Eulerian Gaussian beam method in quantum mechanics

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Outline

Schrödinger equation

The time-dependent one-body Schrödinger equation:

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

$$\Psi^\varepsilon(t,\boldsymbol{x})=A(t,\boldsymbol{x})e^{iS(t,\boldsymbol{x})/\varepsilon}$$

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

Numerical difficulties:
$\Psi^\varepsilon(t,\boldsymbol{x})$ is oscillatory of wave length $O(\varepsilon)$.

Methods	Mesh size	Time step
Finite difference [1]	$o(\varepsilon)$	$o(\varepsilon)$
Time splitting spectral[2]	$O(\varepsilon)$	ε-indep.

[1] Markowich, Pietra, Pohl and Stimming

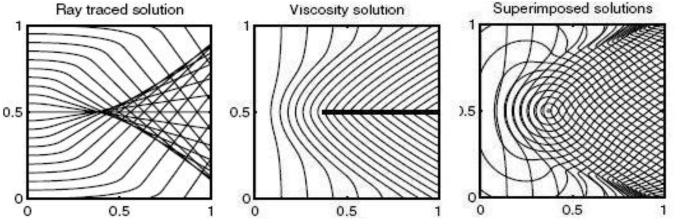
[2] Bao, Jin and Markowich

Geometric optics - WKB analysis

WKB ansatz	$\Psi^\varepsilon(t,\boldsymbol{x}) = A(t,\boldsymbol{x})e^{iS(t,\boldsymbol{x})/\varepsilon}$,
eikonal	$S_t + \frac{1}{2}\lvert\nabla S\rvert^2 + V(\boldsymbol{x}) = 0,$
transport	$\rho_t + \nabla\cdot(\rho\nabla S) = 0, \quad \rho(t,\boldsymbol{x}) = \lvert A(t,\boldsymbol{x})\rvert^2.$

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

Figures from the review paper of Engquist and Runborg:



Caustics   NOT physical   Semiclassical limit

Semiclassical limit + phase correction

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

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

where the phase

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

has finitely many ($K < \infty$) stationary phases ξ_k and $\mathbf{y}_k$:

$$\xi_k = \nabla S_0(\mathbf{y}_k), \quad \mathbf{y}_k = \mathbf{x} - t\nabla S_0(\mathbf{y}_k)\,,$$

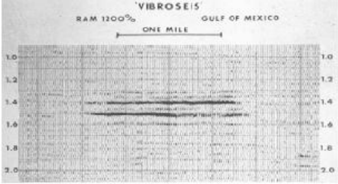
$D^2 S_0$ is the Hessian matrix, and $\mu_k = \mathrm{sgn}(D^2 S(\xi_k, \mathbf{y}_k))$ is the Keller-Maslov index of the kth branch.

Gaussian beam method - motivation

Problems of the semiclassical limit: invalid at caustics

1. the density $\rho(t, \boldsymbol{x}) \to \infty$ in the transport equation,
2. $1 + tD^2 S_0(\mathbf{y}_k)$ is singular in the stationary phase method.

Computation around caustics is important in many applica -tions, for example:



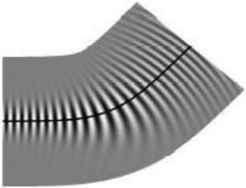
Seismic imaging

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 $S(t, \boldsymbol{x})$:



$$\varphi^{\varepsilon}_{la}(t, \boldsymbol{x}, \boldsymbol{y}_0) = A(t, \boldsymbol{y}) e^{iT(t,\boldsymbol{x},\boldsymbol{y})/\varepsilon},$$

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

beam center: $$\frac{\mathrm{d}\boldsymbol{y}}{\mathrm{d}t} = \boldsymbol{p}(t, \boldsymbol{y}), \quad \boldsymbol{y}(0) = \boldsymbol{y}_0.$$

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 $\varphi^{\varepsilon}_{la}$ has a Gaussian beam profile.

Lagrangian formulation

Apply the beam-shaped ansatz to the Schrödinger equation:

$$
\begin{aligned}
\text{center:} \quad & \frac{\mathrm{d}\boldsymbol{y}}{\mathrm{d}t} = \boldsymbol{p}, \\
\text{velocity:} \quad & \frac{\mathrm{d}\boldsymbol{p}}{\mathrm{d}t} = -\nabla_{\boldsymbol{y}} V, \\
\text{Hessian:} \quad & \frac{\mathrm{d}M}{\mathrm{d}t} = -M^2 - \nabla_{\boldsymbol{y}}^2 V, \\
\text{phase:} \quad & \frac{\mathrm{d}S}{\mathrm{d}t} = \frac{1}{2}|\boldsymbol{p}|^2 - V, \\
\text{amplitude:} \quad & \frac{\mathrm{d}A}{\mathrm{d}t} = -\frac{1}{2}\big(\mathrm{Tr}(M)\big)A.
\end{aligned}
$$

