Eulerian Gaussian beam method in quantum mechanics

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Outline

1. Schrödinger equation and its semiclassical limit
2. Gaussian beam method - Lagrangian formulation
3. Gaussian beam method - Eulerian formulation
4. Numerical results
5. Applications in quantum mechanics
The time-dependent one-body Schrödinger equation:

\[
i\varepsilon \frac{\partial \psi^\varepsilon}{\partial t} + \frac{\varepsilon^2}{2} \Delta \psi^\varepsilon - V(x) \psi^\varepsilon = 0, \quad x \in \mathbb{R}^n,
\]

\[
\psi^\varepsilon(t, x) = A(t, x) e^{i S(t, x)/\varepsilon}
\]

It models: single electron in atoms, KS density functional theory, Molecule Orbital theory ...

Numerical difficulties: \(\psi^\varepsilon(t, x)\) is oscillatory of wave length \(O(\varepsilon)\).

<table>
<thead>
<tr>
<th>Methods</th>
<th>Mesh size</th>
<th>Time step</th>
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<tbody>
<tr>
<td>Finite difference (^1)</td>
<td>(o(\varepsilon))</td>
<td>(o(\varepsilon))</td>
</tr>
<tr>
<td>Time splitting spectral (^2)</td>
<td>(O(\varepsilon))</td>
<td>(\varepsilon)-indep.</td>
</tr>
</tbody>
</table>

\(^1\) Markowich, Pietra, Pohl and Stimming

\(^2\) Bao, Jin and Markowich
Geometric optics - WKB analysis

WKB ansatz
\[ \psi^\varepsilon(t, x) = A(t, x)e^{iS(t, x)/\varepsilon}, \]

Eikonal
\[ S_t + \frac{1}{2} |\nabla S|^2 + V(x) = 0, \]

Transport
\[ \rho_t + \nabla \cdot (\rho \nabla S) = 0, \quad \rho(t, x) = |A(t, x)|^2. \]

Eikonal (Hamilton-Jacobi type) \(\Rightarrow\) singularity (caustics)

Figures from the review paper of Engquist and Runborg:
Semiclassical limit + phase correction

Theorem 1. If $V(x)$ is constant, by the stationary phase method we have, away from caustics,

$$
\psi^\varepsilon(x, t) \sim \sum_{k=1}^{K} \frac{A_0(y_k)}{\sqrt{1 + tD^2S_0(y_k)}} \exp \left( \frac{i}{\varepsilon} S(\xi_k, y_k) + \frac{i\pi}{4} \mu_k \right)
$$

where the phase

$$
S(\xi, y) = \xi \cdot x - \xi \cdot y - (1/2) |\xi|^2 t + S_0(y),
$$

has finitely many ($K < \infty$) stationary phases $\xi_k$ and $y_k$:

$$
\xi_k = \nabla S_0(y_k), \quad y_k = x - t\nabla S_0(y_k),
$$

$D^2S_0$ is the Hessian matrix, and $\mu_k = \text{sgn}(D^2S(\xi_k, y_k))$ is the Keller-Maslov index of the $k$th branch.
Gaussian beam method - motivation

Problems of the semiclassical limit: invalid at caustics

1. the density $\rho(t, x) \rightarrow \infty$ in the transport equation,
2. $1 + tD^2 S_0(y_k)$ is singular in the stationary phase method.

