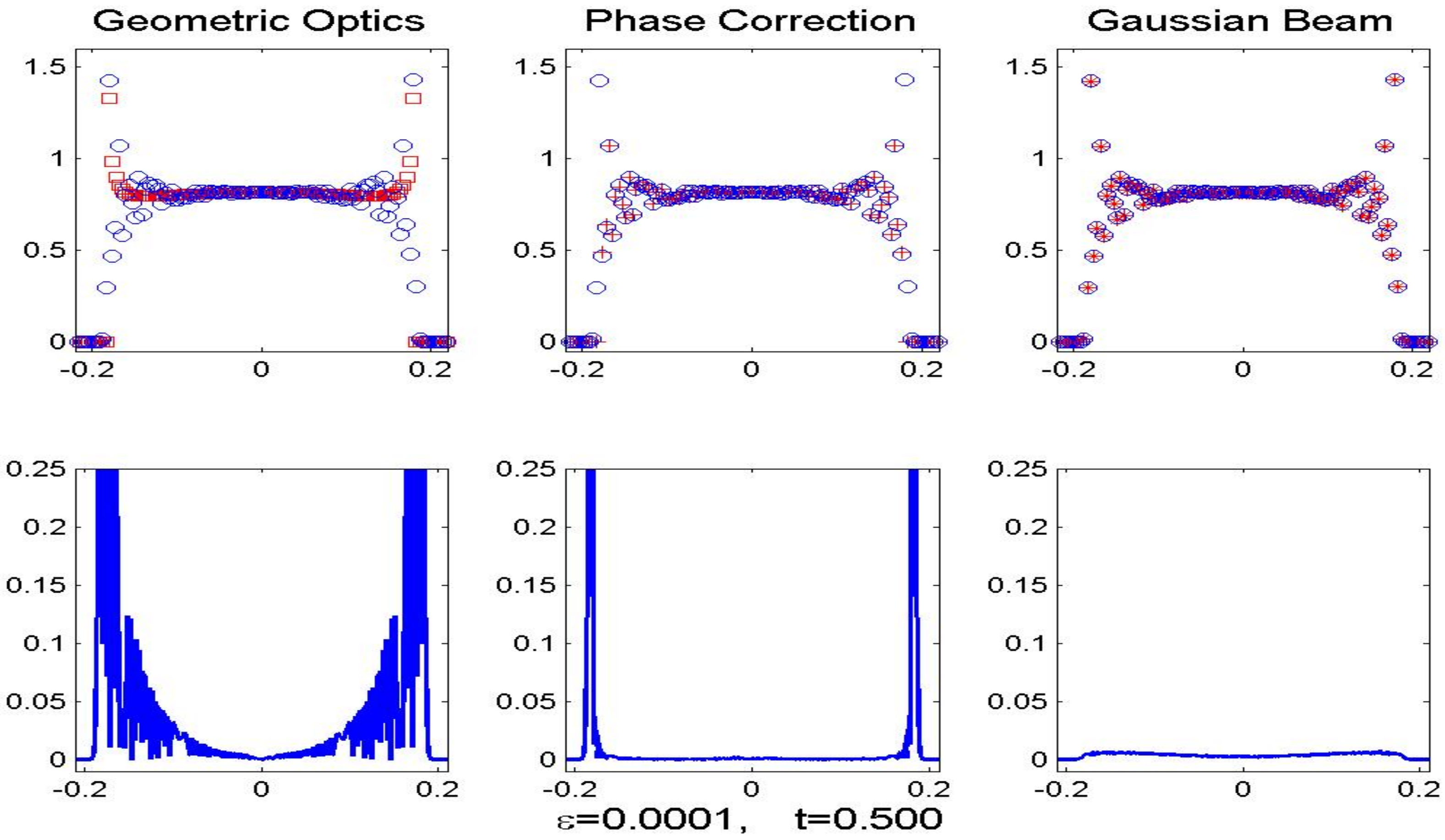
- The direct simulation of the linear Schrodinger equation (via time-splitting spectral): Δ y= $O(\varepsilon)$, Δ t= $O(1)$
  cost: $O(\varepsilon^{-n})$

1d numerical example ($\varepsilon=10^{-4}$)