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:

$$\frac{\mathrm{d}P}{\mathrm{d}t} = R, \quad \frac{\mathrm{d}R}{\mathrm{d}t} = -(\nabla_{\boldsymbol{y}}^2 V)P,$$

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

$$R(0) = M(0) = \nabla_{\boldsymbol{y}}^2 S_0(\boldsymbol{y}) + i\mathrm{I}, \quad P(0) = \mathrm{I}.$$

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

P complexified $\Longrightarrow$ P never singular $\Longrightarrow$ A always finite.

The Gaussian beam summation solution (Hill, Tanushev):

$$\Phi_{la}^{\varepsilon}(t, \boldsymbol{x}) = \int_{\mathbb{R}^n} \left(\frac{1}{2\pi\varepsilon}\right)^{\frac{n}{2}} r_\theta(\boldsymbol{x} - \boldsymbol{y}(t, \boldsymbol{y}_0))\varphi_{la}^{\varepsilon}(t, \boldsymbol{x}, \boldsymbol{y}_0)\mathrm{d}\boldsymbol{y}_0.$$

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 $\boldsymbol{u} = \nabla_{\boldsymbol{y}} S$ into the intersection of zero level sets of phase-space functions $\phi_j(t, \boldsymbol{y}, \xi)$, i.e.

$$\phi_j(t, \boldsymbol{y}, \xi) = 0, \quad \text{at} \quad \xi = \boldsymbol{u}(t, \boldsymbol{y}), \quad j = 1, \cdots, n.$$

$\boldsymbol{\phi} = (\phi_1, \cdots, \phi_n)$ satisfies the Liouville equation:

$$\partial_t \boldsymbol{\phi} + \boldsymbol{\xi} \cdot \nabla_{\boldsymbol{y}} \boldsymbol{\phi} - \nabla_{\boldsymbol{y}} V \cdot \nabla_{\boldsymbol{\xi}} \boldsymbol{\phi} = 0.$$

Eulerian formulation I - semiclassical limit

$$
\begin{array}{ccc}
\text{Lagragian formulation} & \Longrightarrow & \text{Eulerian formulation} \\
\Downarrow & & \Downarrow \\
\text{ODEs} & \Longrightarrow & \text{PDEs} \\
\Downarrow & & \Downarrow \\
\dfrac{\mathrm{d}}{\mathrm{d}t} & \Longrightarrow & \mathcal{L} = \partial_t + \xi \cdot \nabla_{\boldsymbol{y}} - \nabla_{\boldsymbol{y}} V \cdot \nabla_\xi
\end{array}
$$

As shown by Jin, Liu, Osher and Tsai,

$$
\begin{aligned}
\text{velocity:} \quad & \mathcal{L}\phi = 0, \\
\text{phase:} \quad & \mathcal{L}S = \frac{1}{2}|\xi|^2 - V, \\
\text{amplitude:} \quad & \mathcal{L}A = \frac{1}{2}\mathrm{Tr}\left((\nabla_\xi \phi)^{-1} \nabla_{\boldsymbol{y}} \phi \right) A.
\end{aligned}
$$

Eulerian formulation II - semiclassical limit

If one introduces the new quantity

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

then $f(t, \mathbf{y}, \xi)$ 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 ϕ.

Construct the Hessian function

$$\frac{\partial}{\partial \boldsymbol{y}}\phi(t, \boldsymbol{y}, \boldsymbol{u}(t, \boldsymbol{y})) = 0 \quad \Rightarrow \quad \nabla^2_{\boldsymbol{y}} S = \nabla_{\boldsymbol{y}} \boldsymbol{u} = -\nabla_{\boldsymbol{y}}\phi(\nabla_{\boldsymbol{\xi}}\phi)^{-1}$$

$$\Uparrow \qquad \Uparrow \qquad \Uparrow$$

Recall the Lagrangian formulation: $M \quad = \quad R \quad P^{-1}$

Conjecture: $R = -\nabla_{\boldsymbol{y}}\phi, \quad P = \nabla_{\boldsymbol{\xi}}\phi.$