Computation around caustics is important in many applications, for example:

- Seismic imaging
- Single-slit diffraction

Gaussian beam method, developed by Popov, allows accurate computation around caustics.
Beam-shaped ansatz

The key idea of the Gaussian beam method is to complexify the phase function $S(t, x)$:

$$\varphi^\varepsilon_{la}(t, x, y_0) = A(t, y) e^{i T(t, x, y)/\varepsilon},$$

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

beam center: $$\frac{dy}{dt} = p(t, y), \quad y(0) = y_0.$$

Here $S \in \mathbb{R}$, $p \in \mathbb{R}^n$, $A \in \mathbb{C}$, $M \in \mathbb{C}^{n \times n}$. The imaginary part of $M$ will be chosen so that $\varphi^\varepsilon_{la}$ has a Gaussian beam profile.
Lagrangian formulation

Apply the beam-shaped ansatz to the Schrödinger equation:

<table>
<thead>
<tr>
<th>Equation</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \frac{dy}{dt} )</td>
<td>center: ( p ),</td>
</tr>
<tr>
<td>( \frac{dp}{dt} )</td>
<td>velocity: ( -\nabla_y V ),</td>
</tr>
<tr>
<td>( \frac{dM}{dt} )</td>
<td>Hessian: ( -M^2 - \nabla^2_y V ),</td>
</tr>
<tr>
<td>( \frac{dS}{dt} )</td>
<td>phase: ( \frac{1}{2}</td>
</tr>
<tr>
<td>( \frac{dA}{dt} )</td>
<td>amplitude: ( -\frac{1}{2} (\text{Tr}(M)) A ).</td>
</tr>
</tbody>
</table>

The first two ODEs are called ray tracing equations, and the Hessian \( M \) satisfies the Riccati equation.
Validity at caustics and beam summation

\( M, A \) could be solved via the dynamic ray tracing equations:

\[
\begin{align*}
\frac{dP}{dt} &= R, \\
\frac{dR}{dt} &= -(\nabla_\mathbf{y}^2 V)P,
\end{align*}
\]

\[
M = RP^{-1}, \quad A = \left( (\det P)^{-1} A_0^2 \right)^{1/2},
\]

\[
R(0) = M(0) = \nabla_\mathbf{y}^2 S_0(\mathbf{y}) + iI, \quad P(0) = I.
\]

Ralston (82, wave-type eqn), Hagedorn (80, Schrödinger) proved the validity of the Gaussian beam solution at caustics:

- \( P \) complexified \( \Rightarrow \) \( P \) never singular \( \Rightarrow \) \( A \) always finite.

The Gaussian beam summation solution (Hill, Tanushev):

\[
\Phi_{la}^\varepsilon(t, \mathbf{x}) = \int_{\mathbb{R}^n} \left( \frac{1}{2\pi \varepsilon} \right)^{n/2} r_\theta(\mathbf{x} - \mathbf{y}(t, \mathbf{y}_0)) \varphi_{la}^\varepsilon(t, \mathbf{x}, \mathbf{y}_0) d\mathbf{y}_0.
\]
Level set method

The level set method has been developed to compute the **semiclassical limit** of the Schrödinger equation. (Jin-Liu-Osher-Tsai)

The idea is to build the velocity \( u = \nabla_y S \) into the intersection of zero level sets of phase-space functions \( \phi_j(t, y, \xi) \), i.e.

\[
\phi_j(t, y, \xi) = 0, \quad \text{at} \quad \xi = u(t, y), \quad j = 1, \ldots, n.
\]

\( \phi = (\phi_1, \ldots, \phi_n) \) satisfies the Liouville equation:

\[
\partial_t \phi + \xi \cdot \nabla_y \phi - \nabla_y V \cdot \nabla_\xi \phi = 0.
\]
Eulerian formulation I - semiclassical limit

As shown by Jin, Liu, Osher and Tsai,

velocity: \( \mathcal{L}\phi = 0, \)

phase: \( \mathcal{L}S = \frac{1}{2} |\xi|^2 - V, \)

amplitude: \( \mathcal{L}A = \frac{1}{2} \text{Tr} \left( (\nabla_\xi \phi)^{-1} \nabla_y \phi \right) A. \)
Eulerian formulation II - semiclassical limit

If one introduces the new quantity

\[ f(t, y, \xi) = A^2(t, y, \xi) \det(\nabla_{\xi}\phi), \]

then \( f(t, y, \xi) \) satisfies the Liouville equation

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

The level set method for the semiclassical limit still suffers caustics where \( \det(\nabla_{\xi}\phi) = 0 \).