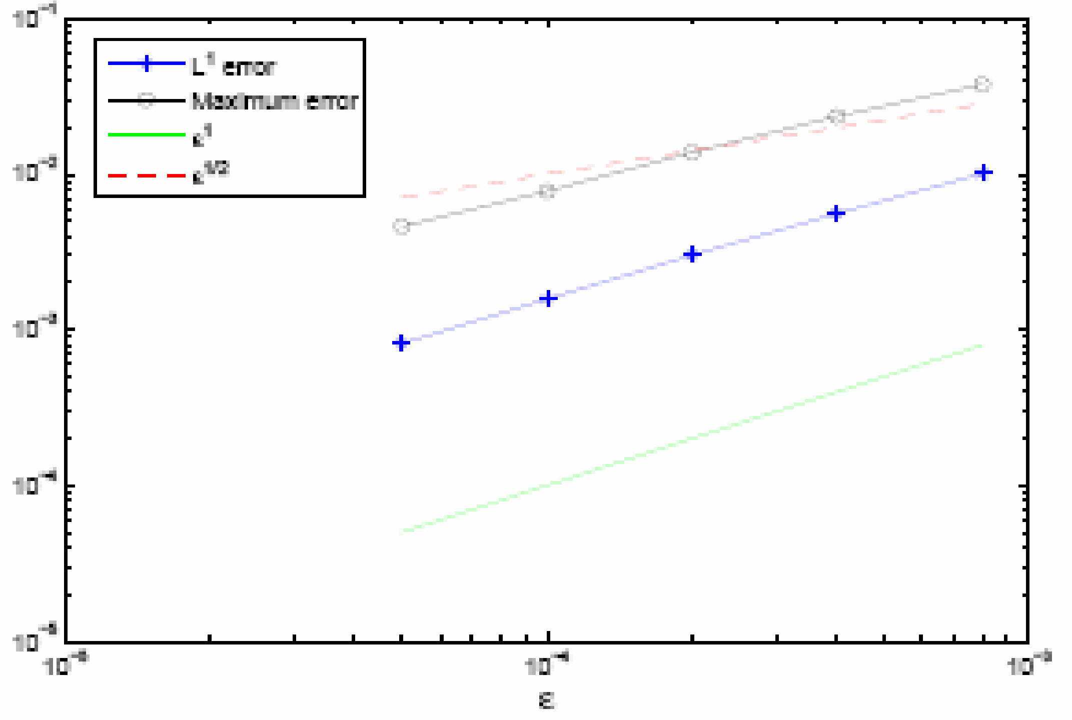




Error comparison



Error rate of Gaussian beam



An 2D example

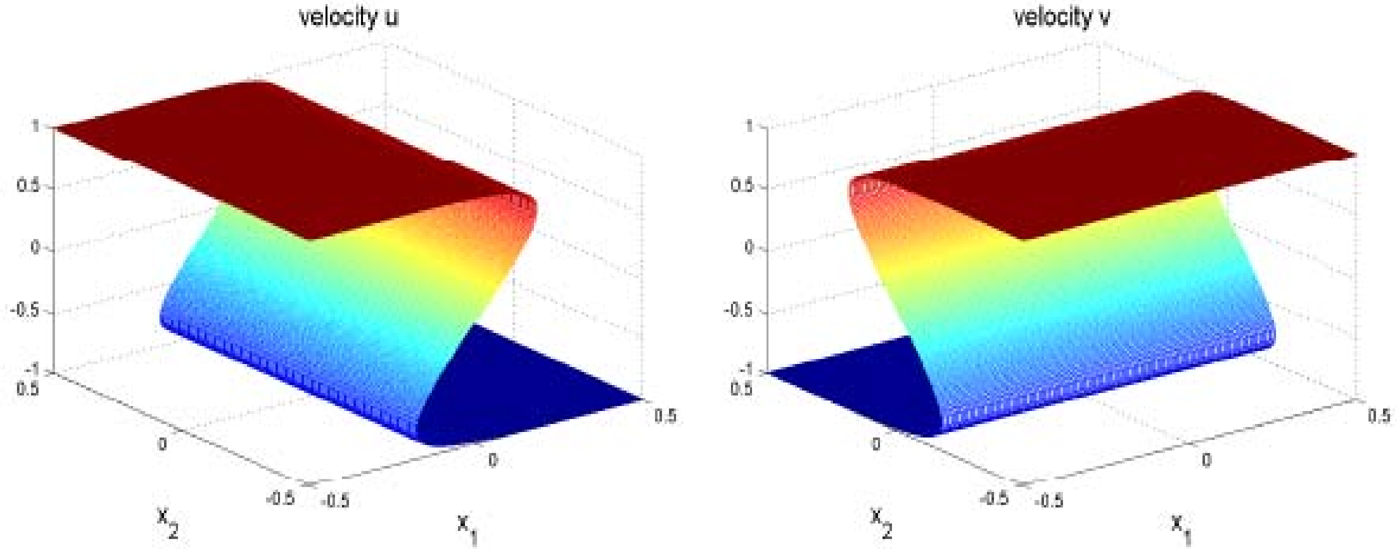


Figure 9: Example 4, the two components of the multivalued velocity at $t = 0.5$.