Complex R and $P \Longrightarrow$ complex ϕ

Conjecture verification

$$
\begin{array}{ccccc}
\mathcal{L}R = -(\nabla_y^2 V)P & \longrightarrow & M = RP^{-1} & \longleftarrow & \mathcal{L}P = R \\
\Updownarrow & & \Updownarrow & & \Updownarrow \\
\mathcal{L}(-\nabla_y\phi) = -\nabla_y^2 V \nabla_\xi \phi & \longrightarrow & M = -\nabla_y\phi(\nabla_\xi\phi)^{-1} & \longleftarrow & \mathcal{L}(\nabla_\xi\phi) = -\nabla_y\phi \\
 & \frac{\partial}{\partial y}\nwarrow & \uparrow & \nearrow\frac{\partial}{\partial \xi} & \\
 & & \mathcal{L}\phi = 0 & &
\end{array}
$$

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

$$
\phi_0(\boldsymbol{y}, \xi) = -i\boldsymbol{y} + (\xi - \nabla_{\boldsymbol{y}} S_0)
$$

$$
R(0) = \nabla_{\boldsymbol{y}}^2 S_0(\boldsymbol{y}) + i\mathrm{I}, \quad P(0) = \mathrm{I}.
$$

Eulerian formulation - Gaussian beam

Step 1: $\mathcal{L}\phi = 0, \quad \phi_0(\boldsymbol{y}, \xi) = -i\boldsymbol{y} + (\xi - \nabla_{\boldsymbol{y}} S_0).$

Step 2: compute $\nabla_{\boldsymbol{y}}\phi$ and $\nabla_{\xi}\phi \quad M = -\nabla_{\boldsymbol{y}}\phi(\nabla_{\xi}\phi)^{-1}.$

Step 3: solve S either by $\mathcal{L}S = \frac{1}{2}|\xi|^2 - V$ or

path integral $S(t,x) = \int_a^x u(t,s)\,\mathrm{d}s + \text{Constant}.$

Step 4: $\mathcal{L}f = 0, \quad f_0(t, \boldsymbol{y}, \xi) = A_0(\boldsymbol{y})^2,$

Step 5: $A = (\det(\nabla_{\xi}\phi)^{-1} f)^{1/2}.$

Parallel to Ralston's proofs,

ϕ complexified $\Rightarrow$ $\nabla_{\xi}\phi$ non-degenerate $\Rightarrow$ A never blows up

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

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

Eulerian Gaussian beam summation formula:

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

r_θ 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 ξ out first:

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

where $\boldsymbol{u}_k$, $k = 1, \cdots, K$ are the velocity branches.

Problem: $\det\left(\mathrm{Re}[\nabla_{\boldsymbol{\xi}}\phi]\right) = 0$ at caustics.

Solution: Split the integral into two parts:

$$\begin{aligned} L_1 &= \left\{\boldsymbol{y} \middle| \left|\det(\mathrm{Re}[\nabla_{\boldsymbol{p}}\phi](t,\boldsymbol{y},\boldsymbol{p}_j))\right| \geq \tau\right\} \\ L_2 &= \left\{\boldsymbol{y} \middle| \left|\det(\mathrm{Re}[\nabla_{\boldsymbol{p}}\phi](t,\boldsymbol{y},\boldsymbol{p}_j))\right| < \tau\right\} \end{aligned}$$

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:

Methods	Mesh size	Time step
Finite difference	$o(\varepsilon)$	$o(\varepsilon)$
Time splitting spectral	$O(\varepsilon)$	ε-indep.
Gaussian beam	$O(\sqrt{\varepsilon})$	$O(\varepsilon^{\frac{2}{p}})$

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

Gaussian beam method

Xu Yang

1D example

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

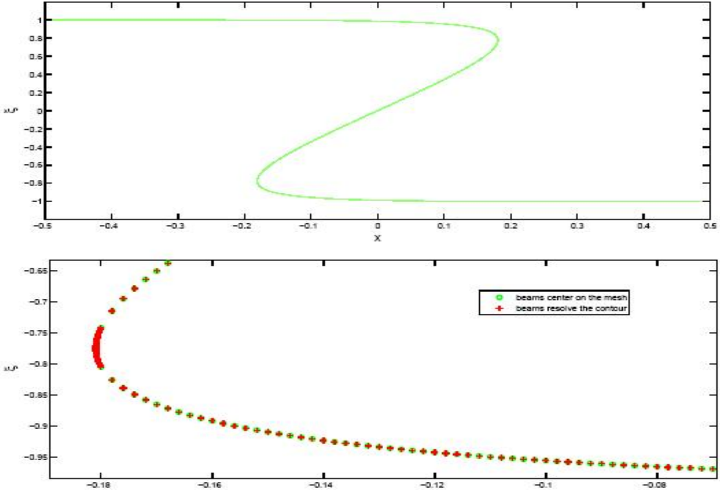
$$A_0(x) = e^{-25x^2}, \; S_0(x) = -\frac{1}{5}\log(2\cosh(5x)).$$

which implies that the initial density and velocity are

$$\rho_0(x) = |A_0(x)|^2 = \exp(-50x^2),$$
$$u_0(x) = \partial_x S_0(x) = -\tanh(5x).$$