Motivated by the Gaussian beam method, we need to complexify the Liouville equation for \( \phi \).
Construct the Hessian function

\[
\frac{\partial}{\partial y} \phi(t, y, u(t, y)) = 0 \quad \Rightarrow \quad \nabla^2_y S = \nabla_y u = -\nabla_y \phi (\nabla_\xi \phi)^{-1}
\]

Recall the Lagrangian formulation:

\[M = R P^{-1}\]

Conjecture:

\[R = -\nabla_y \phi, \quad P = \nabla_\xi \phi.\]

Complex \(R\) and \(P\) \(\implies\) complex \(\phi\)
Conjecture verification

The first two lines are equivalent to each other once they have the same initial conditions:

\[
\phi_0(y, \xi) = -iy + (\xi - \nabla_y S_0)
\]

\[
R(0) = \nabla_y^2 S_0(y) + iI, \quad P(0) = I.
\]
**Eulerian formulation - Gaussian beam**

<table>
<thead>
<tr>
<th>Step 1:</th>
<th>( \mathcal{L} \phi = 0 ), ( \phi_0(y, \xi) = -iy + (\xi - \nabla_y S_0) ).</th>
</tr>
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<tr>
<td>Step 2:</td>
<td>compute ( \nabla_y \phi ) and ( \nabla_\xi \phi ), ( M = -\nabla_y \phi (\nabla_\xi \phi)^{-1} ).</td>
</tr>
<tr>
<td>Step 3:</td>
<td>solve ( S ) either by ( \mathcal{L} S = \frac{1}{2}</td>
</tr>
<tr>
<td>Step 4:</td>
<td>( \mathcal{L} f = 0 ), ( f_0(t, y, \xi) = A_0(y)^2 ),</td>
</tr>
<tr>
<td>Step 5:</td>
<td>( A = (\det(\nabla_\xi \phi)^{-1} f)^{1/2} ).</td>
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Parallel to Ralston’s proofs,
\[ \phi \text{ complexified} \Rightarrow \nabla_\xi \phi \text{ non-degenerate} \Rightarrow A \text{ never blows up} \]
Eulerian Gaussian beam summation

Define

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

where

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

Eulerian Gaussian beam summation formula:

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

\( r_{\theta} \) is a truncation function with \( r_{\theta} \equiv 1 \) in a ball of radius \( \theta > 0 \) about the origin.
Computing the summation integral

**Method 1:** Discretized delta function integral (Wen, in 1D).

**Method 2:** Integrate $\xi$ out first:

\[
\Phi_{e\xi u}^\varepsilon(t, x) = \int_{\mathbb{R}^n} \left( \frac{1}{2\pi\varepsilon} \right)^{n/2} r_\theta(x - y) \sum_k \frac{\varphi_{e\xi u}^\varepsilon(t, x, y, u_k)}{|\text{det}(\text{Re}[\nabla_\xi \phi]|_{\xi = u_k})|} dy,
\]

where $u_k$, $k = 1, \cdots, K$ are the velocity branches.

**Problem:** $\text{det}(\text{Re}[\nabla_\xi \phi]) = 0$ at caustics.

**Solution:** Split the integral into two parts:

\[
L_1 = \left\{ y \mid \left| \text{det}(\text{Re}[\nabla_p \phi](t, y, p_j)) \right| \geq \tau \right\}
\]

\[
L_2 = \left\{ y \mid \left| \text{det}(\text{Re}[\nabla_p \phi](t, y, p_j)) \right| < \tau \right\}
\]

The integration on $L_1$ is regular; the integration on $L_2$ could be solved by the semi-Lagrangian method (Leung-Qian-Osher).
Efficiency and accuracy

**Efficiency:**

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<td>Gaussian beam</td>
<td>$O(\sqrt{\varepsilon})$</td>
<td>$O(\varepsilon^2)^{\frac{2}{p}}$</td>
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$p$: numerical orders of accuracy in time.