Wave amplitude

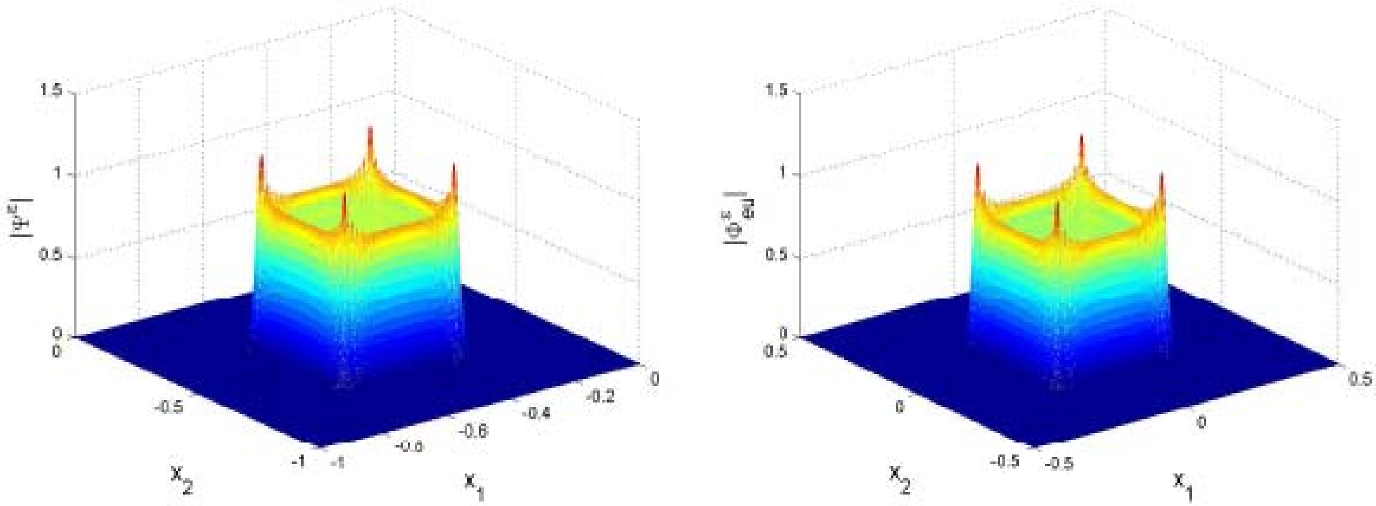


Figure 10: Example 4, the comparison of the wave amplitude between the Schrödinger solution Ψ^ε on the left and the Eulerian beams solution Φ^ε_{eu} on the right for $\varepsilon = 0.001$ and at $t = 0.5$.

Maximum error ~ $O(\varepsilon^{1/2})$

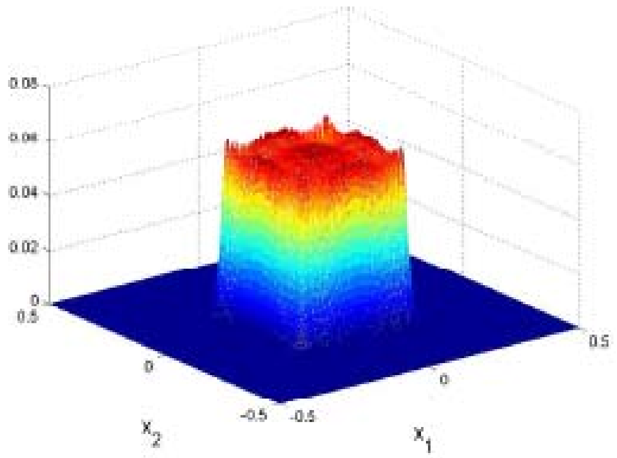


Figure 11: Example 4, the error plot of $||\Psi^\varepsilon| - |\Phi^\varepsilon_{eu}||$.

Schrodinger equation with periodic potentials

- Joint with *Wu-Yang-Huang*

$$i\varepsilon\frac{\partial\Psi^\varepsilon}{\partial t} = -\frac{\varepsilon^2}{2}\Delta\Psi^\varepsilon + V_\Gamma\left(\frac{x}{\varepsilon}\right)\Psi^\varepsilon + U(x)\Psi^\varepsilon, \quad x\in\mathbb{R}^n,$$

- Motion of electrons in periodic media generated by ionic cores
- Photonic crystal; Bose-Einstein condensations, elastic waves, etc.