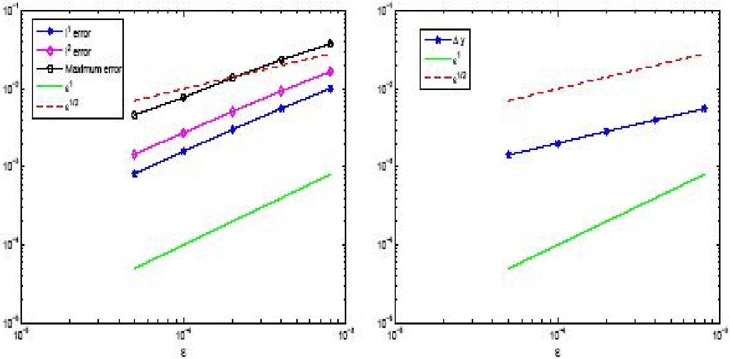
This allows for the appearance of cusp caustics.

Velocity contour



circle: Schrödinger square: Geometric optics cross: Phase correction star: Gaussian beam

Convergence rate and mesh size



Convergence orders: 0.9082 in ℓ^1 norm, 0.8799 in ℓ^2 norm and 0.7654 in ℓ^∞ norm.

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

2D example

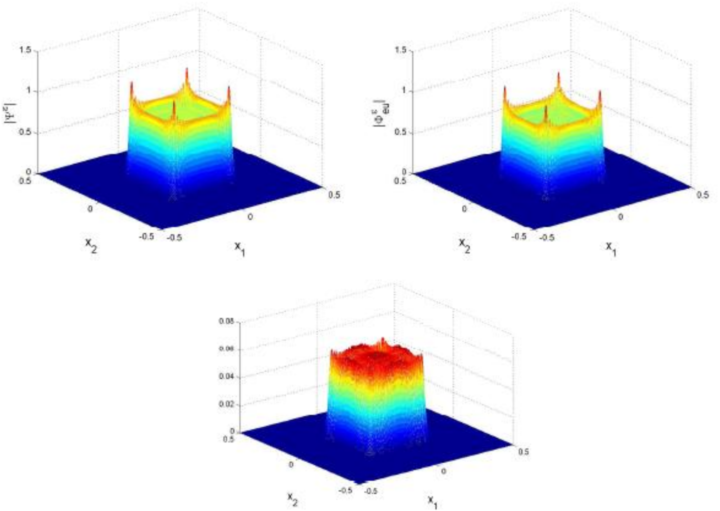
Take the potential $V(x_1, x_2) = 10$ and the initial conditions of the Schrödinger equation as

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

then the initial density and two components of the velocity are

$$
\rho_0(x_1, x_2) = \exp(-50(x_1^2 + x_2^2)),
$$
$$
u_0(x_1, x_2) = -\tanh(5x_1)
$$
$$
v_0(x_1, x_2) = -\tanh(5x_2).
$$

Amplitude at $\varepsilon = 0.001$ and $T_{final} = 0.5$



Schrödinger equation with periodic structure

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

It models: electrons in the perfect crystals

Bloch band decomposition:

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

$$H(k,z)\chi_m(k,z) = E_m(k)\chi_m(k,z),$$

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

Modified WKB ansatz:

$$\Psi^\varepsilon(t,x) = \sum_{m=1}^{\infty} a_m(t,x)\chi_m(\partial_x S_m, \frac{x}{\varepsilon})e^{iS_m(t,x)/\varepsilon}.$$

Equations in the m-th band

Eikonal-transport equations:

$$\partial_t S_m + E_m(\partial_x S_m) + U(x) = 0\,,$$

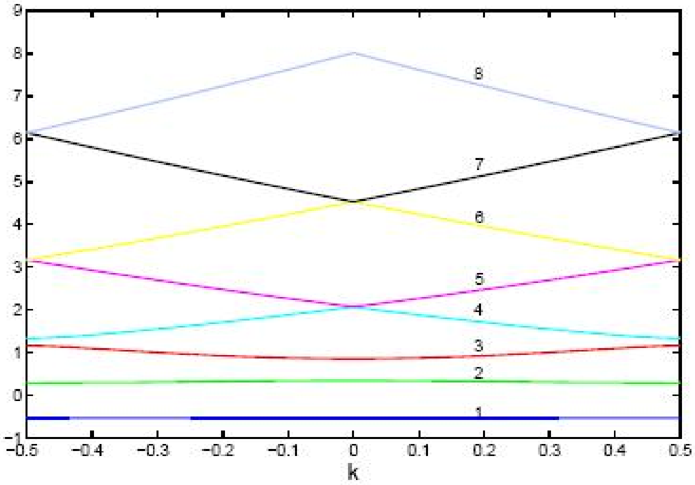
$$\partial_t a_m + E'_m(\partial_x S_m)\partial_x a_m + \frac{1}{2} a_m \partial_x \big(E'_m(\partial_x S_m)\big) + \beta_m a_m = 0.$$

Liouville-type equations:

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

β_m, γ_m are constants related to χ_m.

Band structure for $V_\Gamma(z) = \cos(z)$



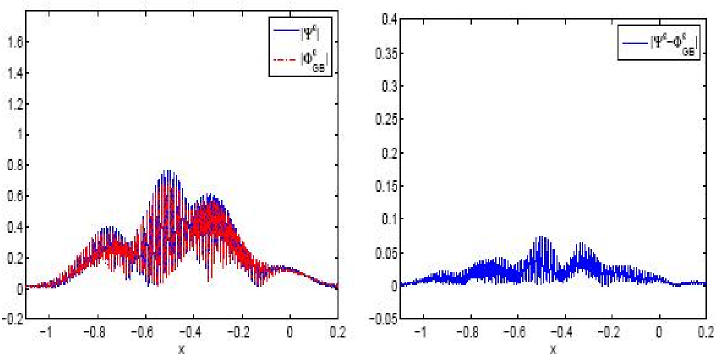
Mathieu's model

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

$$
\begin{cases}
i\varepsilon \Psi_t^\varepsilon &= -\dfrac{\varepsilon^2}{2}\Psi_{xx}^\varepsilon + V^\varepsilon(x)\Psi^\varepsilon, \\
\partial_{xx} V^\varepsilon &= K\left(\dfrac{\sqrt{2\pi}}{10} - |\Psi^\varepsilon(x,t)|^2\right), \quad E^\varepsilon = \dfrac{\partial V^\varepsilon}{\partial x}.
\end{cases}
$$

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

$K = +1$	Focusing potential
$K = -1$	Defocusing potential

Initialization:

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

Convergence results

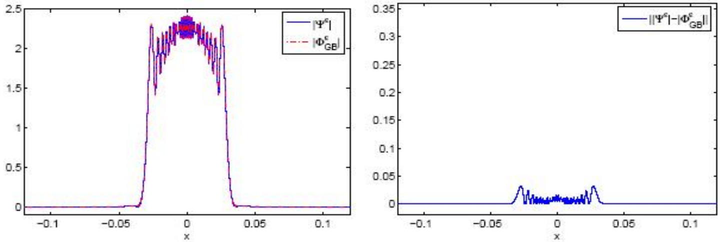
(ε, N_y)	$(\frac{1}{256}, 128)$	$(\frac{1}{1024}, 256)$	$(\frac{1}{4096}, 512)$
l^1 error	1.12×10^{-2}	3.93×10^{-3}	9.22×10^{-4}
l^2 error	4.09×10^{-2}	1.47×10^{-2}	3.80×10^{-3}
l^∞ error	3.09×10^{-1}	1.09×10^{-1}	3.09×10^{-2}

focusing potential

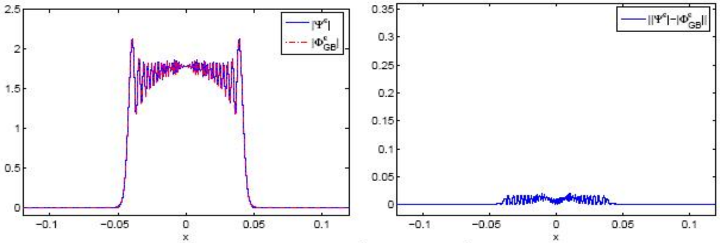
(ε, N_y)	$(\frac{1}{256}, 128)$	$(\frac{1}{1024}, 256)$	$(\frac{1}{4096}, 512)$
l^1 error	8.16×10^{-3}	2.60×10^{-3}	8.35×10^{-4}
l^2 error	3.20×10^{-2}	9.24×10^{-3}	2.94×10^{-3}
l^∞ error	1.74×10^{-1}	5.30×10^{-2}	1.95×10^{-2}

defocusing potential

Numerical simulation $\varepsilon = 1/4096$



focusing potential



defocusing peotential

Thank You!

Questions?