**Accuracy:** $O(\sqrt{\varepsilon})$ in caustic case, $O(\varepsilon)$ in no caustic case.

It could be easily generalized to higher order Gaussian beam methods by including more terms in the asymptotic ansatz.

Tanushev-Runborg-Motamed
1D example

Free motion particles with zero potential \( V(x) = 0 \). The initial conditions for the Schrödinger equation are given by

\[
A_0(x) = e^{-25x^2}, \quad S_0(x) = -\frac{1}{5} \log(2 \cosh(5x)).
\]

which implies that the initial density and velocity are

\[
\rho_0(x) = |A_0(x)|^2 = \exp(-50x^2),
\]

\[
u_0(x) = \partial_x S_0(x) = -\tanh(5x).
\]

This allows for the appearance of cusp caustics.
Velocity contour
Gaussian beam method

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Schrödinger equation

Gaussian beam method - Lagrangian formulation

Gaussian beam method - Eulerian formulation

Numerical results

Applications in quantum mechanics

circle: Schrödinger  square: Geometric optics  cross: Phase correction  star: Gaussian beam
Convergence rate and mesh size

Convergence orders: 0.9082 in $\ell^1$ norm, 0.8799 in $\ell^2$ norm and 0.7654 in $\ell^\infty$ norm.

Mesh size: $\Delta y \sim O(\sqrt{\varepsilon})$
2D example

Take the potential \( V(x_1, x_2) = 10 \) and the initial conditions of the Schrödinger equation as

\[
\begin{align*}
A_0(x_1, x_2) &= e^{-25(x_1^2 + x_2^2)}, \\
S_0(x_1, x_2) &= -\frac{1}{5}(\log(2 \cosh(5x_1)) + \log(2 \cosh(5x_2))).
\end{align*}
\]

then the initial density and two components of the velocity are

\[
\begin{align*}
\rho_0(x_1, x_2) &= \exp(-50(x_1^2 + x_2^2)), \\
u_0(x_1, x_2) &= -\tanh(5x_1) \\
v_0(x_1, x_2) &= -\tanh(5x_2).
\end{align*}
\]
Amplitude at $\varepsilon = 0.001$ and $T_{\text{final}} = 0.5$
Gaussian beam method

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Schrödinger equation

Gaussian beam method - Lagrangian formulation

Gaussian beam method - Eulerian formulation

Numerical results

Applications in quantum mechanics

Schrödinger equation with periodic structure

\[ i\varepsilon \frac{\partial \psi^\varepsilon}{\partial t} = -\frac{\varepsilon^2}{2} \frac{\partial^2}{\partial x^2} \psi^\varepsilon + V_\Gamma \left( \frac{x}{\varepsilon} \right) \psi^\varepsilon + U(x) \psi^\varepsilon, \quad x \in \mathbb{R}, \]

It models: electrons in the perfect crystals

Bloch band decomposition:

\[ H(k, z) := \frac{1}{2} (-i \partial_z + k)^2 + V_\Gamma (z), \quad z = \frac{x}{\varepsilon} \]

\[ H(k, z) \chi_m(k, z) = E_m(k) \chi_m(k, z), \]

\[ \chi_m(k, z + 2\pi) = \chi_m(k, z), \quad z \in \mathbb{R}, \quad k \in (-1/2, 1/2). \]

Modified WKB ansatz:

\[ \psi^\varepsilon(t, x) = \sum_{m=1}^{\infty} a_m(t, x) \chi_m(\partial_x S_m, \frac{x}{\varepsilon}) e^{i S_m(t, x)/\varepsilon}. \]
Equations in the $m$-th band