Bloch decomposition

$$H(k,z) := \frac{1}{2}(-i\partial_z + k)^2 + V_\Gamma(z),$$
$$H(k,z)\chi_m(k,z) = E_m(k)\chi_m(k,z),$$
$$\chi_m(k,z+2\pi) = \chi_m(k,z),\ z \in \mathbb{R},\ k \in \mathcal{B}.$$

- $E_m(k)$: m-the energy band
- $\chi_m(k)$: corresponding eigenfunctions

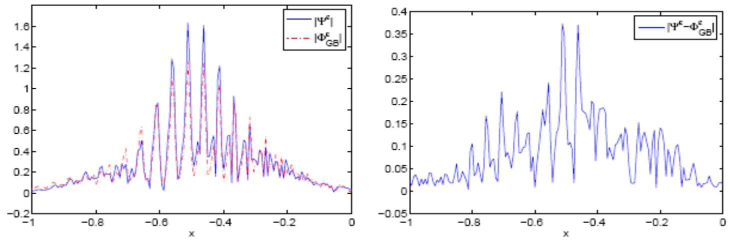
Semiclassical limit

- When $\varepsilon \rightarrow 0$, the semiclassical limit is the superposition of Liouville equation for each Bloch band
- Analytic study of Gaussian beam for Bloch electron (*Dimassi-Guillot-Ralston MPAG 06*)
- Use of Bloch basis for numerical computation (*Huang-Jin-Markowich-Sparber, SISC 07*) better than Fourier spectral method when resolving oscillations
- Computation of the limit using level set: (*Liu-Wang, JCP 09)*

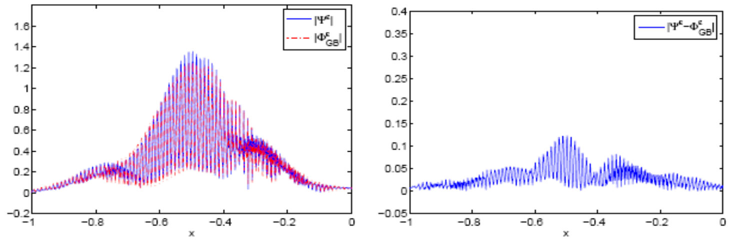
Bloch-decomposition based Gaussian beam method

- We combined the Bloch decomposition with our Eulerian Gaussian beam methods
- important since every band may generate caustics: there are many caustics!

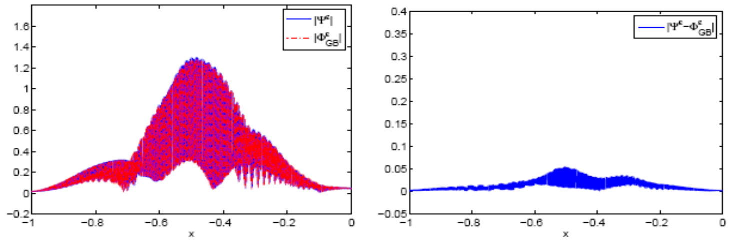
Mathieu's model: $V_{\Gamma}(x)=\cos(x)$



(a) $\varepsilon = \frac{1}{128}$



(b) $\varepsilon = \frac{1}{512}$



(c) $\varepsilon = \frac{1}{2048}$

Figure 3: Example 2, the Schrödinger solution $|\Psi^\varepsilon|$ versus the Gaussian beams solution $|\Phi^\varepsilon_{GB}|$ at $\varepsilon = \frac{1}{128}, \frac{1}{512}, \frac{1}{2048}$. The left figures are the comparisons of the wave amplitude at $t = 0.2$; the right figures plot the errors $|\Psi^\varepsilon - \Phi^\varepsilon_{GB}|$.

Extensions

- Schrodinger-Poisson equations
- Interface (partial transmission/reflection)
- Elastic waves through periodic arrays
- Quantum chemistry applications (surface hopping etc)

Open problems

- Can one derive these complex valued Liouville equations from the Schrodinger equations using Wigner type of transformation?
- Using Gaussian beam ansatz, can one derive new quantum hydrodynamic equations (QHD) that are more accurate than the the QHD using Madelung transformation?
- What kind of regularizations does the Gaussian profile provide to the QHD?

Conclusions

- A new Eulerian Gaussian beam method

  1) in dimension n, based on solving only n complex-valued and 1 real-valued homogeneous Liouville equation

  (solving 7 homogeneous equations in 3D rather than 40 inhomogeneous equations)

  2) Gaussian beam method now as easy as geometric optics (for the time evolution)

- Future applications in many interesting problems in high frequency waves and quantum chemistry