Eikonal-transport equations:

$$
\partial_t S_m + E_m(\partial_x S_m) + U(x) = 0,
$$
$$
\partial_t a_m + E'_m(\partial_x S_m)\partial_x a_m + \frac{1}{2} a_m\partial_x(E'_m(\partial_x S_m)) + \beta_m a_m = 0.
$$

Liouville-type equations:

$$
\mathcal{L}_m = \partial_t + E'_m(\xi) \cdot \partial_y - U'(y)\partial_\xi,
$$
$$
\mathcal{L}_m \phi_m = 0,
$$
$$
\mathcal{L}_m S_m = E'_m(\xi)\xi - E_m(\xi) - U(y),
$$
$$
\mathcal{L}_m a_m = \frac{1}{2} \frac{\partial_y \phi_m}{\partial_\xi \phi_m} a_m - \gamma_m a_m.
$$

$\beta_m$, $\gamma_m$ are constants related to $\chi_m$. 
Band structure for $V_\Gamma(z) = \cos(z)$
Numerical simulation for $\varepsilon = 1/512$

Initial conditions:

$$A_0(x, z) = e^{-50(x+0.5)^2} \cos z, \quad S_0(x) = 0.3x + 0.1 \sin x.$$  

External potential: $U(x) = 0$
Schrödinger-Poisson equations

\[
\begin{align*}
    i\varepsilon \psi_t^\varepsilon &= -\frac{\varepsilon^2}{2} \psi_{xx}^\varepsilon + V^\varepsilon(x)\psi^\varepsilon, \\
    \partial_{xx} V^\varepsilon &= K \left( \frac{\sqrt{2\pi}}{10} - |\psi^\varepsilon(x, t)|^2 \right), \quad E^\varepsilon = \frac{\partial V^\varepsilon}{\partial x}.
\end{align*}
\]

A simple model of the radiation-matter interaction system, for example, in nano-optics, mean field theory...

\[K = +1 \quad \text{Focusing potential}\]
\[K = -1 \quad \text{Defocusing potential}\]

Initialization:

\[A_0(x) = e^{-25x^2}, \quad S_0(x) = \frac{1}{\pi} \cos(\pi x).\]
## Convergence results

<table>
<thead>
<tr>
<th>((\varepsilon, N_y))</th>
<th>(\left(\frac{1}{256}, 128\right))</th>
<th>(\left(\frac{1}{1024}, 256\right))</th>
<th>(\left(\frac{1}{4096}, 512\right))</th>
</tr>
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<tr>
<td>(l^1) error</td>
<td>(1.12 \times 10^{-2})</td>
<td>(3.93 \times 10^{-3})</td>
<td>(9.22 \times 10^{-4})</td>
</tr>
<tr>
<td>(l^2) error</td>
<td>(4.09 \times 10^{-2})</td>
<td>(1.47 \times 10^{-2})</td>
<td>(3.80 \times 10^{-3})</td>
</tr>
<tr>
<td>(l^\infty) error</td>
<td>(3.09 \times 10^{-1})</td>
<td>(1.09 \times 10^{-1})</td>
<td>(3.09 \times 10^{-2})</td>
</tr>
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**focusing potential**

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<tr>
<td>(l^1) error</td>
<td>(8.16 \times 10^{-3})</td>
<td>(2.60 \times 10^{-3})</td>
<td>(8.35 \times 10^{-4})</td>
</tr>
<tr>
<td>(l^2) error</td>
<td>(3.20 \times 10^{-2})</td>
<td>(9.24 \times 10^{-3})</td>
<td>(2.94 \times 10^{-3})</td>
</tr>
<tr>
<td>(l^\infty) error</td>
<td>(1.74 \times 10^{-1})</td>
<td>(5.30 \times 10^{-2})</td>
<td>(1.95 \times 10^{-2})</td>
</tr>
</tbody>
</table>

**defocusing potential**
Numerical simulation \( \varepsilon = 1/4096 \)
Thank You!

Questions?